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 agreements RI-261557, RI-283493 and RI-312763. For more information, see www.prace-ri.eu.

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# PRACE Annual Report 2012

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PRACE: great changes for greater achievements!

Since its inception in 2010, PRACE has steadily developed its offer of access to leading edge computational systems. Both academia and industry can now take advantage of Europe’s top-level Tier-0 resources consisting of 6 systems in 4 countries (France, Germany, Italy, Spain) surrounded by high value services in training, user support and application enabling. Our unified European Peer Review Process is unique on the continent, providing a single portal to request access to one or more of these 6 supercomputers (read more about this on pages 30 to 32) representing an aggregated cumulated amount of resources of more than 5.5 billion cpu hours allocated since mid 2010.

Access to those leading-edge systems has allowed hundreds of excellent scientific projects to come to fruition and yield unprecedented results. For this edition of the PRACE Annual Report, we have again lined up several high-level projects that received large PRACE allocations and stood out for their novelty. You can read more on the way HPC accelerates climate modelling, how it helps to understand the secrets of supernovae, how PRACE supports mathematical discovery and much, much more.

The 2012 PRACE Annual Report is published at an encouraging time for our organisation: PRACE IP Projects are in their final stages after almost 6 years of successfully building the PRACE brand and services, while the Association is preparing to pass from the initial period into PRACE 2.0. Furthermore, PRACE has created an Industry Advisory Committee intended to provide the PRACE Council with advice on relations with industry at European level (read more on page 7). The discussions of this Committee will feed into the further development of the Open R&D Access that PRACE offers to industry starting with the 5th Regular Calls for Proposals.

I would like to take this opportunity to thank the PRACE Implementation Phase Project partners without whom we could not have come this far.

They have steadily built PRACE from the ground up since 2008 and continue to support the PRACE staff in Brussels, who provide scientists and researchers with a single point of contact on all matters related to PRACE, its resources and its access programmes.
PRACE Scientific Case
Key recommendations

► NEED FOR HPC INFRASTRUCTURE AT THE EUROPEAN LEVEL

The scientific progress that has been achieved using HPC since the “Scientific Case for Advanced Computing in Europe” was published in 2007, the growing range of disciplines that now depend on HPC, and the technical challenges of exascale architectures make a compelling case for continued investment in HPC at the European level. **Europe should continue to provide a world-leading HPC infrastructure to scientists in academia and industry, for research that cannot be done any other way, through peer review based solely on excellence.** This infrastructure should also address the need for centres to test the maturity of future Exascale codes and to validate HPC exascale software ecosystem components developed in the EU or elsewhere.

► A LONG TERM COMMITMENT TO EUROPE-LEVEL HPC

Major experiments depend on HPC for analysis and interpretation of data, including simulation of models to try to match observation to theory, and support research programmes extending over 10-20 year timeframes. Some applications require access to stable hardware and system software for 3-5 years. Data typically need to be accessed over long periods and require a persistent infrastructure. Investment in new software must realise benefits over at least 10 years, with the lifetime of major software packages being substantially longer. **A commitment to Europe-level HPC infrastructure over several decades is required to provide researchers with a planning horizon of 10-20 years and a rolling 5-year specific technology upgrade roadmap.**

► INTEGRATED ENVIRONMENT FOR COMPUTE AND DATA

Most application areas foresee the need to run long jobs (for months or years) at sustained performances around 100 Pflop/s to generate core data sets and very many shorter jobs (for hours or days) at lower performances for pre- and post-processing, model searches and uncertainty quantification. A major challenge is the end-to-end management of, and fast access to, large and diverse datasets, vertically through the infrastructure hierarchy. Most researchers seek more flexibility and control over operating modes than they have today to meet the growing need for on-demand use with guaranteed turnaround times, for computational steering and to protect sensitive codes and data. **Europe-level HPC infrastructure should attach equal importance to compute and data, provide an integrated environment across Tiers 0 and 1, and support efficient end-to-end data movement between all levels.** Its operation must be increasingly responsive to user needs and data security issues.

► ALGORITHMS, SOFTWARE AND TOOLS

Most applications targeting Tier-0 machines require some degree of rewriting to expose more parallelism and many face severe strong-scaling challenges if they are effectively to progress to exascale, as is demanded by their science goals. There is an on-going need for support for software maintenance, tools to manage and optimise workflows across the infrastructure, and visualisation. Support for the development and maintenance of community code bases is recognised as enhancing research productivity and take-up of HPC. **There is an urgent need for algorithm and software development to be able to continue to exploit high-end architectures efficiently to meet the needs of science, industry and society.**

► PEOPLE AND TRAINING

There is grave concern about HPC skills shortages across all research areas and, particularly, in industry. The need is for people with both domain and computing expertise. The problems are both insufficient supply and low retention, because of poor career development opportunities for those supporting academic research. **Europe’s long-term competitiveness depends on people with skills to exploit its HPC infrastructure. It must provide on-going training programmes, to keep pace with the rapid evolution of the science, methods and technologies, and must put in place more attractive career structures for software developers to retain their skills in universities and associated institutions.**

► THEMATIC CENTRES

Organisational structure is needed to support large long-term research programmes, bringing together competences to share expertise. This could take the form of virtual or physical Thematic Centres which might support community codes and data, operate dedicated facilities, focus on co-design, or have a cross-cutting role in the development and support for algorithms, software, or tools. While some existing application areas have self-organised in this way, new areas such as medicine might achieve more rapid impact if encouraged to follow this path. **Thematic Centres should be established to support large long-term research programmes and cross-cutting technologies, to preserve and share expertise, to support training, and to maintain software and data.**

► LEADERSHIP AND MANAGEMENT

The development of Europe’s HPC infrastructure, its operation and access mechanisms must be driven by the needs of science and industry to conduct world-leading research. **This public-sector investment must be a source of innovation at the leading edge of technology development and this requires user-centric governance. Leadership and management of HPC infrastructure at the European level should be a partnership between users and providers.**

► Visit www.prace-ri.eu/PRACE-The-Scientific-Case-for-HPC
The Gauss Centre for Supercomputing (GCS) in Germany features Europe’s most powerful High Performance Computer to date. HPC system JUQUEEN, installed at Jülich Supercomputing Centre (JSC), a member of GCS, is the first system in Europe to boast a peak performance of 5.87 Petaflops/s. The system reaches now a peak performance of around 6 Petaflops/s and JUQUEEN is currently on 5th position on the TOP500 list (November 2012). The Jülich HPC system is also one of the most energy efficient supercomputers in the world: With a performance/power ratio of approximately 2 Gigaflops/s per Watt, JUQUEEN holds 5th place on the current Green500 ranking.

Since its entry into service in May 2012, JSC’s Queen of European Supercomputers was gradually expanded from initially 8 to finally 28 racks (January 2013). Equipped with 458,752 compute cores JUQUEEN, an IBM BlueGene/Q system, is especially designed for compute intensive, highly scalable applications which can run in parallel on a very high number of compute cores. “JUQUEEN is targeted to tackle comprehensive and complex scientific questions, called Grand Challenges”, explains Prof. Thomas Lippert, Director of JSC. “Projects from various scientific areas can profit from the system’s performance, e.g. in the areas of neuroscience, computational biology, energy, or climate research. Moreover, it enables complicated calculations in quantum physics, which were not possible before.”

PRACE offers a large number and variety of training opportunities for researchers. These target a wide range of audiences and cover HPC-related topics from programming paradigms, optimisation, debugging, architectures, numerical libraries/modelling to scientific visualisation. It runs a series of seasonal schools (every spring, summer, autumn and winter since 2011) and community-targeted workshops at locations all over Europe.

In 2012, six PRACE Advanced Training Centres (PATCs) were established in Finland, France, Germany, Italy, Spain and the UK. Annually, the PATCs devise a joint curriculum that represents approximately 60 training courses catering for entry-level to advanced HPC users. These PATC courses are disseminated and open to all European researchers.

PRACE also collaborates with third parties such as XSEDE (USA), and in 2013 also with RIKEN (Japan), in organising an annual series of HPC summer schools with an international mix of presenters and participants, e.g. the EU-US Summer School 2012 in Dublin, Ireland and the International Summer School 2013 in New York, USA.

Apart from organising training events, PRACE also maintains a Training Portal that provides HPC training information, including a repository of training material: www.training.prace-ri.eu
The Barcelona Supercomputing Center

The Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC) hosts MareNostrum, the first phase Tier-0 system contribution from Spain to PRACE and with a peak performance of 1 Petaflops/s it ranks number 36 in the world. Unique in the world as it is installed in a chapel, MareNostrum counts with 48,448 Intel Sandy Bridge processors in 3,028 nodes interconnected through a high speed interconnection network: Infiniband FDR10. It also has more than 94,625 TB of main memory and 1.9 PB of disk storage. MareNostrum is an IBM IDPX system with rear door heat exchanger to have a PUE on the high level standards. MareNostrum has provided support to more than 2,000 research projects in areas such as Earth Sciences, Biomedicine, Chemistry, Materials Sciences, Physics, Engineering, Earth Sciences and Astronomy Space. For example, MareNostrum has helped to study the interactions between protein-protein and protein-ligand in order to improve the design of new drugs, it has helped to understand how the physical properties of DNA modulates the biological functions of molecules, to find similarities among different genomes (such as the human and rat genomes), to predict the air quality of the Iberian Peninsula, to model the emission and transport of natural dust from the Saharan desert until the European continent, to study the impact and consequence of the climate change in Europe, to simulate the universe formation, to study the turbulences in an air plane wing inside the turbines, to investigate in the hadrons properties, to design nano fibres structurally stabled, to study the plasma physics confined magnetically or to optimize and scale monitoring, analysis and visualization tools in order to understand the behaviour of the parallel applications in supercomputers such as MareNostrum.

