The Partnership for Advanced Computing in Europe (PRACE) is an international non-profit association with its seat in Brussels. The PRACE Research Infrastructure provides a persistent world-class high performance computing service for scientists and researchers from academia and industry in Europe. The computer systems and their operations accessible through PRACE are provided by 4 PRACE members (BSC representing Spain, CINECA representing Italy, GCS representing Germany and GENCI representing France). The Implementation Phase of PRACE receives funding from the EU’s Seventh Framework Programme (FP7/2007-2013) under grant agreement RI-312763 and from the EU’s Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 653838.

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The PRACE Annual Report 2015 continues PRACE’s tradition of highlighting scientific and industrial advances made by the projects it supports.

The success stories that form the core of each PRACE Annual Report underline the importance of high performance computing (HPC) for a wide variety of scientific domains and industrial disciplines. From chemistry to fundamental physics, and from mathematics to medicine, every researcher who is in need of high-level computational power is welcome at PRACE.

We have also been able to secure the cooperation of two important figures from politics and science who have put their stamp on the development of HPC in Europe and therefore on PRACE: Roberto Viola, Director General of DG CONNECT at the European Commission, and Mateo Valero, Director at the Barcelona Supercomputing Center (BSC). Pages 27 to 30 will tell you more about their vision and outlook.

I would like to use this opportunity to digress slightly from the PRACE Annual Report itself and point you towards some of our other publications and informational materials, such as the PRACE Digest, the PRACE Brochure, and the newly created PRACE Fact Sheets. You can find all of these and more on the “Press Materials” page of the PRACE website (www.prace-ri.eu/press-materials).

The website and press materials are products of the PRACE Implementation Phase Projects that allow us to do so much more than provide access to Europe's highly advanced HPC infrastructure. I invite you to read pages 38 to 41 to find out more about the work of the PRACE IP Projects, which includes diverse activities such as Pre-Commercial Procurement (PCP), the PRACE Advanced Training Centres (PATCs), the PRACE Summer of HPC (SoHPC), and much more.

This annual report will be launched at PRACEdays16, which will be held from 10 to 12 May 2016 in Prague, Czech Republic. This year’s event will be held under the umbrella of the European HPC Summit Week, organised by the European eXtreme Data & Computing Initiative (EXDCI - www.exdci.eu). Besides PRACEdays16, the week will include an EXDCI Workshop, a workshop by EuroLab4HPC, and an Extreme-Scale Demonstrators (EsDs) workshop organised by ETP4HPC.

More information on the other events that PRACE organises and participates in can be found on pages 49 to 51.

Alison Kennedy
Chair of the PRACE Board of Directors
EXDCI

Horizon 2020 is built around three pillars: support for excellent science including grants for individual researchers from the European Research Council and Marie Skłodowska-Curie fellowships; support for industrial leadership including grants for small and medium-sized enterprises and indirect finance for companies; support for research to tackle societal challenges.

High-Performance Computing (HPC) is a strategic resource for Europe’s future. The European Commission recognised the need for an EU-level policy in HPC to optimise national and European investments, addressing the entire HPC ecosystem. In this sense, the European project called European eXtreme Data & Computing Initiative (EXDCI) will complement the Horizon 2020 calls and projects in achieving of a globally competitive HPC ecosystem in Europe. Following the EC’s vision for HPC, this ecosystem is based on three pillars: HPC technology provision, HPC infrastructure and HPC application resources.

About EXDCI
EXDCI’s objective is to coordinate the development and implementation of a common strategy for the European HPC Ecosystem. Started on 1 September 2015, the two most significant HPC bodies in Europe, PRACE and ETP4HPC, join their expertise in this 30-month project with a budget of €2.5 million. Its mission is to foster collaboration among the key players in the HPC ecosystem, including the Centres of Excellence (CoEs), the European Exascale projects and the FETHPC projects. EXDCI aims to support the road-mapping, strategy-making and performance-monitoring activities of the ecosystem, i.e.:

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

More information on www.exdci.eu
The Scientific Steering Committee

2015 was a transitional year for PRACE, with the first phase ending and a new one in preparation. PRACE has been very successful in establishing a European HPC community, which has strengthened European science and competitiveness.

Five years after PRACE’s inception, more than 400 projects have been awarded in all scientific fields. The amount of very high-quality results obtained is impressive and illustrates the impact PRACE has had on scientific research from various domains. The 2015 report demonstrates the range of applications and scales that are possible thanks to PRACE and the wide diversity of high-end applications enabled by PRACE.

During the past year, the Scientific Steering Committee of PRACE has reaffirmed its support for a long-term sustained European computing infrastructure and its expectation that PRACE will continue to deliver access to resources that are competitive at the international level. The continuous improvements of numerical algorithms and simulation tools combined with growing computational power available for scientific analysis is promoting unprecedented investigations into topics as diverse as nanotechnology, new materials, aircraft design and fundamental studies of galaxy formation. Simulations and extensive data analyses that rely on HPC help mankind to answer long-standing physics questions, design better materials, synthesise new drugs and address societal challenges, such as health and climate change. In all domains, further improvement in computing power is essential to progress in science and innovation, as was shown in the 2012-2020 scientific case. World-class supercomputers in Europe are required to solve important new problems that were previously considered inaccessible and thus provide researchers with international visibility. Larger size of domains and more complex physical, chemical and biological systems, will be addressed with increased computing power. Access to world-class Tier-0 machines is also crucial to gain experience on new types of machines and remain competitive at the international level.

2015 has been marked by reduced resources available for projects as a result of the transition between the end of the initial five-year agreement and the start of a new phase of PRACE. Such a reduction is damaging to the scientific community and as chair of the SSC I had to convey our worries. The importance of PRACE for science is, however, well perceived by the PRACE Council and I do hope a solution will be found rapidly.

My mandate of one year as chair of the SSC comes to an end. It has been an honour to serve PRACE. I welcome Petros Koumoutsakos, professor in computational science, as the new Chair, and Erik Lindahl, professor in computational biophysics, as the new Vice-Chair of the SSC. I am sure they will strongly promote the importance of PRACE for science!
Modelling the sun

The area beyond the surface of the sun, known as the outer solar atmosphere, is the home of eruptive events such as solar flares that govern near-Earth space weather and affect mankind’s technological environment. Understanding why the solar atmosphere is so hot and energetic compared to the surface of the sun is the focus of Professor Mats Carlsson’s work.

The outer part of the solar atmosphere is a puzzling place. It is much hotter than would be expected, and nobody knows why. The rest of the sun acts more predictably. At the centre is the solar core — the location of the thermonuclear reactions that keep our solar system warm — which clocks in at a blistering 15 000 000K. As one moves further away from this energy source towards the surface of the star, the temperature gradually drops down to a relatively cool 6 000K. But move beyond the surface and into the corona — the aura of plasma that is visible during a total solar eclipse — and the heat suddenly rises back up to around 1 000 000K.

This unintuitive rise in energy is known as the coronal heating problem, and is one of the most famous unsolved problems in physics. However, despite the name of this celebrated conundrum, it is at a layer of the sun’s atmosphere slightly further in — known as the chromosphere — where the heating begins. “The temperature of the chromosphere can reach 8 000K. This is not nearly as hot as the corona, but it actually takes around ten times more energy to heat due to its higher density,” explains Professor Mats Carlsson of the University of Oslo, Norway. “So although it is known as the coronal heating problem, many of its answers will likely be found by studying the chromosphere.”

The source of the energy is quite clear; convectively unstable areas found inside the sun cause parcels of gas to rise in bubbling motions. The energy from this convective motion is more than enough to heat the chromosphere and the corona. What is not fully understood is how the energy is transported from the convection zone and up into the outer solar atmosphere. Working out the process by which this happens is the focus of one of Carlsson’s recent projects.

Mechanisms for heating

Two mechanisms have been shown to facilitate this transfer of energy. Magnetic fields that stretch across the solar surface occasionally rearrange themselves in what are known as reconnection events. “This can be imagined

The numerical simulation as if viewed through a filter onboard NASA’s Interface Region Imaging Spectrograph (IRIS). The filter only shows light emitted by plasma that is at a temperature of about 20 000 Kelvin. The region shown is twice as large as the Earth.
much like the breaking of an elastic band,” explains Carlsson. “A lot of energy is stored inside a band when it is stretched, so when it snaps, this energy is released. In terms of the sun, this means some of the magnetic field’s energy is converted into thermal energy.”

The other mechanism involves magneto-acoustic waves, which are launched in the solar interior and carry energy out to the chromosphere and corona. “These waves, along with the reconnection events, are the likely source of energy transfer to the outer solar atmosphere, but we do not yet fully understand how either of the processes contribute,” says Carlsson.

**Modelling the sun**

Carlsson’s group is world-leading in modelling the solar atmosphere as one system. Although it is possible to observe magnetic fields in the chromosphere and corona, tracking and measuring them is not possible at present. The next generation of solar telescopes, such as the four-metre diameter Daniel K Inouye Solar Telescope in Hawaii, will be able to measure these magnetic fields, but until they become functional, simulations such as those done by Carlsson’s group can provide some insight into their behaviour.

**“Even with a small three-dimensional section of the sun, it would take longer than the age of the universe to calculate one hour of solar time by brute force due to the coupling effects of radiation”**

Carlsson’s group can provide some insight into their behaviour. The transition between the photosphere (the visible surface of the sun) and the outer solar atmosphere makes simulating this area of the sun problematic. In the photosphere the gas dominates, so when the gas moves around the magnetic field is swept along with it. In the corona the opposite is the case; the magnetic field dominates the gas. The transition from one to the other happens in the chromosphere. This transition means that it is not possible to extrapolate where energy from further inside is dumped and then dissipated. “This is a problem both observationally and computationally,” says Carlsson. “Radiation has the effect of coupling things that are far apart. These distance forces mean that instead of individually solving equations at each point on our grid, we have to solve all of the points simultaneously as one big system. This type of global coupling is very computationally demanding.”

Simulating the entire sun would be impossible, so instead a section of the sun is simulated in a computational box. Even with this small section, if one were to try and solve a three-dimensional version by brute force it would take longer than the age of the universe to calculate one hour of solar time due to the coupling effects of radiation. Some of the complex physics of the system must therefore be simplified but without losing the main properties. A large enough volume of the sun must be simulated to encompass the large chromospheric structures, while a high enough resolution must be used to capture the dynamics of the system. Carlsson’s team used trial and error until a suitable balance was found, after which it was scaled up and run on a supercomputer.

**Higher resolution, more turbulence**

A number of simulations were run, using a massively parallel code called Bifrost and 34 million core hours on SuperMUC hosted by GCS at LRZ.
Germany. “What we found from these experiments was that the results we got depended on the numerical resolution we used,” says Carlsson. “With a higher resolution, using a cell size of 3km, you see more turbulence and more swirling, twisting motions which were not there with our normal resolution of 30km.

“In the lower resolution runs, we made a parameter space which looked at various magnetic field outputs, and then compared this with actual observations. The spectral line from the observations was broader, which tells us that we need to use higher resolution if we want to achieve the levels of turbulence needed to make meaningful comparisons between our simulations and observations. Somewhere in the region of 6km would probably be enough.”