PRACE fosters links with industry for greater European competitiveness

Currently PRACE is in the process of setting up an Industrial Advisory Committee (IAC). The objective of IAC will be to provide the PRACE Council with advice on relations with industry at European level. Whereas the operational requirements of industrial users related to PRACE resources will be conveyed by the newly created PRACE User Forum, the objective of the IAC is to advise the PRACE Council from a strategic standpoint.

Its role will be to gather and relay the high-level expectations of the industry in general and advise the PRACE Council on the directions and measures that might best suit the needs of industry and foster European competitiveness and innovation.

This includes:
- Trends and needs to be related to the domain of industrial HPC resource use (i.e. applications, products, new business models and services, training, etc.)
- Technological transfer between academia and industry
- Training curricula focused on industrial users
- Development of new relations with emerging industries
- Strategies for a broader industrial sector engagement (e.g. large companies and SMEs)

The IAC will help the PRACE Council in lobbying actions at the EC and national government level in order to setup European (in the field of H2020) or national initiatives for promoting the use of numerical simulation and HPC by industry.

The 11 members of IAC will represent European companies who have a significant actual and potential interest in HPC development. The process of nominating and selecting IAC members ensures fair coverage of industrial areas, countries and company types.

The industrial domains to be covered by the IAC are:
- Aeronautics / Aerospace
- Automotive / Transport
- Energy, Oil & Gas
- Engineering / Manufacturing
- Finance / Insurance
- Life Sciences / Pharmaceutics
- Materials / Chemistry
- Renewable Energy
- Telecommunications / Electronics

Industrial users are already invited to apply for HPC resources via the PRACE Open R&D model. The PRACE Industrial Executive Seminars further the co-operation between PRACE and Industry:

www.prace-ri.eu/PRACE-Industrial-Seminars
PRACE Campus Schools

PRACE Campus Schools focus on students aged between 15-18 years. Applying various approaches, these events are envisaged as a key to demystify supercomputers, to describe how they are built and what they are used for in Science, Technology, Engineering, and Mathematics (STEM). Two Campus schools have already been organised by the PRACE-3IP project in Slovenia (November 2012) and Ireland (January 2013).

As part of the 1st PRACE Campus School held in the University of Ljubljana, Slovenia on 15-17 November 2012, experienced trainers presented the benefits of high performance computing. Simple programmes in various parallel languages describing comprehensible problems were given e.g. calculation of Pi with Monte Carlo and integration. Additionally, an introduction to the Ansys simulation software with broad outlook to the real engineering and scientific problems was presented. Multiphysics simulations in the field of structural mechanics and CFD were also presented during the event.

In contrast, during the 2nd PRACE Campus School at the BT Young Scientist & Technology Exhibition (BTYSTE), 10-12 January 2013, in a more informal environment the Irish Centre for High-End Computing (ICHEC) showcased all things supercomputing to primary and secondary level students at the RDS, Dublin, Ireland. Over 45,000 students attended the exhibition with over 200 schools visiting the ICHEC stand to understand the utility of supercomputing. Students and teachers attended from schools from all across Ireland.

The first zone of the stand displayed an eight-way Raspberry Pi cluster built especially for the event where the inner workings of a parallel machine were visible to the attendees. A parallel version of Conway’s Game of Life was run across the machine to describe the software layer.

Presentations were delivered to students in the second zone describing the need for supercomputing and the resources that Europe has to offer in terms of hardware. Weather models over Ireland and the UK were presented in 3D as ICHEC runs the national weather forecast for Met Éireann (Irish Meteorological Service).

Within the third zone of the stand live Molecular Dynamics simulations and other interactive demos provided by NVIDIA were run on a NVIDIA K20. While a Sudoku demo, one that searched for 17 clue grids, allowed the direct comparison of the new Intel Xeon Phi and the Intel Sandy Bridge.

Within the third implementation phase of PRACE (PRACE-3IP), two additional PRACE Campus Schools will be held in Bulgaria (Autumn 2013) and the Czech Republic (Winter 2014) as well as several one-day visits in schools called HPC Classes plus PRACE presentations at scientific events such as the EU Contest for Young Scientists in September 2013, Prague, Czech Republic.
Preparatory Access with User Support (Type C)

**PRACE Preparatory Access** allows researchers to optimize and test applications to prepare their codes for PRACE Regular Project Access.

A special type of Preparatory Access – called type C – gives the applicants the possibility to apply not only for preparatory access to the systems, but also for dedicated support from PRACE technical experts to optimize the application code.

For example, PRACE experts are assisting in ongoing type C projects in the following tasks:

- Implementation of numerical libraries in the codes
- Code optimization via the use of parallel I/O
- Efficient usage of GPUs

When a proposal is accepted for Preparatory Access type C, a PRACE support expert is assigned to the project. He/she will work closely together with the project members in all stages of the project:

- Understanding bottlenecks through code profiling
- Discussing the optimization strategy
- Implementation
- Testing
- Reporting

The optimization work and results of the project may also be published in the form of a White Paper on the PRACE web page: [www.prace-ri.eu/white-papers](http://www.prace-ri.eu/white-papers)

The overall goal is to support the projects to cross the gap from Tier-1 to Tier-0 which was done successfully for many projects in the past. And many successful applications for PRACE Regular Access followed based on the work done during PRACE Preparatory Access.

In this way PRACE provides researchers a unique opportunity to improve the parallel performance of their codes and to get ready for large scale production usage of PRACE resources.

The Preparatory Access Call for Proposals is a rolling call: every three months there is a cut-off for evaluation of the proposals. The proposals for type C are evaluated by the technical experts of the centres that are addressed in the proposal, and by the PRACE optimization group in terms of the requested support work. The maximum allocation period is 6 months and the amount of possible person months for support per project varies from 1 to 6.

Potential applicants to type C are advised to contact the PA type C support group at [prace-optimization@fz-juelich.de](mailto:prace-optimization@fz-juelich.de) prior to submitting their project to understand if their request can be accommodated by the PRACE code optimisation experts.

For more information on PRACE Preparatory Access Type C – or on Type A and Type B, please visit: [www.prace-ri.eu/Call-Announcements](http://www.prace-ri.eu/Call-Announcements). If you want to know more about past projects under PRACE Preparatory Access, go here: [www.prace-ri.eu/Preparatory-Access](http://www.prace-ri.eu/Preparatory-Access)

PRACE Summer of HPC

*The PRACE Summer of HPC is an outreach programme targeting early-stage postgraduate and late-stage undergraduate students. It offers up to twenty undergraduate and postgraduate students summer placements at HPC centres across Europe. Participants will spend two months working on projects related to PRACE technical or industrial work to produce a visualisation or video for use in outreach activities. Flights, accommodation and a stipend will be provided to successful applicants and prizes will be awarded to the best participants.*

To date the programme has been incredibly popular, attracting 189 applicants from 25 different European countries and representing 45 nationalities. The highly competitive selection process is now underway, with many high-quality applicants being considered for 20 summer placements. Successful applicants will be announced in early April and the programme will begin in July 2013. Once the programme has begun, participants will engage in an outreach activity of their own by describing their experiences via social media and a blog at: [www.summerofhpc.prace-ri.eu](http://www.summerofhpc.prace-ri.eu)
Catherine Rivière, CEO of GENCI (France), became Chair of the PRACE Council in June 2012 taking over the baton from Dr. Achim Bachem. Her mandate will run from 2012 to 2014, a period in which PRACE is transitioning to a persistent HPC infrastructure.

▶ Ms. Rivière, can you tell us which the major achievements of PRACE in 2012 were?

Catherine Rivière. Above all, I’d like to say that PRACE’s first successes are due to the personal commitment of Dr. Achim Bachem as the first Chair of the PRACE Council. Thanks to his experience and his conviction that PRACE was a necessity, the inevitable political difficulties of getting PRACE up to the level of a real tangible service to users have been overcome.

I’d also like to point out the role played by the PRACE IP projects and the valuable work they continue to do to put PRACE on track. And now, after only two years of operation, PRACE is a well-known HPC player, not only at European level but also worldwide.

With access to 15 Pflops on 6 world-class systems fully available since end 2012 in four countries (France, Germany, Italy and Spain), PRACE gives scientists and engineers from around the world the possibility to use leading-edge supercomputers and services to find suitable solutions to tackle societal challenges such as ageing population, climate change and energy efficiency.

Since 2010, more than 5.5 billion core hours were awarded to more than 200 projects selected for their scientific excellence through a rigorous but fair peer-review process. Moreover, the request for core hours on PRACE systems increases with each call and largely exceeds what PRACE can offer. This clearly indicates that the scientific community sees the added value of PRACE resources and, more specifically, acknowledges the need for those resources to achieve their goals.

This is a real success for a “young” infrastructure!

▶ Which are the main scientific achievements obtained with PRACE resources?

CR. I will just give two examples, representative of the science computed on PRACE resources. The first one comes from the climate domain, which is a worldwide question. 144 million core hours were awarded to a UK Met team on supercomputer Hermit, in Stuttgart (Germany). This unique amount of core hours will help this team to improve their models and gain 3 years in the development of those.

My second example comes from biophysics and concerns health, which is another issue of interest to every country. With a total amount of 70 million core hours (28 million on Curie in France and 42 million on SuperMUC in Germany), a French team will explore how the nervous impulse is propagated within neurons through ion channels. More precisely, French researchers will investigate at molecular level - using atomistic molecular dynamics simulations – various aspects of the function of these channels, with the scope to contribute to the design of drugs that will modulate their activity.

▶ Are PRACE resources only accessible to academic users?

CR. This was the case in the beginning but since 2012, PRACE has begun to offer its resources and services to industry according to an “Open R&D” model. The only condition for industrial users to access PRACE resources: they must commit to publishing their results at the end of their project. The selection of the projects remains the same as for scientists, on the merit of their scientific
excellence. It was very important to put in place such a bridge to foster technology transfer between academia and industry and it is already fruitful since 7 industrial projects were awarded by PRACE in 2012, to big companies as well as to SMEs.

The strengthening of links between PRACE and industry is also the result of the yearly industrial seminars, organized by PRACE since 2008 to bring academic and industrial users closer to HPC in general and PRACE in specific. The 2013 PRACE Industrial Seminar was held in Stuttgart on the 15th and 16th April.

► How does PRACE ensure that this “success story” will continue?
CR. Already in 2012, the strategic role of PRACE in Europe was recognized by the European Commission in a communication issued in February 2012. In this paper, entitled “High Performance Computing: Europe’s place in a global race”, the EC highlights the importance for Europe to “stay in the HPC race”, saying that HPC is a strong enabler for both scientific discoveries and industrial innovation and asking main actors like PRACE to play a key role in developing HPC.

It is a very important milestone for PRACE and a unique opportunity to secure Europe’s place in HPC. Even if PRACE has won its initial “bet” to give scientists and industrials access to world-class computers, it is necessary right now to prepare for the future... At international level, we face many major players (USA, China, Japan, and Russia) and some new ones (Korea, India...) in a dizzying technological race towards exascale.

► How do you intend to prepare for that future?
CR. PRACE is already working on its strategy towards 2020. We have one main objective: build a persistent HPC infrastructure beyond 2015 and make HPC a strong element of European scientific, economic and social politics. This is particularly vital for PRACE because the initial agreement that freed-up its resources in four hosting countries ends in 2015 as will the PRACE IP projects funded by the EC. PRACE will have to stand on its own feet and we are working hard to do it properly.

► How would you summarize PRACE’s priorities for the coming years?
CR. We have to achieve three main goals. The first of these is that we need to augment and solidify a sustainable European HPC ecosystem to secure Europe’s place in HPC; second, it is necessary to help European scientists to be ready for exascale by providing them continual access to leadership class computers; and the third we have to continue to develop HPC usage as far as possible, to boost science and innovation in Europe.

► Have you got a closing remark?
CR. To conclude, I’d like to add that PRACE is not only an infrastructure offering core hours on supercomputers. It is also a fantastic human adventure, bringing together people from 25 countries! PRACE would not be what it is today without their commitment.

“PRACE is a fantastic human adventure, bringing together people from 25 countries! PRACE would not be what it is today without their commitment”
Interview with Robert Madelin, European Commission Director-General for Communications Networks, Content and Technology

Mr. Madelin, could you tell PRACE more about why you have put High Performance Computing (HPC) high on the policy agenda of DG Communications Networks, Content and Technology?

Robert Madelin: High Performance Computing can help Europe respond to the growing complexity of everyday life for 500 million EU citizens and deal with the increasing number of challenges and problems that our modern society is facing. In February last year the Commission recognised the importance of HPC in the Communication “High-Performance Computing: Europe’s place in a Global Race”. We are now working with European leaders in the field to implement European policy in this strategic area.

What is your interest in HPC technology in the context of your current appointment?

RM: My current job involves working to create the best possible digital future for all of Europe’s half-billion citizens. It covers a broad range of fascinating topics, from broadband to digital copyright, future networks and technologies to smart cities, and HPC for many of those themes. HPC technology is key enabler for innovation which can improve society and make Europe more industrially competitive. As for EU funded research, in Horizon 2020, HPC is an important element of the overall Computing landscape that links to key applications in Societal Challenges.

Advances in HPC are closely linked to other critical technologies, for example data servers and Cloud Computing, multicore and embedded systems, high-end mobile computers, and Key Enabling Technologies like micro and nanotechnology and photonics. HPC and simulation are also critical to industrial innovation, in particular SMEs, as shown by the Factory of the Future (FoF) initiative.

Could you tell us more about the process that the European Commission is following towards achieving a leadership position for Europe in HPC for Horizon 2020?

RM: We expect to support the EU’s HPC strategy in 2020 with a Public-Private Partnership. This will combine three main elements: (a) developing the next generation of HPC towards exascale computing; (b) providing access to the best supercomputing facilities and services for both industry and academia; and (c) achieving excellence in HPC applications; these elements should be complemented with training, education and skills development in HPC.

Who do you see as the most important players in this process? Where would you want to see PRACE in this ecosystem?

Ensuring European leadership in HPC by 2020 is a challenge which depends on joint efforts of Member States, industry and the scientific community in cooperation with the Commission. The European Technology Platform for HPC (ETP4HPC) gathers the main players on the technology supply side. The future Centres of Excellence in HPC will structure the users of HPC applications. Finally, PRACE is vital to the development of a true European policy to provide access and expertise for a world-class HPC computational infrastructure for science and industry. PRACE has to define European supercomputing needs, both in terms of system capacity and of technology requirements, thus linking European demand and supply.

Which sectors and usages do you see as important or emerging for the growth of HPC in Europe?

RM: Traditional HPC application areas such as fundamental physics, earth sciences or transport will still require increasingly large scale computational power to satisfy their needs.
But the upcoming generation of exascale computing systems will be also driven by novel emerging domains like Global System Science, the modelling of complex human functions as in the Virtual Physiological Human initiative or in the Human Brain Project. HPC will also be called on by Big Data for high-end commercial analytics or for urban planning; for example, in the near future, transport infrastructures in smart cities will analyse huge amounts of data and provide multivariable decision and data analytics support to your mobile or car in real time.

**Why is it so important to support European competitiveness through High Performance Computing (HPC)?**

**RM:** Industry is increasingly depending on HPC to help it innovate in products and services. We need to attract newcomers to using simulation, visualisation and prototyping with outreach and capacity building activities for non-users. Spreading and customising “HPC as a service” is essential to increasing competitiveness, in particular for SMEs.

The capability to master the technologies will also support growth and competitiveness in the ICT industry and the economy in general. European industry has to fully commit both as a user and supplier of HPC systems, technologies and services based on HPC. Both roles are important in making Europe more competitive.

**What are the consequences if we fail?**

**RM:** The consequences could be severe. Failure could mean a fragmented and underdeveloped European HPC eco-system with insufficient capacity to meet demand of the science, innovation and industrial communities, and with a subcritical European supply industry, designing and building HPC systems and services. If this happens, research may relocate outside Europe. Nobody wants to see this, which is why the Commission is so active.

**Where do you think Europe currently stands in terms of HPC, overall? Is it significantly behind its competitors?**

**RM:** We have to face facts. In recent years, Europe has been falling behind other regions of the world due to under-investment in the HPC ecosystem. The EU has spent on acquiring high-end computing systems only half as much as the US. New competitors like China, India and Russia have declared HPC to be a strategic priority and have also massively increased their efforts.

Europe has a wealth of HPC experience and talent. We have the technical and human-skills, and world-leading capabilities in critical technologies for the next generation of exascale computing such as power-efficient microelectronics, interconnects and processor designs, as well as unique software tools and applications. These strengths can and must be exploited to re-establish European industry as a leading-edge supplier.

**Are you able to quantify how much investment in the field of HPC is needed?**

**RM:** We need to roughly double the current annual effort - from both national and EU budgets and industrial users.

The question is not only the amount of money, but how smartly you invest it. For example, Pre-commercial Procurement and Public Procurement for Innovation are powerful instruments linking the supply and the demand of HPC that have been underutilised in Europe. Pooling national and EU pre-commercial procurement resources could help advance the EU’s HPC capabilities and to develop the exascale technology that no single Member State can afford.

**Why is it so important that this is a long-term investment?**

**RM:** The global race in HPC is not a 100 meter sprint. There is a clear need for long-term access and tools for a world-class HPC computational infrastructure. We have also to grasp the opportunity of the technology change to reach exascale, and shift the balance of trade in HPC technologies.

We need to develop novel extreme-scale pilot applications, develop an e-Infrastructure for HPC application software and tools, and spread the use of HPC in industry, in particular for SMEs. And all of these require long-term investment to ensure Europe’s position on the global scene.

**What is the return on investment that you expect from HPC?**

**RM:** There are extremely high returns on investment in HPC at a macroeconomic level. Companies and countries which invest the most in HPC are leaders in scientific and economic terms.

Furthermore, advances in the area of HPC such as new computing technologies, software, energy efficiency, storage applications, feed into the broader ICT industry and the consumer mass market, becoming available in households within a few years of their introduction in high-end HPC.