Interpreting observations from satellites
The Interface Region Imaging Spectrograph (IRIS) is a tiny solar satellite that was specially designed to look at the chromosphere. The results from Carlsson’s group’s simulations were used as part of the original proposal to build the satellite, and are now being used to interpret its observations. This synergy of numerical modelling and observations has explained several of the findings of the IRIS mission. “Even though our simulations are not at the resolution needed to totally match the observations, they are crucial for helping us to make inferences on conditions in the atmosphere,” explains Carlsson.

“Mass and energy loading processes that occur at the chromosphere trigger solar outbursts that govern near-Earth space weather and affect mankind’s technological environment”

Data from one of the simulations has been published online and is available to anyone who wants to download it and use it for their own analysis. Carlsson’s group will also spend the next few years analysing their high-resolution runs, quantifying the turbulence and working out how waves are generated in the simulation. “Each snapshot in time is several gigabytes worth of data, and we have already had 20 papers published in journals from 2015 says Carlsson. “So we still have a lot to do, but what we have seen so far looks promising.”

The chromosphere remains an enigmatic area of the sun that continues to fascinate the heliophysicists that study it. The mass and energy loading processes that occur there not only define the heating of the corona, but also affect the acceleration and the composition of the solar wind, and the energetics and triggering of solar outbursts (filament eruptions, flares, coronal mass ejections) that govern near-Earth space weather and affect mankind’s technological environment. As simulations of the sun edge become more complex, our understanding of the characteristics of our solar system becomes richer.

**Project title:** Physics of the Solar Chromosphere

**Project leader:** Mats Carlsson, Institute of Theoretical Astrophysics, University of Oslo, Norway

**Project details:** Awarded 34 million core hours on SuperMUC hosted at GCS at LRZ, Germany

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**SuCCEss StoRiEs**

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Solar convection shown as vertical velocity (bright is downflow) at the visible surface showing that increasing the resolution from a grid size of 48km to 3km dramatically increases the small scale structure. This has a corresponding effect on how the convective energy can be transported to the outer solar atmosphere. The region shown is about half the diameter of the Earth on the side.
The enzyme of life

Photosystem II is the most important enzyme involved in the conversion of sunlight into chemical energy that occurs in plants, algae and cyanobacteria. As a side product it generates oxygen, making it hugely important in terms of the composition of the Earth’s atmosphere and the development of life. Professor Leonardo Guidoni has been using quantum and molecular mechanics simulations in order to elucidate part of the mechanism of this crucial process, which could also lead to ways to improve material design in artificial photosynthesis.

Two and half billion years ago when the Earth was barely recognisable, cyanobacteria in the ocean began to use water and sunlight as a source of energy, developing the capability to split two water molecules into protons, electrons and oxygen. The oxygen would eventually begin to accumulate in the atmosphere, triggering one of the most significant extinction events in Earth’s history (oxygen was toxic to the majority of organisms alive at the time). But at the same time it would also permit the development of the vastly more efficient aerobic metabolisms in life forms that are seen today.

This process of splitting water to produce oxygen is a fairly challenging process from a chemical point of view, and unusually it seems that only one biological blueprint for it has ever evolved in nature. Photosystem II, the protein complex in which photosynthesis begins in all phototrophs, has a catalytic core made by an inorganic manganese cluster, and has almost no variation among species.

For Professor Leonardo Guidoni of the University of L’Aquila, Italy, this represents an interesting area of study. His interest lies in the conversion of solar energy into fuel as a means to provide a renewable source of energy, and he believes that through modelling photosystem II — the protein that achieves this in nature — it may be possible to develop ideas to design economically viable solutions to current energy concerns. He and his team have modelled the entire enzyme at a classical mechanics level and the active site at the quantum level in order to describe the actions of electrons and developing chemical bonds during the reaction.

The mechanism of the oxygen evolving reaction and the organisation of its constituent parts remains one of the biggest challenges to photosynthesis researchers. The outline of the reaction cycle, known as the Kok-Joliot cycle, has been known since the 1970s, but there are several steps that have yet to be fully clarified. The steps of the cycle are numbered S0 to S4, each which represent intermediate states of the Mn4Ca catalytic core and the water molecules involved in the reactions, differing by geometries and oxidation state. Guidoni’s recent work has been looking at the passage between S2 and S3.

“A lot of experiments have been done on this small step because it involves large movements and lots of changes in the structure of the active site,” explains Guidoni. “We used multiscale modelling and techniques that can exploit the capabilities of PRACE infrastructure, which has helped us interpret the results of many experiments done since the 1980s that up until now had been somewhat mysterious.”

Using 6.5 million core hours on Curie hosted by CEA at GENCI, France, Guidoni and his team have been able to describe the molecular changes occurring in the S2 to S3 transition in great detail. They now have a mechanism that is consistent with most of the experimental work that has been done on the transition, providing a clear interpretation of the previously puzzling data.

“Significant changes occur in the coordination of the metal centre, the arrangement of the hydrogen bonding network, and the water binding,” says Guidoni. “Many water molecules were shown to exist in the crystal structure when it was presented in a 2011 paper, but it was not clear which one was going to bind the catalytic cluster between S2 and S3 states. We now have identified this water and, as a consequence, we now know the two water molecules that are needed as a substrate in the reaction.”
These findings have shown much about how the enzyme works and the parts of its structure that are important for catalysis. Researchers involved in artificial photosynthesis are looking for stable, efficient, and economically viable materials to produce fuels, such as hydrogen or other organic molecules, using sunlight. Their knowledge of the biological machines can inspire the development of inorganic, biomimetic motifs that can do the same job but on an industrial scale. “In parallel with our work on Photosystem II we are always working on materials to improve solar energy conversion,” says Guidoni.

Although similarities do exist between the way in which artificial mimics and Photosystem II work, Guidoni and his colleagues believe that there remains more to find out about the natural system if the same efficiency is to be achieved artificially. “Our feeling is that the protein is really finely-tuned. All the details, including the conformation of the amino acids around the active site, and the hydrogen-bonding network, are that way in order to make it incredibly efficient. So there is still a lot more to learn from nature.

“They used multiscale modelling and techniques that can exploit the capabilities of PRACE infrastructure, which has helped us interpret the results of many experiments done since the 1980s that up until now had been somewhat mysterious”

In terms of further work in this area, the researchers will be looking at amorphous solid manganese based catalysts. “Manganese is the same metal that is used in the natural system which is good because it is relatively green and abundant,” says Guidoni. “The challenge is to understand the differences and see if we can tune the properties of the metals in order to let them be as efficient as natural systems.”

The artificial photosynthesis community is currently exploring numerous strategies for connecting sunlight with catalysis. Photovoltaic electricity can also be used to drive water splitting, and light absorption can be integrated inside the catalysis. It is not yet apparent which solution will eventually prove to be the most effective, so many different methods will continue to be explored in the coming years.

The information garnered from this work is, of course, also very interesting in terms of the basic understanding of the mechanisms behind photosynthesis. “It is amazing to think that this system has existed without much variation for over 2.5 billions years,” says Guidoni. “It is a unique protein that has produced all of the oxygen we are breathing now, so it has been hugely important in terms of the development of oxygenic life. Now, using computer simulations, we can finally see how it works.”

Project title: Water oxidation by photosynthesis: dynamics and reactivity of the manganese cluster in the Photosystem II complex explored by Quantum Mechanics / Molecular Mechanics simulations
Project leader: Leonardo Guidoni, Università degli Studi de L’Aquila, Dipartimento di Scienze Fisiche e Chimiche, L’Aquila, Italy
Project details: Awarded 6 million core hours on Curie hosted by CEA at GENCI, France
Gatekeepers of the cell

Membrane proteins are known as the gatekeepers of the cell, regulating the influx and efflux of molecules and information. Professor Mark Sansom has been simulating these proteins in order to gain deeper insight into the relationship between their structure and function.

Membrane proteins play a key role in cell biology as ion channels, drug receptors and solute transporters. It has been estimated that around 25 per cent of genes code for membrane proteins, and that around 50 per cent of potential new drug targets are membrane proteins. Mutations in membrane proteins may result in diseases ranging from diabetes to cystic fibrosis.

Professor Mark Sansom of the University of Oxford, UK, leads a group that employs computational techniques to explore the relationship between structure and function of membrane proteins and related systems. In particular the group is interested in ion channels, membrane transport proteins, and bacterial outer membrane proteins. They have regularly utilised PRACE infrastructure to investigate these topics using massive coarse-grained molecular dynamics simulations. “Computer simulations allow membrane proteins to ‘come alive’,” says Sansom. “We can simulate the motions of membrane proteins and use this to explore the relationship between structure and dynamic function. This
After this initial phase of experimentation, Koldsø began looking at how different proteins organise themselves within the membrane. The S1P1 receptor is the target of a pharmaceutical drug that ameliorates some of the effects of multiple sclerosis, and Koldsø’s findings on this membrane protein were published in the Journal of the American Chemical Society.

“A complete model of the influenza viral envelope has been created for the first time”

The team initially applied for applied for Preparatory Access, which allowed them to test out different machines in PRACE as well as to develop and scale out their simulation. Scalability of code is a requirement for access to Tier-0 systems. As Sansom puts it, “if you’re going to commit to using this many processors at once, you want to check you’re doing it efficiently first!” The preparatory access bid allowed the researchers to demonstrate that their proposed simulation was technically feasible, which led to the subsequent award of time on PRACE supercomputers.

Clusters cause curvature

Cell membranes are extremely multifunctional. The wide variety of lipids present and their irregular distribution helps to achieve this, but most simulations to date have focused on relatively simple lipid compositions. Research fellow Dr Heidi Koldsø was able to show that if multiple species of lipid molecules are simulated within a cell membrane, some striking features begin to form. “What we saw was that the lipids were not evenly distributed, but were clustered together by type,” says Sansom. “These clusters cause spontaneous curvature of the membrane. These findings were published in PLOS Computational Biology.”
Ultimate turbulence

Rayleigh-Benard flow — the flow in a box heated from below and cooled from above — and Taylor-Couette flow — the flow between two counter-rotating cylinders — are the two paradigmatic systems in the physics of fluids, and many new concepts have been tested with them. Professor Detlef Lohse and his colleagues from the Physics of Fluids group at the University of Twente have been carrying out simulations of these systems to try and improve our understanding of turbulence.

Turbulent flow — the irregularly fluctuating flow of fluid seen everywhere from blood moving through arteries to air moving past aircraft wingtips — is abundant in nature and technology. A topic notorious for its complexity, it has proven frustratingly difficult to pin down and describe fully in mathematical terms. Understanding it is of great practical use in many fields, but getting meaningful experimental data is difficult. Numerical simulations on supercomputers have recently helped researchers move further than ever before towards unlocking the secrets of this elusive phenomenon.

Professor Detlef Lohse of the University of Twente has devoted much of his academic work to studying turbulence, specifically two systems — Rayleigh-Benard (RB) flow and Taylor-Couette (TC) flow. Much like the fruit fly Drosophila in biological research, RB and TC flow are the go-to experimental systems in the field of fluid dynamics.

RB convection systems involve the turbulent flow seen in a closed box that is heated from below and cooled from above. Investigations seek to understand how much heat transfer occurs depending on the difference in temperature between the top and bottom. RB systems are one of the classical problems of fluid dynamics, and various concepts of fluid dynamics have been tested using it.