**How important is education in furthering HPC competitiveness?**

**RM:** Education and skills in HPC are essential to maintain Europe’s competitiveness in science and industry. We need a large workforce well trained in HPC, especially in parallel programming, and more scientists specialised in computational tools and applications. HPC skills must be broadly included in curricula to increase the number of trained personnel in the long run, so that Europe can fully exploit the innovation capabilities offered by HPC.
With the 6th Regular Call for Proposals completed at the end of 2012, PRACE is making good progress in enabling world-class research in a wide range of scientific domains. A large number of scientific projects have been completed, and an important task for the SSC has been to evaluate the quality of those projects. The SSC is impressed with the overall quality of the results obtained: World-class research is being made possible by the PRACE Tier-0 computing resources, and some of the most successful projects are presented here in the annual report. Although this attests to the quality of the processes established by the SSC for selecting projects that gain access to the Tier-0 resources, the SSC will continue to monitor the selection process to ensure that the best projects are selected, keeping in mind that high-risk, high-gain projects will not always reach all of their goals.

“PRACE has by now demonstrated that great science is made possible through access to Tier-0 resources”

Based on the request of the user communities and recommendations of the SSC, PRACE started in the 6th Call to allow for multi-year project allocations for projects for which long-term access to Tier-0 resources is necessary. Several projects requesting multi-year access were approved in the 6th Call. In addition to requesting significant Tier-0 resources in the first year of operation, most of these projects are in need of even larger resources in the second year, limiting the availability of CPU hours for new projects in future calls, though a cap has been placed on the maximum number of multi-year projects. PRACE is committed to providing the necessary Tier-0 resources to the projects of highest scientific quality, and the SSC will in the coming year carefully monitor the balance between regular projects and multi-year access proposals in order to ensure that this goal is met.

Making computer codes run on ever larger computers, as well as new scientific communities to take advantage of the scientific advances that can be enabled through high-performance computing, requires a tight integration of software development and access to Tier-1 and Tier-0 resources. PRACE and the SSC are exploring different avenues for ensuring that these goals can be achieved, both through advanced training programs as well as through more integrated activities towards selected, large HPC communities in order to ensure that the full innovative potential in these scientific domains can be exploited.

PRACE has by now demonstrated that great science is made possible through access to Tier-0 resources. As work is progressing in defining the strategy for PRACE 2.0, the SSC will support the work on creating a sustainable infrastructure for Tier-0 resources in Europe by promoting the great science that has been achieved so far in the PRACE project and the scientific questions that remain unsolved due to the need for even greater HPC capacity in Europe, as identified in the Scientific Case for HPC in Europe.
The PRACE User forum

The PRACE User Forum was set up at the end of 2011 and has held several user sessions at meetings such as the PRACE Scientific Case workshop in March 2012, and the PRACE Scientific Conference at ISC’12. The User Forum was also involved in the development of the PRACE Scientific Case throughout 2012. It is now a reasonably-resourced User Forum with a social media presence on LinkedIn and Twitter, and well-defined lines of communication into the PRACE organisation.

In the coming year we will hold our first full General Meeting. This will give the PRACE user community an opportunity both to express its views on the activities of PRACE and to elect new members of the Programme Committee of the User Forum. This is an important step as the Forum is now moving from a start-up phase into a more evolved situation in which both the internal organisation and communication lines have been defined, leaving more room for development of policy objectives. It will be important for computational science in Europe that fresh, enthusiastic people join the Programme Committee to push forward its development over the following two years. Discussions are ongoing with regard to the venue of the General Meeting, and this will be communicated as soon as the information is confirmed.

The User Forum website will also be established fully, and this will be the main mode of operation of the Forum on a day-to-day basis: suggestions for policy changes to be made to PRACE will be developed and discussed here. Depending on the scale of the proposal, these proposals will either be brought directly to PRACE, or may be brought to General Meetings of the User Forum for ratification and communication to PRACE in a more formal manner.

Additionally, discussion boards will facilitate the informal sharing of experiences by users. We expect 2013 to be a significant year for the User Forum and we look forward to seeing many users at the User Forum General Meeting towards the end of this year.

Dr Turlough Downes, Chair of the User Forum
Cryptography: Making elliptic communication cryptic

Information is power, which makes data security increasingly important. Mathematical research that utilises high performance computing is being used to develop procedures for encrypting data and to ensure that these encryption protocols are secure.

The quantity of sensitive information now regularly exchanged over the Internet might astound previous generations. This places high demands on secure data handling. Encrypted data exchange generally requires a key sequence that can be used to encode and decode the transmitted data. The challenge is to develop encryption protocols where this key cannot be cracked by a third party attempting to intercept the data exchange. To this end mathematicians have been working to identify problems which are relatively simple to confirm given the solution, but hard or impossible to solve without it.

“All the keys we are using in cryptography fit into this scheme,” explains Professor Antoine Joux, a researcher at the Université de Versaille in France. His work investigates the use of ‘discrete logarithms’ in cryptography. “Take an integer $x$ and a number mod $P$ and calculate $J$ to the power $x$,” he explains. “This is easy to compute but finding $x$ (given the value of $J$ and $J$ to the power $x$) is difficult. Finding $x$ is called finding the discrete logarithm.”

Yet, although finding $x$ is “difficult”, progress in the development of more efficient algorithms over the past 20 to 30 years have raised questions over the security of cryptography protocols based on this kind of discrete logarithm known as “finite field” logarithms. As a result large key sizes are required for implementing these cryptography protocols. The increasing tractability of these problems to solution has stimulated research in a different type of discrete logarithm based on elliptical curves.
“An elliptic curve is a very classical mathematical object, which has been used in mathematics since the 19th century,” explains Professor Joux. The points on such a curve can be handled just like usual numbers, in the sense that you can add them, using a fixed recipe, which is not complicated at all to use (but took quite a lot of mathematical sophistication to figure out in the first place). Given a fixed point P on the curve, you can then easily find P, P+P, P+P+P and so on. What is difficult, though, given another point Q on the curve, is to determine how many times you have added P to itself to obtain Q (even if you are given the information that Q is the result of adding P to itself a finite number of times). “There is no easy way to do this”, says Professor Joux.

Finding this value in elliptical curve problems is described as the elliptical curve discrete logarithm and has been used in cryptography since the mid 1980s. In fact with their added complexity these protocols provide cryptographic keys, which are now used in secure shell (SSH, a network protocol for secure communication) and smart cards and are significantly more efficient than those based on finite field discrete logarithms. “Nowadays I think most governments recommend using at least 2000 bits key size,” says Professor Antoine Joux referring to cryptography protocols based on finite field discrete logarithms. “For elliptical curves the equivalent recommendation is around 256 bits.”

In fact, some of Professor Joux’s recent research has suggested that some elliptical curve discrete logarithms may in fact be less difficult to solve than had been previously believed. He and his colleague Vanessa Vitse, now assistant professor at the University of Grenoble, have worked on a type of elliptical curve found over a finite field of P to the power 6. They showed that by transforming the problem to a different curve over a smaller field two previously reported methods of attacking the problem could be combined to find a solution, clearly compromising its security. “And we showed this by just computing the discrete logarithm for a curve of this form at sizes which should not have been possible,” says Professor Joux.

This sort of research is very important. “By doing this kind of cryptography you remove branches that are hopeless,” he explains. It prevents people working to optimise protocols—finding specific ways of computing in the cryptographic path more efficiently or making the smart card algorithm smaller—when the protocol is not secure in the first place. “What you want to do is to remove the dead ends.”

Professor Joux’s collaboration with Professor Vitse in this work also typifies the size of collaborations in this field. Researchers working on similar problems span most of the world including Germany, France the UK and Canada, and many other countries. Yet broadly international collaborations seem rare. “It’s much easier to collaborate on the theoretical ideas than it is when you are dealing with real-life implementations,” explains Professor Joux. “Because you need quite a close-knit team if you want to programme it all and run it on a machine.”

He also emphasises how the field has benefited from the development of cluster computing, where several machines may run in parallel. “You can have 1000 machines run for a day to see if something will work or not,” explains Professor Joux. “With classical computers it would take months or a year to confirm an idea but with the big machine you can get confirmation very quickly which is very useful.

“An elliptic curve is a very classical mathematical object, which has been used in mathematics since the 19th century”

for research.” To date, the researchers have been awarded 750,000 hours on each of the CURIE FN, CURIE TN (both at GENCI@CEA) and JUGENE (GCS@Jülich) supercomputers.

His current research is moving away from the elliptical curves and revealing further limitations of finite field discrete logarithm cryptography. “I really think it is no longer a good option unless you use a really huge key,” he concludes, providing examples of the key sizes that have been solved and hence found no longer secure. “Just to give you an idea of the dimensions, right now the record is close to 2000 bits.” In fact, just a few days after our interview, Professor Joux was able to announce that he had succeeded in work on a much larger record of over 4000 bits. In this exciting and ever evolving field, it seems the bar for secure complexity is constantly rising.

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SUCCESS STORIES

Project title: Discrete logarithm on a 160-bit elliptic curve over F(p^6)
Project leader: Prof. Antoine Joux, PRISM - Université de Versailles, France
Project details: This project was awarded 750,000 core hours on each of CURIE FN and CURIE TN @ GENCI@CEA, France and 750,000 core hours on JUGENE @ GCS@Jülich, Germany
Exploring the properties of supernovae through 3D simulation

Not even stars are immortal; at the climax of their vast existences, these luminous beacons explosively burn to cinders, their debris sewing the seeds for new stars. Yet only now are the properties of these detonations being understood. Using supercomputing resources, HPC models are helping to reveal the enigmatic properties of thermonuclear supernovae.

Ranked highly amongst the universe’s most wondrous spectacles, supernovae – for all their conspicuous glory – can also be included in the most inscrutable. Positioned millions of miles away from terrestrial spectators, there’s a significant shortfall in the observable data gathered from these heavenly lightshows. Without sufficient information, their physics will remain an enigma to us.