In an RB system, an increasing temperature gradient at first causes some diffusive transport of heat. Then, the onset of convection rolls occurs. These convection rolls become more intense, after which pattern formation begins. Finally, spatio-temporal chaos turbulence begins. This final turbulent regime is the area that Lohse is interested in. “There is a particular transition from the point where there is turbulence in the bulk of the flow but it is still of laminar type in the boundary layers, to a new regime where there is also turbulence in the boundary layer,” says Lohse. “This is known as the ultimate regime, where heat transport...
is enhanced greatly. If you extrapolate this to real geophysical and astrophysical applications, this can become quite significant.”

Lohse has been studying the nature of this transition – when it happens, and what the flow organisation looks like. Experiments have been done on this, but Lohse’s work aims to complement experimental work with numerical simulations. “Experimental work is limited because it isn’t possible to get full flow information; you can only measure global or local quantities, but you cannot look at the whole temperature and velocity field, and certainly not simultaneously. With numerical simulations, all of this is possible.”

“Access to PRACE supercomputers has allowed Lohse and colleagues to study this particular transition in greater detail than ever before”

Numerical simulations of turbulence are, unsurprisingly, computationally demanding. Access to 11.1 million core hours on Curie hosted at GENCI at CEA, France in and 7.5 million core hours on Hermit hosted at GCS at HLRS, Germany has allowed Lohse and colleagues to study this particular transition in greater detail than ever before.

Another well-studied convection system is (TC) Taylor-Couette flow – the flow between two counter-rotating cylinders. Although this involves the transport of angular momentum rather than heat, it can be shown to be mathematically analogous to RB flow. Numerical simulations of TC flow thus offer insight into the workings of RB flow. This is because mechanical driving is more efficient than thermal driving, so it is less computationally demanding to see TC flow reach the transition to ultimate turbulence. “Experimentally, RB flow reaches the transition at a Rayleigh number [a higher Rayleigh number indicates a more strongly driven RB system] of 10^14,” says Lohse. “Unfortunately, we can only currently achieve 10^13 in simulations, where we see indications that the transition is setting in but do not see it fully. But, in the analogous TC flow we can see and now understand the transition and the enhanced transport.”

Knowledge of turbulence can be applied almost everywhere, from astrophysical processes to the heating of buildings. The Gulf Stream – the Atlantic Ocean current originating at the tip of Florida that has a warming effect on the climate of Western and Northern Europe — illustrates the important role that turbulence plays in the real world. The current is affected by both salt concentration and temperature concentration – a so-called double diffusion system. Competing density gradients within such a system cause the organisation of the flow to be complex, and changing conditions within the Gulf Stream mean that this flow could potentially change, with far reaching consequences. Lohse explains: “At the equator you have hot water which is very saline due to evaporation from the surface, whereas at Greenland you have cold water which is less saline due to melting ice. Changes in these conditions have led to speculation that at some point the flow..."
may turn around. Having a detailed understanding of turbulence allows people to test how robust the Gulf Stream system is and whether there really is a chance that this change in flow may occur.”

Lohse is keen to stress that the support that he has received from PRACE has not only come in the form of CPU hours. Staff from SURFsara, the Dutch member of PRACE that offers support to those using HPC infrastructure, were invaluable in helping Lohse and his colleagues with efficient parallelisation. “It is not only hardware that you need – you also need knowledge from the people who know how to use it. I am a fluid dynamics physicist, but I could not tell you a lot about the details of computer architecture. This is a crucial but overlooked service that PRACE provides. Take China, for example – they have the fastest computers, but the support given to use those computers is not nearly as good as what you receive here in the Netherlands by SURFsara.”

The code developed by Lohse’s team is currently the highest quality around, and it has now been made public domain so that others can use it. In the future he hopes to push simulations of RB flow to higher Rayleigh numbers in order to see the transition to the ultimate regime of turbulence. He is also planning to carry out simulations of turbulence that are both thermally and shear driven. “This is a much more realistic simulation of flow. What we work with now are idealised systems that help us understand fluid dynamics, but they do not look like flows that we see in the natural world. I expect that adding this extra element of driving will mean that the ultimate regime is reached at a lower Rayleigh number.”

**Project title:** RBTC - Towards ultimate Rayleigh-Benard and Taylor-Couette turbulence  
**Project leader:** Detlef Lohse, University of Twente, Netherlands  
**Project details:** Awarded 7.5 million core hours on Hermit hosted at GCS at HLRS, Germany and 11.1 million core hours on Curie hosted at GENCI at CEA, France

"It is not only hardware that you need – you also need knowledge from the people who know how to use it"
Cloud computing

Forecasting weather at a local level is notoriously difficult. Small-scale processes such as cloud formation, turbulence and surface interactions are difficult to simulate, but Professor Harmen Jonker has been using the power of GPUs to achieve this at higher resolutions than ever before. This work has led to a spin-off company that provides accurate weather forecasts to renewable energy companies.

Graphics processing units, or GPUs, were originally designed for the computer graphics and image processing demands of gaming. They achieve this with highly parallel structures that make them more effective than general purpose CPUs. “GPUs have developed on a different trajectory than ordinary CPUs,” explains Harmen Jonker, a professor of atmospheric physics at Delft University of Technology. “CPUs have become more complex and heavy with each new generation, whereas GPUs have become much faster and nimble. They’re very straightforward; they’ll do one task but do it very fast in parallel.”

Around ten years ago Jonker and his colleagues decided to try using GPUs to run the fluid mechanics and meteorological solvers that are designed to accurately model weather systems. Seeing that this worked well using just
one GPU, they then decided to apply for use of the Curie machine in Paris. Consisting of around 300 GPUs that operate at the same time, the machine gave them computational power far beyond what had been available to them before.

The atmosphere is essentially a fluid. The fluid mechanics calculations used to simulate cloud formation and wind are extremely computationally demanding, especially at the scales Jonker and his colleagues have been working on. “In an ordinary meteorological model you would have a resolution of around 10km,” says Jonker. “We are using a resolution of 50-100m, which is a huge step up in terms of the computational power required.”

Processes such as cloud formation, precipitation and turbulence all occur on a fine scale, and so increasing the resolution allows for a much more accurate and useful picture. Through the power of brute-force computing, the researchers have moved beyond modelling the processes and are now simulating them. “The great thing about this is that we are able to use a first-principals approach which makes hardly any assumptions,” says Jonker. “You just set certain parameters and then let the computer run.”

Traditionally these kinds of simulations have only been used in an academic setting to try and understand cloud formation better and to gain a better idea of 

Clouds over the Netherlands on 6 July 2004. The image shows the simulated cloud field, with the corresponding satellite image as inset.
“Supercomputers allow us to use a first-principals approach which makes hardly any assumptions. You just set certain parameters and then let the computer run”

how turbulence affects the weather. Now, because of GPU technology, it can be used for forecasting. “Its amazing how far things have progressed since we started our academic work on this ten years ago. PRACE facilities have really helped us to show that this approach to forecasting is feasible. It is still one for the future but will be a reality sooner than people think.”

The success of these simulations has led to the creation of a spin-off company called Whiffle. Describing its service as “finecasting” for renewables, the company uses the fast atmospheric simulation platform to provide weather forecasts for renewable energy companies at an unmatched resolution. Whiffle is currently targeting wind energy companies, which use wind forecasts to estimate in advance how much electricity they will produce the next day. “The energy of tomorrow has already been traded today,” says Jonker, “so accurate forecasts are valuable to these companies.”

“Unpredictable supply is one of the main challenges that renewable energy companies face. Traditional fossil fuel power plants can switch generators on and off to meet demand, but this is not possible when energy generation is dependent on the weather. For these companies, marginally better weather prediction can save them a lot of money. Our data on clouds and turbulence can be used to calculate how fast the wind will be blowing at the height of the turbines, so we have a lot of people interested.”

The company is now in talks with wind energy customers who are interested in contracting pilot projects over the course of a few months to assess how much they can reduce their operational costs by. “The company is still at it starting phase, so we need to work out what it is we can provide and a suitable pricing scheme,” explains Jonker. “But it is a truly exciting challenge to be taking these simulations out of an academic context for the first time and seeing how they fare in an operational setting.”

Solar energy companies will also be taking a keen interest in such accurate simulations of cloud cover. “This is the area where we believe we can make the biggest difference,” says Jonker. “Traditional models for wind are pretty good and although we can certainly make improvements, they will only be by a small amount. Solar forecasts, although trickier, are where we can have a greater impact and have real traction. There is still a lot of work to be done to develop these solar forecasts, but I believe that they can be of real use to solar energy companies in the near future.”

For the time being, the team are working with their code and assessing just how good their forecasts are and how they can improve them before they begin with their initial pilots. After that, it will be straight in at the deep end as they try and change the world of weather forecasting with their high-resolution simulations.

Project title: Large-Eddy Simulation of tornado formation by a supercell
Project leader: Harmen Jonker, Delft University, Netherlands
Project details: Awarded 500,000 GPU hours on Curie hosted by CEA at GENCI, France
The search for new physics

The Standard Model of particle physics is one of the great scientific achievements of the 20th century. After confirmation of the existence of the Higgs boson in 2013, physicists are now keen to see whether there is anything beyond the theory. Laurent Lellouch of CNRS and Aix-Marseille University has been leading a team that has been using lattice QCD to see whether a certain experimental measurement is indeed a glimpse of new fundamental physics.

The Standard Model of particle physics — the theory that classifies all known subatomic particles — has stood the test of time well. No experimental evidence has conclusively contradicted it since its current formulation was finalised in the mid 1970s. Despite this, there are a number of theoretical features of the model that have lead many to believe that it does not tell the complete story. Scientists around the world are searching for clues for what lays beyond it, the most prominent example being the work taking place at the Large Hadron Collider, which famously confirmed the existence of the final piece of the theory – the elusive Higgs boson.

Problems arise when trying to probe the Standard Model because some processes are so complex theoretically that they cannot be solved by the more traditional “pen and paper” approaches. That makes it very difficult to determine whether phenomena incorporating these processes are consistent with the predictions of fundamental theory. One such example of a measurement that could potentially deviate from the theory is the anomalous magnetic moment of the muon, a close cousin of the electron.

What is this measurement? Fundamental particles that carry spin, such as the muon, behave like tiny magnets. This effect is characterized by the magnetic moment of the particle. However, for more accurate values of this property to be calculated, the relativistic quantum effects of particles spontaneously flitting in and out of existence in the vacuum must be taken into account. These quantum fluctuations lead to small corrections which are collectively known as the anomalous magnetic moment. Most of these corrections can be predicted from first principles, but the hadronic contributions — the contributions from the strong nuclear force that holds quarks together to form particles such as protons and neutrons — are only beginning to be computed directly from the fundamental theory due to the need for new methods and the limitations of supercomputing power.

The most accurate experiment to date measured the anomalous magnetic moment of the muon with a relative precision of $5 \times 10^{-7}$. An experiment that will make a measurement four times as precise is currently being prepared. The most accurate prediction of the value had a precision of $4 \times 10^{-7}$. Interestingly, these values do not agree. “This is one of the best-known discrepancies between the Standard Model and experiments,” says Christian Hoelbling of the University of Wuppertal. “But, the current prediction of the value is based on models and interpretations of other experimental data. What we and other teams have been doing is using HPC resources to predict this value from first principles, directly from the underlying theory of the strong interaction. In this, our first attempt, we seek to compute the largest hadronic correction with sufficient accuracy to verify that the current determinations, based on other experimental data, are consistent with the fundamental theory. Eventually, the methods that are being developed will allow us to know for certain whether the experimental value actually deviates from the Standard Model.”