To overcome this estrangement, a 2012 German-led project employed richly textured models to divulge the secrets of the supernova. Undertaken by the Max Planck Institute for Astrophysics (MPA) in Garching, Würzburg University and the Heidelberg Institute for Theoretical Studies, the study concentrated on one particular type of event – the Type Ia supernova.

“Our aim was to generate the first suite of realistic 3D explosion simulations for this ‘delayed detonation’ variant of supernovae” explains Doctor Ivo Seitenzahl, the Project Leader. “The models we generated, in collaboration with PRACE, encompass a comprehensive modelling chain. They range from the initial explosion, to post-processing, to radiative transfer in the material expelled in a stellar explosion. The hydrodynamic explosion itself is of course a prominent feature, but the nucleosynthesis of the aftermath was also closely examined.” The latter part of the sequence is perhaps even more significant in the context of recent theory, having been perceived as fundamental to the apparent growth of the cosmos.

“...the universe is expanding at an accelerating rate, this discovery was based on scrutiny of Type Ia supernovae”

In 2011, as Seitenzahl recounts, the Nobel prize in physics was jointly awarded to Brian P. Schmidt, Saul Perlmutter, and Adam G. Riess, who showed that the universe is expanding at an accelerating rate. “This discovery was based on scrutiny of Type Ia supernovae” notes the academic. “But, amazingly, the details of the explosion mechanisms are not actually known. So we can’t be entirely sure of their nature. A sound theoretical understanding to underpin this celebrated thesis, and the way associated systems are formed is consequently lacking. This is where we come in.”

One of the common progenitors of a Type Ia supernova, the scientist explains, is that of a compact white dwarf, which finally meets its end in a colossal ‘delayed detonation’. Drawing near to a companion star, it begins to accrete mass from this twin, ultimately approaching the limits of its stability (or ‘Chandrasekar mass’). A complex chain of reactions is thus set in motion, culminating in a stunningly powerful blast. Accumulated density at the heart of the star reaches such high levels that carbon is ignited, creating nuclear fusion and releasing massive amounts of energy – up to 10^30 times the power of the World War Two bomb dropped on Hiroshima.

Beginning to burn, flames initially burst from the white dwarf at subsonic speeds. An instant thereafter, charged by rising energy levels, they propagate outwards at accelerating velocity. Within the turbulent flows of this nuclear cauldron, a further detonation may occur, which converts carbon and oxygen into heavier elements, like the radioactive isotope nickel-56.

It’s the hiatus between the initial deflagration flame and the secondary explosion which earns the model its title, confides Seitenzahl. “Since the initial deflagration
flame is subject to instabilities, this renders analytic approaches impossible” he continues. “These limitations basically leave 3D simulations as the only viable tool for exploration.” Intriguingly, he notes, it isn’t the initial blow-up that causes the celestial fireworks for which supernovae are famed. Rather, the slow decay of radioactive nickel-56, a byproduct of the initial explosion, in fact illuminates the heavens.

Thanks to the co-operation of PRACE, the project was awarded all of the access requested by the research team. 21.6 million core hours were awarded. “It’s essential we were awarded the full allocation we requested, in order to reach our goals. Without sufficient time, the project would not have been feasible” comments Seitenzahl. Four core members based at the Max Planck Institute for Astrophysics operated as the nucleus of the team, with international partners from Northern Ireland and Australia attached to analytic phases of the project and related spin-offs. To glean the necessary data to develop their thesis, the group were able to access JUGENE, an IBM BlueGene/P unit which offers a 144 terabyte memory and a peak performance approaching one PetaFLOP (approximately a thousand trillion operations per second).

Perhaps the most formidable challenge the researchers faced was setting up and maintaining the modelling pipeline, which was processed in linear sequence. “We began with a hydrodynamic simulation, progressed to the nucleosynthesis calculations and, thereafter, scrutinised the emerging radiation” details the Project Leader. “These discrete steps needed to interface smoothly. Any change you make in one of these phases could hence interfere with the veracity of another. Establishing a robust system, and maintaining its integrity, was hence our greatest task.”

Despite these initial concerns, once the project’s workflow was finessed, the boost contributed by PRACE resources allowed the team to transcend their initial objectives. “We delivered” emphasises Seitenzahl. “The project promised to create a full set of 3D-delayed detonation models, and certainly realised this. Moreover, we actually created two models more than anticipated, through speeding up the code. Our success is a first, and truly unique.” Using their own, in-house computing resources, the researchers were also able to make related measurements, which had not been targeted at inception. These revealing tangents included the gamma ray spectrum, x-ray emission lines, gravitational wave and neutrino signal for the models. Hydrosimulation results generated from the test’s virtual environments were published in early 2013, and presentation of the light curve findings is in preparation.

Fleeting though they may be, the data gleaned from a starburst casts light across several other important facets of astrophysics. As such, the discoveries made by the scientists – much like the explosions themselves – have begun to permeate throughout the universe of human knowledge. “Type Ia supernovae are central to many sectors in the field” points out MPA’s Seitenzahl. “In high-energy astrophysics, they provide sources of galactic positrons. In cosmology, they offer standard candles for distance measurements.” In terms of galactic evolution, he observes, “they’re also fundamental to the formations of stars and galaxies, and contribute to the cosmic cycle of matter, by ejecting certain elements.” With the intervention of HPC, quantum leaps in our comprehension of these other-worldly bodies need no longer be regarded as light years away.

Project title: Diversity of Type Ia supernovae from initial conditions of the exploding white dwarf star
Project leader: Dr. Ivo Seitenzahl, Max Planck Gesellschaft (MPG), Germany
Project details: This project was awarded 21.6 million core hours on JUGENE @ GCS@Jülich, Germany
Modeling gravitational wave signals from black hole binaries

The emerging field of gravitational wave astronomy is paving the way for the study of previously unobservable phenomena such as the merging of two black holes. This is achieved due to the ripples of gravitational energy that these events create, causing tiny vibrations in space-time that have only just become measurable.

Almost one hundred years after Einstein’s theory of general relativity revealed space and time to be dynamical entities, gravitational research is about to take another giant leap. Some of the first ever gravitational wave detectors capable of accurately detecting signals from space will be coming online over the next few years, allowing a totally fresh perspective on the universe that will be comparable to the revolution brought about by radio astronomy.

A project from the University of the Balearic Islands, Spain, is based around this new field of gravitational wave astronomy, which aims to marry the theoretical physics behind black holes and general relativity with real observations from space. “Everything we know about the universe at present comes from different bands of electromagnetic waves, including optical, infrared and x-ray,” says Professor Sascha Husa. “What these waves give us is an image of their source. What we are doing now uses the same principle but utilises gravitational waves instead, which will allow us to see objects that we have been unable to access so far, such as black holes and neutron stars.

“However, what these gravitational waves give you is not so much an image of the source, but rather a sound. They create vibrations in space-time, so with an event such as two black holes circling around one another, we will be able to observe the single wave train that this motion produces. We are basically hearing the ripples of gravitational energy that are sent throughout the universe, using incredibly sensitive state-of-the-art equipment.”

Vibrations in space-time can be measured by the fact that they cause tiny fluctuations in the distance between two objects. The relative change in these distances is in the order of 10^{-22}, and so it is only through a huge technological feat using very large laser interferometers that it is possible to measure this. “Before, the event rate of our instruments meant that we did not have sufficient sensitivity to study the field properly,” says Husa. “However, they are now being upgraded and we should be beginning observations in 2015.”

As a theoretical and computational physicist, one of Professor Husa’s roles within the project is to make predictions for what wave trains will ‘sound’ like from different sources. For example, a binary black hole system will have a different mass and spin from other systems, and so it is up to Husa to use data from simulations to create analytical templates that can be used by those who analyse the data from the gravitational wave detectors, so that they can then identify binary systems and calculate their mass and spin.

“The templates that we create will allow our data analysts to sift through the noise produced by the

“Before, the event rate of our instruments meant that we did not have sufficient sensitivity to study the field properly”
universe and compare it to the templates, which will allow them to pinpoint where these binary black holes are and a little bit about their nature,” explains Husa. “It is almost analogous to the music identification apps that are now available on smartphones. These apps are able to match the original audio waves of songs, the equivalent of our binary black hole templates, with songs playing in a noisy bar, and identify what it is.”

For some sources, such as the slow inspiral of widely separated black holes, good analytical approximations for the gravitational waveforms are provided by perturbative post-Newtonian expansion techniques. For the last orbits and merger of two black holes, however, where the fields are particularly strong, and where one has the best chances of discovering entirely new physics, the Einstein equations have to be solved numerically.

Up until recently, it took the use of analytical perturbation theories to do this kind of work, but even this did not allow for the full picture to be shown. In 2005, however, there was a breakthrough that allowed researchers to carry out computer simulations of these types of events that gave measurable results. Since then, it has been a case of using these simulations to provide an improved picture of the wave-trains produced from the last orbits at the merger of two black holes.

These simulations are not cheap, however. A single simulation of a binary black hole can easily cost hundreds of thousands of CPU hours. “Without the top European supercomputers behind us it is not possible to carry out this sort of work,” says Husa. “For a long time there have been large computational resources in the US but not in Europe, so having the resources provided by PRACE - we received 37 million core hours on SuperMUC hosted by GCS @ LRZ - gives us the chance to carry out this research which would not be possible on the national machines you have in most European countries.”