A group led by Dr Laurent Lellouch of CNRS and Aix-Marseille University has been using the JUQUEEN supercomputer in Germany, Fermi in Italy, as well as Turing, a 1.2 Petaflop IBM BlueGene Q system, hosted by GENCI in France., to investigate this potential lead. The group’s method for predicting the value for the hadronic contribution to the anomalous magnetic moment of the muon is a two-stage process, the first of which is generating typical vacuum states of the theory. This involves simulating a small piece of space-time on the supercomputer. “We took a very small volume — no bigger than the volume of a few nuclei — and a very small period of time, and then solved the quantum chromodynamics equations used to describe the strong nuclear force.”

![Pictorial representation (Feynman graph) of the fundamental process responsible for the leading order hadronic contribution to the anomalous magnetic moment of the muon.](image-url)
Quantum chromodynamics (QCD) is very hard to treat numerically: the fundamental degrees of freedom of the theory (quarks and gluons) are very different from the states that occur in nature. Usual perturbative techniques are insufficient. The problem is thus approached using a technique called lattice QCD. The QCD equations are discretised on a space-time lattice, and then the quantum mechanical path integration is performed stochastically. This approach is extremely demanding numerically. The integration has to be performed on a space with a dimension given by the number of lattice points times the internal degrees of freedom. Since the lattice has to be both fine enough to reproduce all essential details and big enough to fit the entire system being investigated, typical dimensions are in the order of several billion dimensions. Even for petaflop-class installations such as JUQUEEN, Fermi and Turing, it is a challenging task to perform this stochastic integration.

This part of the process has now been completed, and the very complex and numerically challenging analysis of the results is now taking place. The results of this analysis are due to be published shortly. Hoelbling explains the possible outcomes: “If we can confirm the experimental number of this magnetic moment, it would mean that the previous estimates of the number, which were not obtained from fundamental theory, were erroneous due to something which had been overlooked. This would basically close the door on the matter and we would be able to say that this measurement is in compliance with the Standard Model and does not require new physics to explain it. This is the most likely outcome, but from our point of view would also be the least exciting!"

“If, on the other hand, the methods used eventually allow us to confirm that there was a real discrepancy, we would have found something very interesting. The first action would be to check whether there is something within the Standard Model, which has so far been overlooked, that can explain this. This seems unlikely, however. After that, we would have to conclude that there was a new particle that was causing this value to differ from what we expect.”

In time, any evidence for a new particle would give a prediction for the mass of the new particle. This could then be looked for directly at the Large Hadron Collider. “Our work would be providing indirect evidence of something new, which would then provide a strong incentive to search directly for this new particle via experiments. If evidence was found for the existence of a new particle, then we would be entering a new realm of physics which would require us to expand on the Standard Model.”

If (or when) the Standard Model is proven to be incomplete, it could well happen through a combination of the complementary fields of lattice QCD and particle accelerator physics. With the LHC already pushing the latter field beyond what has ever been done before, the highest level of supercomputing resources offered by PRACE could potentially do the same for lattice QCD.

**Project title:** Leading hadronic contribution to the anomalous magnetic moment of the muon  
**Project leader:** Laurent Lellouch, CPT/CNRS Marseille, France  
**Project details:** 35.35 million core hours on JUQUEEN hosted by GCS at FZI, Germany and 35.35 million core hours on Fermi hosted by CINECA, Italy.
Magnetic reconnection is one of the most striking processes in the universe. It happens when hot charged gases, called plasma, reconfigure their magnetic field lines. This releases a formidable amount of energy as the magnetic field is converted into heat and kinetic energy, accelerating particles up to close to the speed of light.

The process is thought to be the main way in which magnetic field energy can be released into particles. It happens in a number of astrophysical settings such as on the surface of stars and in jets produced around black holes, but can also occur in laboratory settings. For example, tokamaks — torus (think hollow doughnut) shaped devices designed to confine plasma for fusion reactions — can experience disruption events in which huge (and undesirable) releases of energy can be deposited on the walls of the machine, causing damage. Methods for using magnetic reconnection constructively in order to provide propulsion for long-distance space missions are also being investigated.

The tremendous amounts of energy that are suddenly and explosively released in this way are a topic of great interest for physicists. Professor Giovanni Lapenta of KU Leuven in Belgium has been investigating how these events happen and especially how they occur in such large volumes. “There are a lot of models that explain magnetic reconnection on a microscopic level, where energy is released quickly but in small amounts,” he says. “But to understand how a much larger amount of energy is released so quickly is more of a challenge.”

Large-scale examples of reconnection, known as turbulent reconnection, are seen commonly in solar physics. Areas of the sun can be observed storing up energy, becoming more and more energetic until the energy is released in the form of a solar flare, or in more extreme cases in an event called coronal mass ejection. These ejections can cause shockwaves and particles that, if they reach the Earth, create geomagnetic storms that can disrupt radio transmissions and damage satellites. These solar energetic particles also cause particularly strong instances of aurora around the Earth’s poles and damage transmission and power lines on the ground.

Similar events can occur in the accretion disks of material that orbit around black holes. Energy is released in jets that can be thousands of light years long, emitting electromagnetic radiation across the spectrum. “These jets constantly replenish themselves, all along the jet, so there must be a source of energy fuelling them that is not just found in the black hole,” says Lapenta. Up until recently, scientists had struggled to understand how this process occurs, but Lapenta and his colleagues now think they have a more comprehensive explanation for what is occurring.

By carrying out large-scale simulations on supercomputers, Lapenta and his fellow researchers have concluded that magnetic reconnection events can cause chain reactions that set off subsequent reconnection events. “In our simulations, reconnection begins at one point in space at which magnetic energy starts to be released. This creates a turbulent flow that expands out of the region and causes new reconnection events to take place, progressively feeding bigger and bigger regions in a cascade that can very quickly convert huge amounts of energy.

“It’s really quite an amazing spectacle,” says Lapenta. “People had drawn up sketches of how they thought this happens, but what we have done is to prove this in practice through simulations. To do this properly, we needed to simulate large amounts of energy in a 3D space with dimensions in the regions of millions of

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*“There are a lot of models that explain magnetic reconnection on a microscopic level, where energy is released quickly but in small amounts”*
kilometres, all at a sufficient resolution to be able to observe the tiny regions in which the original reconnection events occur. To do this, we needed a lot of computing power! 25 million core hours on the SuperMUC computer hosted by GCS at LRZ, Germany, were awarded for the project.

Given that the general proof for chain reactions of magnetic reconnection now exists, a number of new lines of investigation can now be explored. “We have the model, so now we need to make predictions from this model that are experimentally verifiable,” explains Lapenta. “For example, there is a current mission from NASA called the Magnetospheric MultiScale (MMS) mission which is measuring the distribution of electrons and ions around the Earth. It will be interesting to see how the observations made on this mission compare with our simulations. Will we be able to predict the distribution? Will we be able to see a difference between original points of reconnection and the subsequent ones generated by the chain reaction?”

When magnetic reconnection events occur, waves are created in the manner of an explosion. Lapenta is interested in what the MMS mission can find out about these waves. “These waves, as well as the high energy particles, also transfer energy from the magnetic reconnection process. What we want to see is how much energy is converted into the particles and how much is converted into these waves that are propagated out? This is the first time we have been able to directly measure these. Currently we are measuring waves characteristic of the secondary reconnection sites from the chain reaction, and trying to link what is seen with the simulations we have done.”

Another satellite mission will be launched to go very close to the sun and observe the effects of magnetic reconnection in the sun. Much of the work done in these simulations was done in preparation for this mission, so it won’t be long before the results of these simulations can be verified with real observations from around the solar system.

**Project title:** Particle acceleration by magnetic reconnection in turbulence  
**Project leader:** Giovanni Lapenta, KU Leuven, Belgium  
**Project details:** Awarded 25 million core hours on SuperMUC hosted at GCS at LRZ, Germany
Modelling a changing world

The Earth’s climate is a vastly complex system, with a huge number of intertwined variables that influence the trends of the future. Modelling climate is no easy task, and is one of the most computationally expensive areas of research. **Professor Francisco Doblas Reyes** has been leading the HiResClim project, which has been running a global climate model at unprecedented levels of detail.

Climate models mathematically represent interactions between the atmosphere, oceans, land surface, ice, and the sun. Using simulation codes to represent the physical processes that govern these enables researchers to see how things might change given various different scenarios.

Professor Francisco Doblas Reyes of the Barcelona Supercomputing Centre (BSC) and formerly of Institut Catal de Cincies del Clima (IC3) is a researcher in the field of climate variability and climate prediction, ranging from one month to several years. He is one of the lead researchers in the HiResClim project, which has been using HPC resources to run climate models at unprecedented levels of detail.

The HiResClim project has been looking to make major advances in the science of estimating climate change and formulating climate predictions. This is done by addressing the
dual requirements of increased climate model resolution and increased number of ensemble realisations of future climate conditions over a range of time scales and for a set of plausible socio-economic development pathways.

The HiResClim: High Resolution Ensemble Climate Modelling project has received more than 50 million core hours and has helped to raise the profile of the European Network for Earth System Modelling community (ENES), especially in the field of climate prediction, both at the European and international level. It uses a seamless multi-model climate modelling approach. This is advantageous not only because it can provide excellent estimates of climate change but also because it uses supercomputing resources efficiently.

“Thanks to HPC resources awarded by PRACE, the researchers have been using an increased model resolution that has been delivering a significant improvement on the ability to simulate key modes of climate and weather variability”

Thanks to HPC resources awarded by PRACE, the researchers have been using an increased model resolution that has been delivering a significant improvement on the ability to simulate key modes of climate and weather variability. This can help provide reliable estimates of future changes in this variability. “The project took place over three years starting in 2013,” says Doblas Reyes. “We were working with the MareNostrum supercomputer in the Barcelona Supercomputing Centre (BSC). “We took a couple of new models and used them to perform a number of experiments on a global scale at 50km resolution – a resolution that had never been tested before. The experimental set up was unprecedented in that we used the same model to perform experiments that are not typically done together.”

The multi-model ensemble approach acknowledges the inherent uncertainty in estimating changes in climate over seasonal to centennial time scales, particularly in phenomena that are highly variable and which have rare intense events which can impact society and nature the most. To provide credible risk assessment on these phenomena, such as extra-tropical and tropical cyclones, heat waves, droughts and floods, a combination of high climate model resolution and a multi-model ensemble approach is unavoidable. HiResClim has approached this using a seamless multi-model climate modelling approach. This is the most efficient way to utilise HPC resources and improves the realism of climate simulations, and is also the only way to provide robust estimates of climate change.

Some of the experiments involved simulating the climate of the 21st century. “We were also trying to assess our ability to predict the climate, from the level of a few months all the way to ten years in advance. These experiments are very expensive computationally because they are not only trying to make a forecast but at the same
time are looking at how well this can be used to predict climate. By doing this many times, we can then estimate how well we can predict the climate in the near future, when a wide range of users need to make decisions.” The team also carried out similar experiments on a larger time scale, looking at how well their climate models predicted the slow-down or speed-up of global mean temperature over the course of a decade.