This work with PRACE is part of a longer project which started in 2005, and it will be keeping these researchers busy for the foreseeable future. “We’re hoping that in around 3 to 5 years we will have confirmed our first discovery of a binary black hole system, and will have been able to use our algorithms to calculate data about its spin and mass,” says Husa.

“Having this sort of data will be a huge coup for astrophysics, as it will begin to answer questions about the history of stars, about what happens in clusters and globular clusters of stars, and about what happens when stars burn out, amongst other things.”

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Project title: Modeling gravitational wave signals from black hole binaries
Project leader: Prof. Sasha Husa, University of the Balearic Islands, Spain
Project details: This project was awarded 37 million core hours on SuperMUC @ GCS@LRZ, Germany

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“We’re hoping that in around 3 to 5 years we will have confirmed our first discovery of a binary black hole system, and will have been able to use our algorithms to calculate data about its spin and mass”
Increasing the fidelity of global climate solutions through massive HPC simulations

When destructive weather events begin to wreak unforeseen, elemental havoc, the importance of understanding mechanisms of the Earth’s climate system becomes self-evident. Analysing extreme events in detail requires complex high-resolution climate models that are computationally very demanding and require sustainable high-performance computing facilities. Through the support of PRACE, the UPSCALE research project has faced such a challenge by producing climate simulations using a global climate model in unprecedented detail.

Catastrophic tempests such as hurricane Katrina seem to reveal the cruel, capricious face of nature. Yet such events can be discerned as the product of a holistic, interactive global weather system. According to climate scientists, we can assess the causes of these phenomena, and how they interact at a global level, by making use of sufficient observational data and model simulations.

Launched by JWCRP-HRCM, a joint team between the University of Reading and the UK Met Office in January 2012, the UPSCALE project seeks to better understand high-impact weather and climate risks – and how best to deploy our technology to enhance that understanding. This yearlong venture is led by Professor Pier Luigi Vidale and supported by four full time staff members. UPSCALE was allocated an extensive 144 million core hours to produce and interpret colossal volumes of “synthetic weather” data. The team were granted access to the HERMIT Tier-0 supercomputer in Stuttgart hosted by GCS @ HLRS, who offered personnel and logistical support. Through PRACE, the researchers were able to produce several 27-year simulations for present and future climates with a global climate model at a detailed 25km (and experimentally 12km) resolution to discern local and regional weather patterns. Such long model datasets with such detail is unprecedented.

“UPSCALE was allocated an extensive 144 million core hours – the largest allocation to date in the world”

“Standard global climate models are often unable to distinguish regional differences, beneath a certain scale” illustrates Professor Vidale. “They also omit, or miscompute certain weather and environmental phenomena.” These include such critical features as clouds, their interactions with radiation, and accurate rainfall times. “As these local occurrences emerge,” he continues, “we need to determine what impact they might have on the global climate, and, indeed, whether or not the global climate is different due to their emergence.” The UK Met Office’s global weather forecast model currently runs at 17km resolution, for 15-day weather forecasts, making the UPSCALE team’s 12km resolution climate model a rare trailblazer in this respect. “Typically, you take the weather forecast model to its maximum resolution, as it only needs to be run for a few days” notes Vidale. “A global climate model is invariably more complex and needs to be run for tens to hundreds of years, and thus would tend to be executed with less detail”.

Another aim of the project is to determine what effective resolution is required for each simulated phenomenon, and decide at which resolution extra information on the phenomenon becomes superfluous. Beyond a certain resolution, the fidelity of simulated phenomena will ultimately cease to increase, so that the extreme computational cost will not be justified by scientific benefits. Leaping from a climate modelling resolution of 25km to one of 12km requires a tenfold increase in HPC and data storage usage and, correspondingly, cost. Establishment of benchmarks is consequently a key concern for the global community, which is seeking to unify its standards.

Operating at the 12km resolution, the Reading-Met Office team could disable convective parameterisation – a key component of climate models, albeit introducing strong uncertainty in the simulation of the climate system. “We showed that at 12km, and without convective parameterisation, the diurnal cycle of precipitation can be predicted extremely accurately” discloses the Project Leader. “This is very significant, as most climate models, using convective parameterisation because of their coarse resolution, erroneously depict rainfall as occurring locally at 12 noon. The convective parameterisation estimates the time of day that is most likely to be generating the greatest near-surface atmospheric instability and immediately triggers precipitation. Of course, in reality, clouds and rainfall may often build up slowly, and gradually transform into large rain events. Our 12km model convincingly accommodates this”.

“Another shortfall in current models, also caused by that limitation, is what happens to the rain when it falls,” he adds. “Water from rainfall eventually seeps into the soil, which plants use for growth and survival. If rain hits the ground at noon, it would tend to re-evaporate immediately, due to the amount of energy (heat) present on the surface. The proportion of evaporation, runoff into rivers and the water transpired by plants are miscalculated by orthodox models, which use coarse grid resolution. They over-emphasise instant evaporation from the land surface, at the expense of other mechanisms.” Calculation of a correct diurnal cycle...
ensures that the model supersedes these limitations. The propagation of convection is also, he highlights, discernible at 12km resolution, which, when viewed globally, reveals intriguing patterns. “Convection organises itself so that the clouds are dynamically aware of one another. They don’t just form in the same region, but actually move together, like a herd of sheep; particularly over Africa and the tropics” the scientist explains. Sometimes such organised formations intensify and, over the ocean, may become the catalyst for hurricanes, which is what emerges in our simulations. The UPSCALE high-resolution model simulations thus reveal interconnected events at various scales – ranging from cloud formations to hurricanes and large-scale extreme weather events. “We have started to see evidence of interaction with the large-scale environment, which strengthens our understanding of key processes in the global climate system” enthuses Vidale. To demonstrate this, the scientists have shown how the simulated extreme precipitation, associated with an especially high frequency in hurricanes in the north Atlantic region, can co-exist with droughts over the Amazon. These phenomena are seemingly connected by atmospheric circulation - and recreated conditions that were actually witnessed when Katrina struck in 2005.

“Our experience with PRACE was very positive” summarises Vidale. “Access to the PRACE (HERMIT) HPC represented a major step-up in our simulation capability, about 33 times our national HPC allocation at the time, which means that we would never have undertaken this project without access to PRACE resources. The HERMIT supercomputer operated continuously and reliably, which is of fundamental importance in a project of this magnitude; HLRS were always able to accommodate our specific needs, and their technical support was very good.

“Also, we generated a vast amount of data – around 0.4 petabytes – which is hard to archive and transfer”. This is, he notes, almost a third of what the entire international community produced for the forthcoming IPCC report (CMIP5, an international state-of-the-art exercise to review climate models, produced 1.8 Petabytes of data). The Project Leader gratefully acknowledges the assistance of the British Atmospheric Data Centre, where the simulations data are stored, in facilitating this epic migration.

“We were faced with conveying an unprecedented amount of data on such a short time scale. Every day, this entailed moving four or five terabytes of data from Germany to the UK, using highly developed techniques and tools. PRACE not only helped us to manage the simulations, but also supplied utilities to conduct this sensitive transfer. If this were interrupted at any time, it would have been extremely disruptive because our climate model would run out of storage space and would simply stop. Without such a reliable, stable platform, we would not have completed the project.” Encouraged by their success, the collaborators are considering a major new submission to the organisation, which will ask for two or three years of access to include another important feature – interactive eddy-resolving oceans – within their 12km resolution model.

Once the preliminary analysis is formally concluded by the Principal Investigator, the simulation results will be made accessible to the scientific community – a move which promises to yield further insights over many years. “The British Atmospheric Data Centre is one of the worldwide nodes that provide access to the shared IPCC data” elaborates Vidale. “Shortly, our work will be made available to all. The consolidated data will become a long-term resource for the global community – for them to comprehensively analyse for our collective scientific benefit”.

**Project title:** Joint Weather and Climate High-Resolution Global Modelling: Future Weathers and their Risks  
**Project leader:** Prof. Pier Luigi Vidale, University of Reading, United Kingdom  
**Project details:** This project was awarded 144 million core hours on Hermit @ GCS@HLRS, Germany

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**SUCCESS STORIES**

**Snapshot of a tropical cyclone making landfall in Louisiana and a “companion” extra-tropical cyclone in the West Atlantic ocean, moving to the N-NW. Both storms were simulated by a Global Climate Model (HadGEM3-A) at a resolution of N512 (~25 km) and had originally developed in the tropical Atlantic ocean. Colours show humidity with winds shown as vectors, coloured by local temperature at 500 mb (top left), 200 mb (top right), 925 mb (bottom left) and 850 mb (bottom right).**

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Examining branch point polymer motion in designing new materials

Polymers share common attributes, but for scientists, mastering the subtleties of their architectures is integral to devising new applications for such compounds. At the molecular level, polymer structures are extremely diverse, with common forms including stars, combs and dumbbell arrangements. These formations integrate during a process of synthesis, in which small molecules, or monomers, are bonded into chains and networks, forming an interconnected mesh. Where individual units intersect and cohere in repeating patterns determines their overall properties, such as strength, density and flexibility.

“We need to know how to manipulate these qualities” pledges Dr Angel Moreno, a senior researcher from the Spanish Scientific Research Council (CSIC). “They are primarily determined by the large-scale motions of polymer chains. These are long macromolecules with a rich internal dynamic behaviour. It’s important to understand how their dynamics work, and to comprehend the microscopic origins of attributes like viscoelasticity.” To determine the origins of this characteristic, the Spanish institutions Center of Materials Physics (Centro de Física de Materiales, or CFM-CSIC) and University of the Basque Country (UPV/EHU) collaborated on a recent project supported by the PRACE infrastructure.