The team have carried out most of the experiments they had planned using the MareNostrum supercomputer, but at the same time they used computing resources from the partner’s institutions to carry out the same experiments at the lower, standard resolution used commonly in the field of climatology. “What we found was that although we obtained better results using the increased resolution, the gains we were getting were not as much as expected. This is due to the fact that we have not carried out as many experiments at this high resolution as we do at the standard resolution, so we cannot yet properly understand the behaviour of the system at this level.”

“What we need to do is carry out more work to improve the model at this level. We are still using parameters that were designed to be used at the standard resolution configuration – a resolution that all climatologists have been many years working with and have had a lot of time to perfect. These parameters are not necessarily suitable to the higher resolution and are thus causing it to underperform. We will need more time on supercomputers in the future to improve this new tool so that it is fit for purpose. At the moment it is like having a brand new car, but its engine has not yet been tuned and it is using the wrong kind of fuel.”

Doblas-Reyes and his colleagues will be submitting a proposal for PRACE’s 13th Call for Project Access with the hope that they can continue to work on improving their model at a higher resolution and improve the parameters. One of the case studies they will be proposing will be looking at the ability to accurately predict the levels of sea ice in the late summer Arctic.

**Project title:** HiResClim: High Resolution Ensemble Climate Modeling  
**Project leader:** Francisco Doblas-Reyes, Barcelona Supercomputing Center (BSC-CNS), Spain  
**Project details:** Awarded 50.44 million core hours on MareNostrum 3 hosted at Barcelona Supercomputing Center (BSC-CNS), Spain
Q&A: Roberto Viola

What is the EC currently doing in relation to HPC activities?

Roberto Viola: President Juncker stressed the importance of HPC by stating the EC’s ambition to place Europe in the world top 3 in HPC by 2020. In this line, the EC has substantially increased the planned financing levels for HPC-related initiatives in Horizon 2020.

In Horizon 2020, the EU framework programme for research and innovation, the commission has pledged €700 million of EU contribution to a contractual public-private partnership (cPPP) on HPC with the European Technology Platform on HPC (ETP4HPC). The main goal of this investment is to address the development of the next generation of exascale technologies and to achieve excellence in HPC application delivery and use. For the period 2014-2017, €224.4 million has been committed for this cPPP on HPC.

Preparing Europe for the exascale generation

High performance computing in Europe has received funds from the European Commission, with a commitment of €700 million from the Horizon 2020 programme. Roberto Viola, Director General of DG Connect in the European Commission, believes that this investment can help make the EU one of the world’s top supercomputing powers, and that PRACE will be an essential part of this endeavour.
But our support to HPC does not stop here. The next stage is the launch of a European Cloud initiative as part of a broader digital single market technology package that the EC will unveil on 6 April 2016.

The European Cloud initiative comprises the European Open Science Cloud and the European Data Infrastructure. The European Open Science Cloud is a trusted and open environment for the scientific community for storing, sharing and reusing scientific data and results. The European Data Infrastructure is underpinning the Open Science Cloud, combining world-class supercomputing capability, high-speed connectivity, leading-edge data storage and interfaces for cloud-based service delivery. HPC is at the heart of this ambitious initiative that would place the EU among the world’s top supercomputing powers. This would be realised with two exascale supercomputers based on EU technology (including low-power HPC chips) ranked in the first three places in the world.

The initiative will also support quantum technologies, to unlock their enormous potential in the computing, secure data exchanges and networking domains. To accelerate their development and bring commercial products to public and private markets, the EC will start the preparatory steps for a large-scale flagship on quantum technologies.

▶ What can be done to ensure that Europe competes with the US and the rest of the world?

RV. HPC is at the core of major advances and scientific and industrial innovation in the digital age. It is the base of sound policy-making to tackle key societal challenges like climate change. This is well understood by our competitors worldwide; the U.S., China, Japan, Russia, and India have declared HPC an area of strategic priority. They have specific national programmes to develop their own HPC ecosystem towards exascale computing (hardware, software, applications, skills, services, etc.) and to deploy state-of-the-art supercomputers.

Europe has to participate in the HPC race in line with its economic and knowledge potential. We need to invest in the establishment of a full European HPC ecosystem to avoid the risk of being delayed or deprived of strategic know-how and critical technology. It is not only about having the fastest systems, but also mastering the next generation of exascale technology and making the new computing power available to our scientists, industrial users and business.

Member states in isolation do not have the resources to develop the necessary HPC ecosystem and acquire exascale capabilities in competitive timeframes. I therefore welcome the joint initiative taken by a group of member states (Luxembourg, France, Italy and Spain) who presented their plans to launch an Important Project of Common European Interest (IPCEI) on HPC and big data enabled applications. The declared objective is to support the development of new usages of HPC by the industry and to guarantee access to world-class HPC facilities for public and private research.

“We need to invest in the establishment of a full European HPC ecosystem to avoid the risk of being delayed or deprived of strategic know-how and critical technology”

Building on this initiative and with the support of other member states and the industry, the European Cloud Initiative aims to provide Europe with leading computing and data infrastructure capabilities, giving easier access to HPC to researchers, industry, in particular SMEs, and public authorities everywhere in Europe. Needless to say, we see PRACE as an essential partner in this endeavour.

▶ How can Europe ensure that enough graduates with the right skills to excel in HPC are produced?

RV. Education and skills are critical components of the HPC strategy. PRACE has deployed an important effort through the Advanced Training Centres and the Training Portal. Also, we expect the recently established Centres of Excellence in HPC applications to help in the development of a much larger workforce that is well educated and trained in HPC. But much more is needed at national and European level to develop the skills and expertise for the era of exascale computing.
The image of HPC as a career choice needs to be campaigned at all levels, starting even before the students enter university. HPC should be a part of education in most scientific domains. However there are no practical strategies for integrating HPC into the already crowded scientific and engineering curricula of European universities. Exploiting the HPC opportunities in science and industry also requires creating more HPC-related internships and postdoctoral opportunities, as well as guidelines for HPC on-the-job training.

“Education and skills are critical components of the HPC strategy. PRACE has deployed an important effort through the Advanced Training Centres and the Training Portal”

In our view, the way to go is to promote HPC from a multidisciplinary point of view, combining both the computational and the domain-specific aspects. This is going beyond expanding computer science with HPC elements – it is about integrating computational science methods into the requirements for science degrees. Another important avenue is to exploit the combination of web programming with cloud-based access to HPC resources, tapping into the web-based skills that are much wider than the scarce parallel programming expertise.

How can SMEs be encouraged to use HPC resources?

RV. Considerable progress has taken place in the last few years, with several member states supporting HPC competence centres that facilitate access of SMEs to HPC services. Some of our European supercomputing centres are world leaders in collaboration with industry. For example the PRACE SHAPE programme or Fortissimo helps HPC adoption in SMEs.

However, only a small percentage of European SMEs that could be helped by HPC seem aware of these opportunities, and more effort is needed to reach out to a higher number of new HPC users. We need to support the ‘democratisation’ of HPC resources, exploiting the opportunities offered by the convergence of HPC, big data and cloud technologies. SMEs without in-house capabilities should benefit from easy access to on-demand HPC-powered cloud-based services, parallel codes, data analytics tools, and even more important, skills, guidance and consultancy in HPC.

Giving SMEs cost-effective and easy access to HPC and data capacity via the cloud is one of the main objectives of the European Cloud initiative. It will notably take place via data and software centres of excellence and data services innovation hubs that will be deployed across Europe.

How are PRACE’s activities important to DG Connect’s overall goals in Europe?

RV. PRACE has been instrumental in pooling leadership-class computing systems and making them available to all researchers in Europe for scientific excellence and innovation.

We now need to coordinate national and European investments to deploy an integrated and sustainable world-class HPC infrastructure in Europe. This will include a governance structure for the management and the development of the data and HPC infrastructure and services, decision making on funding, long-term sustainability and security.

The experience and know-how of PRACE in procurement and operations of world-class computers is invaluable. Therefore, we count on PRACE to become a key partner in the governance and the implementation of the European Cloud Initiative.

How will the Digital Single Market be realised in Europe?

RV. The Digital Single Market will be a borderless area where people and businesses can trade, innovate and interact legally, safely, securely, and at affordable cost. It will create opportunities for new start-ups and allow existing companies to grow and profit from the scale of a market of 28 countries.

To realise the Digital Single Market we need to bring down barriers and tackle existing fragmentation in the online world.

This calls for action in many different areas: we will facilitate cross-border e-commerce; adapt our telecom rules to promote the deployment of high-speed broadband networks; review the current rules in the audio-visual sector; assess the role of online platforms; modernise EU copyright law; allow the free flow of data in Europe; and realise the digital transformation of industry, public sector and science, partly by investing in world-class data and HPC infrastructures.

We are working full speed on these initiatives and will deliver on most of them in the course of 2016. Involvement of member states and stakeholders (industry, civil society, the research and innovation community) is essential to help us develop and implement these initiatives and realise the Digital Single Market.
Mateo Valero is a Spanish computer architect and director of the Barcelona Supercomputing Centre, home of the MareNostrum supercomputer. He has been working with PRACE since its inception. We spoke to him about the future of HPC software, the importance of creating a domestic HPC industry in Europe, and the ways in which Europe can continue to support the increasing demand for HPC resources from industry and SMEs.

As director of the Barcelona Supercomputing Centre, what has been your experience of working with PRACE?

Mateo Valero: PRACE as a European Research Infrastructure is great for European scientists, offering the best European machines to the most interesting projects decided by a peer review process. In the few years it has been operating, I think it has proven to be a very valuable tool to promote scientific competition and cooperation within Europe.

The Barcelona Supercomputing Centre (BSC) has always been strongly committed to the creation and implementation of PRACE. Right from the concept stage, we understood it was a necessary extension of HPC services at the European level. Its approach is very similar to the one that the BSC used to promote the development of the Spanish Supercomputing Network in 2007.

PRACE is a multicultural infrastructure which includes German, British, Nordic and Mediterranean partners, with all of their different idiosyncrasies. These partners all work together and benefit from seeing how others use different methods to achieve the same objectives. I’m convinced that the complexity of establishing it has been more than compensated by the many scientific and industrial success stories which
have resulted from the initiative from all around Europe.

▶ It has been said that the applications and codes used in HPC are lagging behind the development of the hardware. How can this be addressed?

MV. Future HPC infrastructures will have a very large computing capacity spread among a wide and heterogeneous set of computing units (CPUs, GPUs, vectors, etc.). As such, data movement across the system must be properly orchestrated to fully use such large computational capacity. From the software perspective, system software must be developed which can reduce the burden of properly expressing at the application source code level how and when data should be moved across the whole HPC system. From the hardware perspective, mechanisms to support some fundamental operating system (OS) and runtime system activities need to be developed. A tight collaboration between the system software (OS, parallel runtime system, etc.) and the hardware is expected to be one of the key aspects of upcoming HPC machines.

▶ How can we encourage the emergence of new European technologies — especially hardware — for HPC?

MV. The HPC market is dominated by technology providers whose headquarters are based outside the EU, who operate in well protected domestic markets and who often receive what are effectively government subsidies in their home countries. This preferential treatment helps to strengthen and consolidate these companies, increasing their ability to sell aggressively in Europe. This has made it more difficult for Europe to build a strong domestic HPC industry.

I think Europe should take a similar approach to the US, Japan and China, and invest big in potential European industrial HPC actors. This should be done by funding at least two major HPC prototype systems built by European industry with different architectures and, as far as is possible, using a full HPC stack from the processor to the system and all the way to the application software.

Developing a genuine domestic HPC industry is important from a business point of view, but some may argue that Europe doesn’t need to be competitive in all market segments. However, and this is what other regions have seen, from a strategic point of view it is essential. It is clear that we are living in a world which is becoming more and more dominated by computing. Computing now pervades all aspects of modern life including health, the right to privacy and the security of citizens. Europe cannot be entirely dependent on foreign technology when these issues are at stake.

“The Barcelona Supercomputing Centre (BSC) has always been strongly committed to the creation and implementation of PRACE”

Europe also needs to create quality jobs for graduates of long and expensive computer science, engineering and applied computing degrees. If Europe had a domestic HPC industry to absorb the talent coming from its outstanding universities, many of our best young HPC professional would not need to emigrate to the US.

▶ HPC resources are being used by a wider variety of sectors than ever before. How can Europe make sure to keep up with increasing demand from industry and smaller businesses?

MV. By buying the best HPC systems the international market can provide in the immediate term, while at the same time developing a domestic HPC offer. Access to HPC resources should be made easier not only for big industries but also for SMEs.

This will require investments in IT education for the wider European workforce, a network of HPC centres with cutting edge performance, such as the centres collaborating in PRACE, an aggressive HPC roadmap, like the one indicated by ETP4HPC, but above all consistent and continued investment from the EU member states and from the European Commission.

The recent announcement by Commissioner Oettinger of an Important Project of Common European Interest on HPC and Big Data (IPCEI HPC BGD) initiated by Luxembourg, France, Italy and Spain and open to the rest of Europe, is a good potential step in the right direction. Much of its success relies on the anticipated funding of €3.5bn over the next few years becoming available soon enough to allow Europe to compete as an equal in the worldwide competition for the predominance of HPC technology, and thus enjoy its resulting benefits.
Key performance indicators

Given the scale of the 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.

In 2014, the PRACE Council approved a set of key performance indicators (KPI) that facilitate the analysis and evaluation of PRACE’s achievements and successes.

PRACE’s impact on evolving research

Number of projects
The number of project applications received via PRACE Calls for Proposals for Project Access exhibit a clear overall upward trend. 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 1). A downward trend of rejected projects below the technical quality threshold is noted, displaying the maturation process of proposal submissions, in which researchers put more effort into the quality of their proposals. 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 1 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.

The overall trend highlights the increasing importance and impact of PRACE Tier-0 service for research.

Project resubmission
PRACE also keeps track of the submission of project proposals by recurrent principal investigators (PIs) (Figure 2). The ratio of recurrence is relatively low: over 41% of PIs who submitted the most recent proposals were recurrent applicants to a PRACE Call for Proposals for Project Access. The upward trend of the ratio of recurrence is visible, particularly from the 6th Call onwards (reaching 57% at the 11th Call), influenced by the downward trend on awarded projects.
International cooperation

A total of 60% of the projects that are awarded with PRACE resources, and two-thirds (63%) of those resources are awarded to “foreign projects” (i.e. projects with PIs from a different country (recorded as the primary institution of the PI) than the machine on which the research is executed). The ratio of awarded foreign projects remains rather stable over time (Figure 3). This suggests that the nationality of the PI’s institution does not impact the chances of a project being awarded and reflects that the PRACE peer review process works with scientific excellence as its main criterion.

This also demonstrates PRACE’s impact on the enhancement of European and international collaboration.

National and international co-funding for PRACE-awarded projects show a downward trend (Figure 4), despite the clear increase in the 10th Call for national co-funding. National co-funding represents the most prevalent form of self-support for the projects awarded by PRACE, overlapped only by EC co-funding in the 9th Call. EC co-funding exhibits a gentle overall upward trend.

The increase of EC support for the projects awarded by PRACE illustrates the outcomes of EC funding policies, aligned with the support to HPC, as key enabler technology.
PEER REVIEW PROCESS

Figure 4 – Ratios of awarded projects with National, EC and International support; and related trend lines

PRACE’s impact on scientific production

Considering that it is only possible to measure the impact of PRACE-supported projects via their scientific production one year after the end of the project, Figure 5 only presents the evolution of scientific production supported by PRACE up to and including the 6th PRACE Call for Proposals for Project Access (mid-2014).

Up to and including the 6th PRACE Call for Proposals for Project Access, PRACE supported 275 MSc and PhD theses, 746 publications and 1363 scientific talks. On top of that, two patents resulting from projects supported by PRACE have been filed. The data reflects an increasing trend in all types of scientific production supported by PRACE.

The increase in scientific production (Figure 5) is partly related to the increase in PRACE HPC resources made available and therefore the possibility of awarding a larger number of project applications. Of course, a higher number of publications raises the chance of a higher impact in science, but a future analysis of the impact-factor of published papers will reveal quantitatively whether the quality of scientific production also improves over time.
PRACE’s impact on growing know-how in Europe

Since 2008 PRACE has aimed to provide top-class education and training for computational scientists in Europe through the PRACE Advanced Training Centres (PATC), the International HPC Summer School, and PRACE Seasonal Schools, with a clear increase of participants registered (Figure 6). A slight decrease is observed between 2014 and 2015.

PATC courses, Seasonal Schools and the International HPC Summer School are offered free of charge to eligible participants.

Between August 2008 and December 2015, PRACE has provided 23,783 person-days of training through attendance-based courses, with an upward attendance trend. PRACE courses were attended by 7,350 unique individuals. This shows the effectiveness of PRACE in attracting, training and retaining competences.

The six PRACE Advanced Training Centres are 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).

The average rate of recurring participation in training is of 30%. This excellent ratio proves that PRACE trainings are not a closed circuit where the majority of attendees are the same people attending repeatedly. It also shows enough recurrence to indicate the attractiveness of PRACE training courses.

In 2015 the number of participants registered in PATCs courses was 1628 (1366 from academia and 262 from non-academia affiliation). More than 83% of participants attending PATCs trainings days have academic affiliation (1366), illustrating the impact of such event 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 2015. As observed in Figure 7, the total number of attendances registered in the first semester (first and second quarters) is significantly higher than during the second semester (third and fourth quarters). This is the result of the varying number of training days and courses available during these periods.

![Figure 6 – Number of person-days registered at PRACE training days between 2008 and 2015](image)
PRACE’s impact on attracting the industrial sector

**Industrial visitors of the PRACE booth at ISC and SC**

The interest of industry in PRACE at high-level international events has increased steadily over the past years (Figure 8). The total number of industrial participants showing interest in PRACE during the two main HPC events (Supercomputing (SC) in the USA, and the International Supercomputing Conference (ISC) in Germany) between 2008 and 2015 was 1233 unique individuals.

**Industrial participants in PATCs**

The average participation of industry in PATC training is 12% between 2012 and 2015 (15% in 2015). The increasing interest from industry in participating in HPC training is visible in Figure 9. A total of 260 industrial participants were trained by PRACE. Eligible industrial participants enjoy the same service as academic trainees and can attend PATC courses free of charge.
Industrial use of PRACE HPC resources
PRACE opened its Calls for Proposals to industrial applicants in mid-2012. Industrial participation can take the form of a project led by a principal investigator coming from an industrial enterprise, or a researcher from industry collaborating in an academia-led project. The reduction and stabilisation of projects awarded after the 7th call has a strong impact on the number of projects awarded with industrial participants (Figure 10).

Regarding SHAPE pilot, PRACE can report 10 success stories of SMEs from 6 different countries benefitting not only from PRACE HPC resources but more importantly, from the know-how in the PRACE centres. The second SHAPE call awarded 11 more projects and a third SHAPE call was opened in November 2015.
Expertise through high-class training

As the performance and the complexity of supercomputers keeps increasing, fully exploiting their capacity is becoming more and more non-trivial. PRACE continues to provide a comprehensive, high-quality training programme in order to help researchers gain a competitive edge from high-end computing.

High-performance computing (HPC) has become an essential tool for scientists and engineers both in research and industry, and well-trained staff are as important as cutting edge hardware. PRACE provides world-class training in HPC and in computational science via the Prace Advanced Training Centres (PATCs), seasonal schools, and on-line training opportunities in the PRACE training portal. During 2015 PRACE has started extensive training collaboration with the recently started EU Centres of Excellence for computing applications.

**PATCs**

The six Prace Advanced Training Centres at BSC – Barcelona Supercomputing Center (Spain), CINECA - Consorzio 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) have been operational since 2012, and have significantly boosted the PRACE training programme.

In 2015, PATCs have offered 75 courses in the PRACE coordinated curriculum (together in the 2014-2015 and 2015-2016 programmes). The PATC curriculum covers a wide range of topics in HPC and scientific computing including basic parallel programming, advanced accelerator utilisation, large scale data analysis, scientific domain based techniques, as well as and more industrially focused topics like one on uncertainties quantification.

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<td>August ‘14-July ‘15</td>
<td>August ‘15-January ‘16</td>
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<td>58</td>
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<td>1 786</td>
<td>405</td>
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<tr>
<td><strong>Female (%)</strong></td>
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<td>8.4</td>
<td>8.4</td>
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</tbody>
</table>

This table shows some key statistics about the PATC curriculum.
Specific PATC highlights in 2015 include:
- More emphasis on data science
- Increasing number of female participants
- Continued industrial focus with increasing number of non-academic participants

PRACE Winter School 2015
Due to the transition from the PRACE-3IP project to PRACE-4IP, only a single seasonal school was held in 2015. The PRACE Winter School 2015 was held on 12 – 15 January 2015 at the VŠB - Technical University of Ostrava, Czech Republic, and it was organised jointly by the National Supercomputing Center IT4Innovations, VŠB - Technical University of Ostrava and PRACE.

Participants at the PRACE Winter School 2015

The topic of the school was “HPC Tools for Data Intensive Processing”. 45 participants learned essential skills for high-performance data analysis. The school offered a portfolio of tutorials on high performance I/O, data analytics with the R language, and visualisation.

In 2016, three seasonal schools will be organised in Slovakia, Ireland, and Austria. More information about the seasonal schools is available at: www.training.prace-ri.eu

International HPC Summer School 2015
For a few years, PRACE has been collaborating with the USA’s National Science Foundation’s eXtreme Science and Engineering Discovery Environment (XSEDE) project, Canada’s Compute / Calcul Canada and Japan’s RIKEN Advanced Institute for Computational Sciences (RIKEN) in organising an international summer school.

The International HPC Summer School 2015 was held on 21-26 June 2015, in Toronto, Canada. 79 students and post-docs from Europe, US, Canada and Japan participated in the school. 30 students came from Europe of whom 29 from PRACE member countries. Topics included HPC challenges by discipline (e.g. earth, life and materials sciences, physics), HPC programming proficientiues, performance analysis and profiling, algorithmic approaches and numerical libraries, data-intensive computing, scientific visualisation, and Canadian, EU, Japanese and US HPC-infrastructures.