“Atoms in solid materials exhibit an elastic response to deformation. Once strain is supressed, they return to their initial positions” explains Moreno. “By contrast, simple liquids such as water just flow”. Polymers, in their melted state (that is to say, during processing conditions) behave in a far more complex way, and this is known as viscoelastic response. In this phase, they’re essentially viscous liquids.” Between January and November 2012, the research team (comprising of Moreno, from CFM-CSIC, and Professor Juan Colmenero and PhD student Petra Bacova, from UPV/EHU) were able to access 3 million core hours of HPC resources via PRACE, and utilise France’s Tier-0 computer, CURIE, to scrutinise the phenomenon. Using detailed simulations, the group were able to test the validity of several theories which attempt to rationalise the ‘branch point motion’ which interlinks molecules.

Current hypotheses often attribute polymer viscoelasticity to ‘reptation’. This is the thermally encouraged motion of long, entangled chains of macromolecules. Because of the uncrossability of the polymer chains, lateral motion is strongly impeded, and the chains are forced to move along their own contour (like repeating snakes). This motion is formally described by the so-called ‘tube theory’. However, as Moreno notes, this picture conceives of polymers as if they existed in exclusive, linear strands. Contrarily, in many industrial applications, different polymer types – such as the star form – are not linear at all. “Many polymer types often exhibit ‘branches’ which bond outside of any common ‘tube’” details Dr. Moreno. “They possess complex architectures, and may even be ‘hyperbranched’ laterally. Consequently, the application of reptation theory to such polymers becomes extremely difficult.” Although, he relates, “new mechanisms to understand the motion of such polymers have been
One proposed alternative is ‘arm retraction’. In this model, molecular limbs withdraw towards their branch points, and poke out along new directions to join adjacent tubes. ‘Tube dilution’ is another hypothesis, which suggests that, in a molecular branch, entanglements of the outermost segments with their inner counterparts are not effective, since the former relax at much shorter time scales. “Consequently, the tube will effectively widen with time” summarises Dr Moreno. A third dimension to this puzzle is suggested by the notion of ‘hopping’ branch points, which are another possible means of molecular diffusion. “These hypotheses are incorporated in tube theories by mathematical formulations, but specific assumptions are still poorly understood” attests the Project Leader. “What we’ve done with our simulations is attempt to vigourously test some of these notions.”

**“Atoms in solid materials exhibit an elastic response to deformation. Once strain is supressed, they return to their initial positions”**

Employing the widely recognised ESPRESSO software to conceive their models, the team was able to exploit the allocation, and undertake thorough simulations of melts of entangled branched polymers. “PRACE’s contribution has been vital. It would have been impossible to conduct this dedicated study without supercomputers” reports Moreno. “We undertook a very systematic investigation, which incorporated various forms including stars, H- and Y-shaped, and comb-like polymers.” The overall properties of a polymer construct depend on not only a few minor details (as uncrossability, molecular weight and architecture). For this reason “we carried out simulations of generic bead-spring polymers” – a well-known methodology in polymer physics. “The amount of time we were awarded is rather singular in the research community” enthuses the scientist. “The rationale behind this is simply that it was essential to securing our objective. Polymers are very long – meaning that extensive simulations were a prerequisite. The unusually slow dynamics of branched polymers, in comparison with their linear counterparts, also entail significant CPU usage, and the formal diversity we embraced meant that several computer cores were simultaneously accessed by the team."

Final analysis of the simulations has already divulged several important results. “We’ve directly observed, for the first time, that there is a broad distribution of relaxation times across the polymer branches” imparts Moreno. “This is consistent with the idea of arm retraction – and an unprecedented discovery. The reason we achieved this breakthrough was because of the time granted to us on supercomputer resources.” Thanks to their extensive HPC access, the researchers were also able to perceive the crossover from retraction to reptation in asymmetric star polymers, another hitherto undetected phenomenon. Motion of branch points was also characterised in detail, and the tests revealed, for the first time, that the little understood branch point hopping only occurs when the adjacent branch is fully relaxed, as proposed by tube theories.

“We’ve been able to observe specific polymer motions which, until now, had only been suggested at a theoretic level” comments the specialist from CSIC. “We now hope that our results will lend themselves to even greater quantitative relevance, once our analysis has been completed.”

(Above) Mean squared displacement of the branch point, normalised by the square root of the time, in some of the simulated systems (see legend). Numbers in the legend represent the number of entanglements in the branches. The horizontal lines indicate the crossover to reptation at long times.

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Success Stories

Project title: Branch point motion in star polymers and their mixtures with linear chains

Project leader: Dr. Ángel Moreno, Centro de Fisica de Materiales, CSIC-UPV/EHU, Spain

Project details: This project was awarded 3 million core hours on CURIE @ GENCI@CEA, France
Optimising the combustion dynamics of transcritical flames

Combustion is essential to modern air and space propulsion. While steady operation of engines under nominal conditions is reasonably well understood and simulated, less is known about the dynamics of combustion and the possible instability problems which may arise in these high performance devices. To optimize engine performance and limit instabilities, investigating their characteristics necessitates detailed computer modelling heavily relying on HPC.

“Today, 85 per cent of the world’s energy is obtained by combustion. The most common applications are found in automotive, industrial gas turbines and aerospace engines, but there are many other usages – such as power plant boilers, furnaces for material processing, domestic heaters...” explains Dr Gabriel Staffelbach, a senior member of the Computational Fluid Dynamics (CFD) group at CERFACS. “If combustion can be replaced by renewable energies in certain cases (to produce electricity for example), there is no other practical alternative to propel an aircraft or a rocket. It is thus important to understand how this process works, so that it can be optimised, and costs minimised.” Efficient conservation of fossil fuels, in response to rarefaction of resources and climate constraints is also a priority for today’s designers.

“One of the biggest problems in combustion analysis, and especially for rocket engine design, is the highly exothermic chemical reaction process inside the system. Conversion is accompanied by the rapid release of heat taking place in thin reactive fronts (a few micrometers thick), and incredibly intense” reports Staffelbach. “Because of this, rocket flames are difficult to observe, or recreate in laboratory scale experimental conditions. Such experiments have been carried out in recent years by the team led by Sébastien Candel at EM2C, CNRS, our partner in the present project. This group was able to observe cryogenic flames formed by liquid oxygen and gaseous hydrogen or methane under conditions prevailing in rocket engines. These experiments were carried out on a testbed located at ONERA and designated as “Mascotte”. Their more recent effort has concerned the coupling of combustion with high amplitude transverse acoustic modes. It was the right time to try to simulate these experiments and examine the interaction mechanisms with state of the art tools. The objective was to gain an understanding of how the flames within this system interact with each other.” High performance engines possess hundreds of injectors, creating numerous small flames that merge and burn at temperatures of more than three thousand degrees. “These flames may respond to an acoustic perturbation in a synchronized fashion and this may lead to a resonance generating high amplitude oscillations, augmented heat fluxes to the walls with potentially dangerous consequences, and can ultimately jeopardise the structural integrity of the thrust chamber continues the scientist. “Flames can behave erratically; bifurcations are present in many combustors, leading to flames which can behave one day in a certain way and the other day in another, much more dangerous manner.” Consequently, anticipating this behaviour – and developing methods to suppress instabilities – can enable industry to develop more reliable systems.

Terminated in June 2012, Staffelbach’s project, was jointly undertaken by EM2C laboratory, CNRS (Ecole Centrale Paris) and by CERFACS (Toulouse). Work was carried out collectively by L. Hakim, A. Ruiz, T. Schmitt, G. Staffelbach, M. Boileau, S. Ducruix, B. Cuenot, T. Poinsot and S. Candel. Through their collaborative efforts, they were able to develop a cutting edge simulation which examined the dynamics of a five-injector combustor, typical of rocket engines, submitted to intense transverse acoustic modes. “This is a world first, to our knowledge, and is especially valuable as we have combined computer modelling with real experiments carried out by the EM2C team asserts the Project Leader. “The real breakthrough in our work with PRACE is that we are looking at multiple turbulent flames under transcritical conditions interacting with an intense transverse acoustic field and that we are able to compare results from our HPC simulations with observable, physical phenomena, and in so doing validate the accuracy of the model. Many of the features observed experimentally were retrieved in the simulation.

It has been found for example that the flames become much more compact when they interact with an intense acoustic field. One of the most remarkable results we found was that, even if the five injectors are identical, neighbouring flames can behave in a different manner. They differ in length, and are deviated because of the proximity of other injectors. This suggests that one can not characterise the operation of a complete engine by generalising the behaviour of a single injector which is the method presently used in current engine design. In an actual engine, complex interactions take place between hundreds of such devices, suggesting that group interactions between flames could change the flow geometry, the performance of the engine and its stability.”
For these high-fidelity simulations, the team employed the AVBP software tool, which was co-developed by CERFACS and IFP Energies Nouvelles and used a real gas version jointly developed with EM2C, CNRS (most notably by T. Schmitt) to account for the specific working fluid characteristics corresponding to the rocket engine range of operating conditions. Optimised to consider unsteady flows in combustor systems, the principles of Large-Eddy Simulation (or LES: a mathematical model for computing fluid dynamics) were exactly fitting the requirements of this study but the practical implementation of AVBP for such a flow was still a challenge. “This type of simulation had never been carried out before under such complex physical conditions” reports Staffelbach. “It was a trial and error process to develop the right mesh size, and obtain a useful resolution.” Large, elaborate meshes require significant CPU resources. Conversely, if they miss certain details, the simulations could be undermined. Fortunately, confirms the researcher, “LES is very useful in turbulent combustion as it exposes the unsteady behaviour of the flows, without having to resolve all the scales. You just need sufficient resolution to observe unsteady behaviour.” Once this equilibrium between precision and resources had been identified, the team was able to access the substantial computing resources at their disposal.