In 2016 the International HPC Summer School takes place in Ljubljana, Slovenia from 26 June to 1 July.
Online training
The main online facility in PRACE training is the PRACE Training Portal which serves as a single hub for the PRACE training events as well as for training material and tutorials. Training material includes recorded lectures, lecture slides and material and model solutions for hands-on exercises when appropriate.

The figure below shows the visitor statistics for the portal for the whole year of 2015. In comparison to year 2014, the number of page views has increased by 24% and the number of users by 45%. It is interesting to note the high traffic from the US.

As a new online-training activity, in 2015 PRACE started the development of massively open online courses (MooCs). The first PRACE MooC will focus on introduction to HPC and management of massive data, and should be available in 2016.

During 2015, PRACE has also been developing a CodeVault repository. The CodeVault contains various code examples and model solutions of common HPC programming tasks. The code samples are released under open source licenses and they can be utilised both in HPC training as well as in building blocks of real-world computing applications. Anonymous read-access is possible for everyone, and registered users can also contribute to the repository. The CodeVault repository was launched in January 2016, and it can be accessed via the PRACE Training Portal.

Visit the training portal at: www.training.prace-ri.eu
PRACE Summer of HPC 2015

The PRACE Summer of HPC (SoHPC) programme is now in its third year of inspiring late-stage undergraduates and early-stage postgraduates in their path to becoming the next generation of HPC users. In 2015, twenty top students were selected through a highly competitive application process to complete projects at ten HPC centres around Europe.

In late June 2015, the successful applicants travelled to the Barcelona Supercomputing Center (BSC), Spain to undertake a week-long training programme in HPC and visualisation.

From Barcelona, students departed to their host sites for eight-weeks, during which time they completed HPC related projects under the supervision of expert mentors. Projects included visualising the surface of Mars, medical and climate visualisations and developing graphical user interfaces for molecular dynamics software. Throughout the programme, the participants blogged about their experiences and project progress with posts on the PRACE SoHPC blog (www.summerofhpc.prace-ri.eu).

At the conclusion of the programme, all participants presented their results. Two exemplary students were chosen by a panel of experts to be recognised for their excellent contributions to the PRACE Summer of HPC and were presented with awards at a dedicated ceremony at BSC in December 2015. Simos Kazantzidis from Greece was presented with the Best Visualisation Award for his superb work on a collaborative interface for in-situ visualisation and steering of HPC molecular dynamics simulations. Alberto García García was presented with the PRACE HPC Ambassador Award in acknowledgement of his excellent outreach efforts.

Once again, the SoHPC programme has successfully provided first-rate opportunities for undergraduate and postgraduate students to develop real-world HPC and visualisation skills. The next edition of the SoHPC will take place in the summer of 2016.

For More Information:
Webpage & Blog: www.summerofhpc.prace-ri.eu
Facebook: www.facebook.com/SummerOfHPC
Twitter: @SummerofHPC
YouTube: www.youtube.com/user/SummerofHPC
The user forum aims to provide a communication channel between the users of PRACE computational resources on the one hand and PRACE RI and the computational centres on the other. This concerns generic issues, such as problems in the review process or during the actual allocation as well as use cases and needs which are currently not catered for.

**Outreach.** The focal point of 2015 was to further increase the number of users actively involved in the forum, starting with the attendance to the annual meeting at PRACEdays. From PRACEdays15 onwards, the user forum will occupy a central time slot. Together with the Scientific Steering Committee, the user forum proposed to reinstate an open call for presentations in order to attract more researchers. This has been put in place for the 2016 edition in Prague.

At the same time, the user forum investigates ways to reach out to (future) users. A mini-symposium was organised at ICCS15 in Reykjavik, which hosted individual research presentations in addition to the actual user forum and a contribution by PRACE RI on peer review. Currently the approach is under evaluation, and any suggestion about candidate conferences or other types of outreach activities would be greatly appreciated.

**Issues.** Too many issues were discussed within the user forum to be listed exhaustively. We will look at some of the longer term recurring issues and their follow-up.

From the outset, the peer review has occupied a very prominent place in the discussions. Since PRACEdays15, the PRACE Peer Review Officer is invited to present the process, answer factual questions, and get direct feedback from the users. These discussions allowed to alleviate some of the concerns of the users and provided input for improvements to the process. Remaining issues concern more detailed guidelines for reviewers and applicants, as well as more detailed feedback to applicants on the final stage of the review.

A second recurring issue concerns (applications for) projects which involve complex work flows, either at the level of the computation or for co-processing purposes. PRACE remarks that tests can be performed within preparatory projects, and that PRACE-4IP features a dedicated work package. In order to follow up this issue, the user forum would be interested in collecting use cases, suggestions or problems encountered in past projects.

Another long term standing point concerns facilities for large data sets, potentially requiring long term storage and/or additional computational resources for the actual post-processing. The 11th Call for Proposals for Project Access featured pilots on this issue. This will be followed up by the user forum, but other use cases are still welcome.

Finally, some users have had problems with the timely consumption of resources due to too high a load of the machines combined with a relatively strict consumption policy. PRACE acknowledges that there may be punctuality issues, and advocates a proactive attitude from the centres by following up the timely resource consumption per project and by notifying users in time concerning issues about availability of resources. As these concerns were specified in very general terms, the user forum is interested in collecting specific examples.

**Conclusion.** For the user forum, 2015 has brought promising evolutions in terms of the outreach activities as well as in the interaction with PRACE. Its contributions to the meetings and the proactive attitude is much appreciated. Special thanks go out to the users that actively contributed to the discussions. We look forward to meeting you again soon.
PRACE projects support the research infrastructure

During 2015, two EC-funded projects, the third and fourth implementation phases of the PRACE project (PRACE-3IP and PRACE-4IP), were active and supported the implementation of PRACE aisbl. The PRACE projects are joint efforts, where 25 PRACE members contribute and work together in order to deliver the best support for PRACE users and for the implementation of the PRACE research infrastructure. Some highlights of the work of the PRACE projects are reported in detail in other parts of this annual report, particularly the extensive training activities of the PRACE Advanced Training Centres, the SHAPE pilot, and dissemination actions such as the organisation of the PRACEdays15 conference or the PRACE presence at numerous high-profile HPC exhibitions and events.

The PRACE-3IP EC review took place in Brussels on 27 October 2015. PRACE-3IP received the highest possible rating, “excellent”, for the entire project. The experts from the European Commission attested that the project has achieved a high degree of work and professionalism at a high level. For most of the work packages it was the final review as only pre-commercial procurement (PCP) related activities continue. The PCP pilot on ‘whole system design for energy efficient HPC’ was planned for 48 months to allow the execution of a full procurement process.

With a back dating of three months the PRACE-4IP project started on 1 February 2015, continuing and extending the successful work and support from PRACE-3IP. Already in 2015 the work for a new proposal for the PRACE-4IP successor project was started. The following presents some highlights of the project work in 2015:

PRACE-3IP pre-commercial procurement

The energy constraints of multi-petascale and subsequent exascale systems will require significant developments from hardware suppliers to integrate energy efficient components at all levels of HPC technology. To address this issue in the most suitable way for PRACE user communities, PRACE is assessing for the first time in the field of European HPC a three-phase pre-commercial procurement (PCP) programme on “whole system design for energy efficient HPC” during the third PRACE implementation project (PRACE-3IP). PCP is the procurement of new innovative solutions before they are commercially available.

The first execution phase, of the PRACE-3IP PCP on “whole system design for energy efficient HPC”, took place from September 2014 to March 2015, with the following vendors:
- BULL SAS, France
- E4 Computer Engineering SpA, Italy
- Maxeler Technologies Limited, United-Kingdom
- MEGWARE Computer Vertrieb und Services GmbH, Germany

During this phase, which focused on solution design, vendors worked on a design specification for new technologies and solutions to be developed within PCP, a high-level design specification for the final system architecture, an application porting strategy, an energy efficiency analysis, and a market analysis. After assessment of their results and visits to their facilities during January 2015, all vendors were invited to submit a bid for phase II of the PCP, which will build on the results of phase I.

This second call for tender was issued from 9 March to 27 April 2015. MEGWARE withdrew from the process, leaving three bids to be assessed. The three remaining bidders scored positively and were awarded the phase II contract. The signature of the contracts was completed on 15 June 2015. The second phase is expected to end on 14 April 2016. In this follow-up phase focused on prototyping, contractors are expected to work on lab prototypes, write a detailed specification of the overall architecture as well as the pilot system, work on performance and energy consumption models and on the porting of real production applications codes in use by PRACE today that will be used as benchmark for the evaluation of improvements in energy efficiency.
The selected applications are part of the European Unified Application Benchmark Suite:

- **BQCD** a quantum physics code that simulates lattice quantum chromodynamics;
- **NEMO** a climate modelling code for oceanographic research and seasonal forecast;
- **Quantum ESPRESSO** a material electronic-structure code;
- **SPECFEM3D** a geodynamic code that simulates 3D seismic wave propagation.

The PCP vendors who were selected for phase I were invited to present their work on HPC energy efficiency at the 6th European Workshop on HPC Centre Infrastructures, which was organised by PRACE-4IP work package 5 (WP5) “best practices HPC commissioning and prototyping” from 10 to 13 May in Stockholm. This was not part of the PCP process and had no link to the assessment of phase I or selection of phase II, but it was an opportunity for the vendors to present their work to a large panel of public and private procurers of HPC and datacentre infrastructures in Europe, US and Australia, and to some key players of the HPC industry. It was noted by the audience that this PCP’s methodology for determining energy efficiency could be followed within future ordinary HPC infrastructure procurements as it allows for a better forecast of the total cost of ownership (TCO).

The third and final phase of the PCP is planned to start in June 2016, last for 16 months, and will be focused on implementing first versions of the final architecture and their deployment as pilot systems in operational centre. These pilot systems will allow the verification of technology readiness and assess the progress in terms of energy efficiency.

**Operational services**

The operation and coordination of the PRACE common services enables the interoperation among different PRACE HPC systems and presents a common interface to the PRACE European level (Tier-0) systems and the national level (Tier-1) systems involved in services for European level (Tier-0) systems.

Six European level (Tier-0) systems and 23 national level (Tier-1) systems were operational in 2015. The operational procedures have continued to be successful in maintaining a reliable and available set of services. The services are divided into seven categories: network services, data services, compute services, AAA and operational security services, user services, monitoring services and generic services. These services are described in the service catalogue, which is a living document, reflecting the evolution of PRACE’s available services.

Important activities have also been undertaken in order to monitor and maintain the availability of the common services and to prepare and discuss changes of the operational status of...
services, including the addition of new services. The PRACE security forum continues to coordinate all the security related issues and to efficiently manage potential security vulnerabilities. The analysis of new services and the investigation of the prototypical implementations of these services at the pre-production level to assess the functionality were also undertaken.

In addition, links with complementary e-infrastructures and Centres of Excellence (CoEs) have been reinforced, to identify commonalities and foster the technical interoperability across their services for the benefit of the users. For example, collaboration with EGi on security topics, and with EUDAT, on data, to identify interoperability in order to guarantee the long-term preservation and sharing of data produced on the PRACE systems.

The support for the enhancement of interoperability between PRACE and XSEDE started in April 2014 and continued until 2015 with three projects:
- Smart data analytics for Earth Sciences across XSEDE and PRACE
- Interoperable high throughput binding affinity calculator for personalised medicine
- UNICORE use case integration for XSEDE and PRACE

These projects involved collaborating teams with members from both Europe and the US. The results and experience have been valuable and can be used to provide support to other collaborating teams that use resources from both PRACE and XSEDE.

**SHAPE supporting industry**

SHAPE, the pan-European SME HPC Adoption Programme in Europe implemented by PRACE, aims to help European SMEs to raise their awareness of the benefits of using advanced numerical simulation and HPC in order to increase their innovation and competitiveness.

Following the successful pilot run of SHAPE under PRACE-3IP, the second call for applications was launched in November 2014 and closed in January 2015. 12 applications were submitted, out of which 11 were found to be appropriate for support through SHAPE following review. They included projects from a broad range of fields such as wind turbine design, plant breeding optimisation and sailing boat performance. The projects are still ongoing and will be formally reported on in April 2016, but initial feedback has been positive.

An example success story from the recent projects is the work with Ergolines s.r.l. This is an Italian SME with expertise in the design and development of advanced technologies for process control in metal casting and foundry. This SHAPE project was concerned with using HPC-based numerical simulations to study the fluid dynamics of liquid steel under the effect of electromagnetic stirring in an electric arc furnace. In collaboration with PRACE, Ergolines have ported their solver to the CINECA’s supercomputer Fermi, which has enabled them to perform simulations in 20 minutes that would have taken them 15 hours on their local systems - thus enabling them to carry out many more extensive and detailed analyses to feed into their design processes.

The third SHAPE call opened in November 2015 and closed in January 2016 with eight proposals being submitted.

The SHAPE programme is achieving good results, contributing to changing the attitude of European SMEs towards HPC, fostering technological transfer between academia and industry, and ultimately increasing European competitiveness.

**PRACE training**

Harnessing the extreme parallelism of supercomputers of today is highly nontrivial, but unavoidable for researchers who wish to gain a competitive edge from high-end computing. A comprehensive training and education programme is thus essential for the impact of the PRACE research infrastructure.

PRACE has been providing training from the very beginning, and state-of-the-art training in HPC and scientific computing has continued during 2015. PRACE training is carried out via the PRACE Advanced Training Centres in Finland, France, Germany, Italy, UK, and Spain, as well as via seasonal schools. Due to the transition from the PRACE-3IP project to the PRACE-4IP project, in 2015 only the winter school on “HPC tools for data intensive processing” in VŠB Technical University of Ostrava, Czech Republic took place, but the organisation of several seasonal schools for 2016 has already started. As a new activity, PRACE has entered into a training collaboration with EU Centres of Excellence for computing applications.

PRACE training material is available on the PRACE Training Portal. A new on-line training activity, the development of massively open on-line courses (MooCs), has been initiated in 2015. In addition, a PRACE CodeVault repository aimed at sharing code examples, model solutions and other tips in HPC programming within the community has been in development, and a pilot service will be launched in January 2016.

A more comprehensive overview of PRACE training activities is given on pages 38 to 40 of this report.

**Evolution of PRACE Applications Enabling Services**

PRACE commits significant expertise to ensure that a good range of important applications are able to exploit PRACE systems effectively. This work has always been a critical part of the activities of PRACE and involves porting, optimisation, scaling and benchmarking of codes on a variety of large HPC systems. As well as working on academic codes, PRACE also supports work on industrial codes via the SHAPE programme.

During the last year, there has been significant evolution in the application enabling services, with an increasing focus on exascale and accelerators. PRACE project partners surveyed a broad range of key tools and techniques, and then exploited promising
techniques on applications of value to PRACE users. In addition, we are producing a version of our benchmark suite that will run on different accelerators, and plan to compare and evaluate the performance against our standard benchmarks.

PRACE is also investigating ways of implementing new services to enable promising scientific or industrial research to access the EU HPC ecosystem. One such service will define a new access route for “Tier-1 service for Tier-0” and will provide a more effective and explicit migration path between the national level (Tier-1) and the European level (Tier-0). This will be particularly suited to new groups of users or new communities with promising science cases who have not previously accessed resources at the pan-European level. Successful applicants will get support from PRACE experts, initial access to national level (Tier-1) systems for development, and access to a European level (Tier-0) system for demonstration runs. This service is planned to start in the first half of 2016.

To maximise the benefits to the European research community from all the applications enabling work, the resulting knowledge and experience is disseminated via best practice guides and whitepapers. These are readily available from the PRACE web site and get an encouragingly high number of downloads.

**Case study 1: Mesh generation on the road to exascale**

Mesh generation and refinement tools were identified as being of crucial importance to several European communities on the road to exascale. We focused on implementing and exploiting a new mesh generation tool, which has enabled massive mesh generation in OpenFOAM for the first time. In particular, meshes with 7 billion elements were generated in approximately 20 minutes using a scalable mesh generator built on top of Netgen. We also demonstrated that mesh refinement as enabled in Code_Saturne, is also a possible option to create huge meshes for future CFD exascale challenges.


*Figure 1: Test geometries and meshes used during the development of new mesh generation and refinement tools in PRACE 3IP T7.2*
Case study 2: Optimising PICCANTE – an Open Source Particle-in-Cell Code for Advanced Simulations on Tier-0 Systems

The main goal of the project was to establish strong and weak scalability of the particle-in-cell code PICCANTE on large European level (Tier-0) systems. Various optimisations have been performed. The complete rewriting of the I/O scheme had very good impact on the overall performance.

When using more than 2048 MPI Tasks the usual MPI-IO routines dramatically slow down the output process up to an unacceptable level on the used BlueGene architecture. By using a limited number of “sub-master” MPI tasks, which collect the data within their group, and switching to one output file per “sub-master” the program provides its best IO performance.


Figure 2: Comparison of the initial and the final output strategy.

Figure 3: Output time improvement by switching to the new output strategy.
Case Study 3: Parallel Subdomain Coupling for non-matching Meshes in Alya

In this project, the strategy was implemented to couple subdomains with non-matching meshes for distributed memory supercomputers within the Alya multi-physics code framework. The method can be explicit (for multi code approaches) or implicit (for single code approaches).

The multi-code coupling does not affect the scalability of each code, because the extra communications are more or less of the same cost as that of one matrix-vector product communication of the normal parallelisation of the code, and it is performed just once each coupling iteration or time step. In the implicit approach, the extra communications is performed after each matrix-vector product, and the impact can be significant.


(Right) Figure 4: Coupling of the solution of two different subdomains.

(Below) Figure 5: Fluid structure interaction (FSI) benchmark to validate multi-physics problem with a multi-code approach.
PRACEdays15, which ran from 26 to 28 May in Dublin, Ireland, marked another successful edition of the annual PRACE Scientific and Industrial Conference. The Irish Centre for High End Computing (ICHEC) hosted the conference and satellite events locally and, with this year’s theme being “Enable Science Foster Industry”, attracted close to 200 experts from academia and industry.

Two satellite events focusing on Women in HPC and Exascale European projects proved very popular on 25 and 26 May and the EES12 Project held its final conference on 28 and 29 May to round off the week. The PRACE user forum invited all participants to an open session on Wednesday afternoon.

Highlights of the week included the keynote presentations given by well-known academic and industrial researchers from Europe and Asia, including the keynote speech by Masahiro Seki, President of the Research Organisation for Information Science and Technology (RIST), Japan. The European Commission added their vision to the programme with a presentation entitled “Implementing the European Strategy on High Performance Computing”. There were six heavily subscribed parallel streams across various scientific and industrial themes. The final panel discussion on 28 May entitled “Science and Industry: Partners for Innovation”, was moderated by Tom Wilkie of Scientific Computing World and brought together high level representatives from the European Commission, industry and academia.

Finally, the PRACEdays15 Award for Best Poster was presented to Panchatcharam Mariappan for his poster entitled “GPU accelerated finite element method for radio frequency ablated cancer treatment”.

The entire programme, all posters and presentations can be found: [www.prace-ri.eu/prace-days15-wrapup](http://www.prace-ri.eu/prace-days15-wrapup)
Panchatcharam Mariappan, Best Poster Winner of PRACEdays15

Announcement of PRACEdays16
PRACEdays16 will be held at the Orea Pyramida Hotel in Prague, Czech Republic from 10 to 12 May 2016.

The event will again offer a fascinating agenda with several very interesting keynote speakers from academia, industry and the European Commission, including Max Lemke, Head of Unit for Complex Systems and Advanced Computing, European Commission. Christoph Gümbel, Director Virtual Vehicle, Porsche A.G. will also give a talk. From academia, one of the largest users of PRACE resources, Hans-Thomas Janka from the Max-Planck-Institute for Astrophysics, will give a keynote presentation.

PRACE supports the Women in HPC initiative, and this is reflected in the conference programme of PRACEdays16 which includes speakers like Carme Rovira Virgili, University of Barcelona, and Sharon Broude Geva, Director of Advanced Research Computing, University of Michigan, United States. Female researchers have also been invited to speak in the parallel sessions.

PRACEdays16 will be the Centre Point of the European HPC Summit Week which includes an EXDCI Workshop, a Workshop by Eurolab4HPC and an ETP4HPC Workshop

ISC15, 13-15 July 2015, Frankfurt, Germany
The PRACE booth at ISC’15 attracted more than 300 visitors with various booth activities including the treasure hunt, mini presentations and a car racing video game called ParallelRACE.

Award
PRACE awarded the best paper submitted to the ISC Research Paper Sessions. This year David Rohr won from the University of Frankfurt with the following paper:

Lattice-CSC: Optimizing & Building an Efficient Supercomputer for Lattice-QCD & to Achieve First Place in Green500.

Memorandum of Understanding
Furthermore a Memorandum of Understanding was signed between WHPC and Compute Canada at the PRACE booth. WHPC proposed an interesting and well-attended workshop during the ISC15.

Alison Kennedy of EPCC and Mark J. Dietrich of Compute / Calcul Canada
PRACE Networking Session @ICT15: High Performance Data Analytics to conquer Europe!

PRACE organised a networking session together with EUDAT and EGI at ICT 2015 - Innovate, Connect, Transform held from 20 to 22 October 2015 in Lisbon, Portugal.

Experts from the fields of HPC, data analytics, infrastructures and archiving and representatives from scientific user communities, government officials, representatives from European projects on related topics joined the session and participated in an active discussion about HPC data analytics after the presentations given by international HPC and big data experts. Furthermore PRACE was part of the EC village to present successful various PRACE activities.

SC15, 15-20 November, Austin, Texas

A highlight - PRACE Open R&D for Industry was awarded the HPCwire Readers’ Choice Award for Best HPC Collaboration between Academia and Industry. Tom Tabor, CEO of Tabor Communications, publisher of HPCwire, presented the award to Alison Kennedy, Chair of the PRACE Board of Directors, in the presence of Stéphane Requena, Oriol Pineda and Florian Berberich, three members of the PRACE Board of Directors, live during SC’15 in Austin, TX at the PRACE booth.

PRACE Booth Team

PRACE booth proposed many different and fascinating activities to the SC visitors. Our experts were on hand to speak about PRACE activities, partners, training and projects. In additional a car racing video game and the traditional PRACE treasure hunt gave visitors the opportunity to connect with PRACE and PRACE partners.

The PRACE Booth Team at SC’15 in Austin, Texas, USs