“Simply put, we could not have completed our work without PRACE. This type of simulation would otherwise have been prohibitively expensive. Moreover, their partnership has enabled us to access current Tier-1 resources simultaneously,” says Staffelbach. Utilising the CURIE supercomputer owned by GENCI, the team was allocated 8.5 million core hours, and, encouraged by their recent success, are hoping to make PRACE a critical part of their next series of cutting-edge tests.

These will expand on their current findings, by widening the scope of the LES models to enhance their realism and, hence, relevance. “After this first numerical and experimental comparison we have been working recently on a multi-injector scenario closer to real engine situations. This will multiply the intricacy of our prior work tenfold, and include complex patterns of injectors within an engine,” says Staffelbach. “We now know that multiple injectors alter the internal dynamics within the engine; but the next big challenge is for us to quantify the contribution of these additional features.”

“Ultimately, given a larger, and more precise setup, we would ultimately like to model a full size engine, including hundreds of injectors” pledges the Project Leader. “Another subject we are considering is the thermal response of solids positioned near the flames. As these are often close to intense heat sources, it is important to be able to estimate the heat load and life duration of the thrust chamber walls.” Cooling, too, is another aspect which must be considered, and adds an extra dimension to the simulation. Unsteady flames are more compact and this can lead to elevated temperatures of the walls under the augmented heat fluxes. Such knowledge, he adds, is vitally needed by the aerospace industry, and particularly the space sector. “In the past fifty years industry has produced many rockets via experiments and costly (indeed, sometimes fatal) trial and error methods. Consequently, understanding how the combustion process works can be used to avoid mistakes at the design stage.” Instead of expensive test rigs, HPC may offer an alternative platform for the technology’s lift-off: “compute them before you build them” remains the first objective here. “This could reduce the cost of new developments. Streamlined, IT enhanced practice could herald the expansion of numerous affiliated industries” Staffelbach muses.

Project title: Large-Eddy Simulation of high-frequency instabilities under transcritical conditions.

Project leader: Dr. Gabriel Staffelbach, CERFACS CFD, France

Project details: This project was awarded 8.5 million core hours on CURIE @ GENCI@CEA, France
Developing innovative catalysts for storing solar energy

Solar power offers one of the brightest hopes for a future in which renewable sources will supply humankind’s growing needs. To realise that ideal, flexible storage systems are required to provide dependable access to light-derived electricity, on demand. One potential solution is artificial photosynthesis – a chemical conversion of molecules which mimics plants, and deposits energy in artificial fuels.

By 2020, the EU has pledged to generate 20% of its energy from renewable sources. To date, it has made significant headway – with the territory boasting over 75% of cumulative global solar energy capacity, and Germany emerging as a world leader. Further expansion depends on performance, but also on all-year round availability. Users are accustomed to having electricity ‘on tap,’ but to replicate this convenience with solar power, latter-day alchemy is needed to transform ephemeral sunlight into fuels which can be whimsically accessed. Such a process is necessary to mitigate one of the fundamental weaknesses of solar energy – the ‘diurnal cycle’, or its inevitable dependence on daylight.

“Storing solar power by means of artificial photosynthesis can emulate what plants do, and is achieved through a series of chemical reactions, driven by solar energy” explains Dr. Simone Piccinin. To refine such devices, comprehending the physics and chemistry involved is a prerequisite. “Finding suitable materials to catalyse the reaction is a big challenge, however” he relates. “They need to be both efficient and stable.” Based at the Istituto Officina dei Materiali of the National Research Council (CNR-IOM) and International School for Advanced Studies (SISSA) in Trieste, the scientist has recently concluded a successful research project investigating such catalysts, using rigorous atomistic modelling. His main collaborators in this pursuit were colleague Stefano Fabris (CNR-IOM), Andrea Sartorel and Marcella Bonchio (University of Padova), Giuliana Aquilanti and Andrea Goldoni (ELETTRA, Trieste).

For the study (recently published on PNAS) Piccinin concentrated on water oxidisation, a key component in the unfolding reaction. “This process is important, because it’s one way solar energy can be stored” the academic details. To initiate this conversion, light is initially shined on a device, which initiates a reaction that begins to transform water into potential fuel sources. These units typically operate using an electric current channelled through an anode, around which the water oxidises, and a cathode, at which new molecules are formed. “By rearranging chemical bonds into their constituents, water molecules can be split. One way of achieving this is to first of all liberate electrons and protons from them” details the Italian expert. These components can then be deployed in new molecular configurations. Hydrogen is one of the most straightforward molecules to engineer, but producing other fuels will require greater mastery of the reactive process.

“Oxidising environments may be quite harsh – so the catalyst can sometimes dissolve itself in water” says Piccinin. “The catalyst inside plants, which helps with photosynthesis, is made of calcium, manganese and oxygen, surrounded in a protein environment. This asset is continuously damaged, but also repeatedly rebuilt by nature. If a self-repairing catalyst is unfeasible, we must instead develop one which is extremely robust.” The materials utilised pose a third challenge. Expensive catalysts based on iridium and platinum are well-known, but scientists are keen to discover ‘earth abundant’ replacements which are ubiquitous, such as the manganese found in plants. “Recently, there has been a lot of progress – and catalysts based on cobalt and nickel have been proposed, and are undergoing testing. There’s optimism that catalysts based on these readily available substances could enter the marketplace relatively soon” enthuses Piccinin.

Identifying a specific class of plentiful, inorganic compounds, the Italian team subjected a variety of materials to rigorous testing. The catalyst they produced was made of manganese, with ruthenium added for catalytic properties. The team then subjected the device to high levels of oxidation, and found that the catalyst remained stable, and produced hydrogen efficiently. They have also developed a model for predicting which materials might work best, and are currently refining it to make it easier to use. They hope to have a fully functional device ready for demonstration by 2022.

“Although we still have a long way to go, we are making good progress” concludes Piccinin. “We are confident that we will be able to develop a working prototype in the next few years, and we are looking forward to seeing how it performs.”
of these materials to rigorous simulation, particularly those based on ruthenium and cobalt. “Using atomistic modelling, we have identified the mechanism by which water is oxidised into molecular oxygen. The main results of our work reveal how this chemical reaction takes place” explains the scientist. The venture also sought to establish their suitability as catalysts, and compare them with alternatives. During this analysis, some unanticipated, but highly significant parallels gradually emerged. “Intriguingly, the mechanism we’ve discovered closely matches that discerned in other systems, like the surfaces of oxides – which are greatly dissimilar.

“Such awareness is important because, if you can understand a catalyst better at a molecular scale, it can hint at why it might function better in heterogeneous cases. From an experimental point of view, this makes it much easier to investigate. Any information which can be transferred between these realms of analysis can help to increase our understanding” emphasises Piccinin, whose team is proposing ultimately to unify the theory of such reactions.

“Showing that there are molecular catalysts that replicate the behaviour of an extended oxide, at this scale, has been truly pioneering.” To achieve this breakthrough, the researchers conducted HPC simulations based on density functional theory and the method of metadynamics (developed by their colleague Alessandro Laio at SISSA), which allows investigators to accurately model reaction mechanisms. Offering a level of detail that complements experimental investigations, these tools enabled the group to ‘zoom in’ on the reaction, and scrutinise how chemical bonds are formed and broken. PRACE’s collaboration was vital to launching this important exercise, as Dr. Piccinin acknowledges. “Carrying out these types of exercises, from a computational point of view, is very demanding. They require several million CPU hours, and we couldn’t have completed our study without the facilities allocated by PRACE.” PRACE awarded 4.8 million core hours on CURIE @ GENCI @ CEA, France In parallel PRACE’s Finnish member CSC awarded 1.5 million core hours on the Tier-1 system LOUHI

Once these properties are determined, the results can be shared with industry – hopefully encouraging the development of cheaper, more effective solar power units. Encouraged by his recent experiences, the scientist is keen to obtain access to further PRACE resources for future projects, which will address other facets of the catalytic conundrum. “Over the next few years, we intend to shift our emphasis from the anodic reaction (the oxidisation of water) to the cathodic one – which can help us to consider how to reduce CO2” he anticipates. “This is, of course, another of the functions performed by organic photosynthesis in plants”.

Although this particular aspect of their exploration has concluded, the group has committed itself to a long-term involvement in the field. “The kind of information we’ve been able to extract from our recent study can be exploited, to consider whether other catalysts work in a similar fashion” informs Piccinin. “If so, we can devise means by which less expensive catalysts can be fabricated, and try to ensure they possess the same efficiency as models reliant on costlier materials.”

Project title: Multicenter cobalt-oxo cores for catalytic water oxidation
Project leader: Dr. Simone Piccinin, CNR-IOM, SISSA - Condensed Matter, Italy
Project details: This project was awarded 4.8 million core hours on CURIE @ GENCI @ CEA, France In parallel PRACE’s Finnish member CSC awarded 1.5 million core hours on the Tier-1 system LOUHI
PRACE project requests and allocations continue to break records

The Partnership for Advanced Computing in Europe provides access to world-class computing resources. These resources are accessible for promoters of successful projects submitted in response to periodic calls for proposals.

Available resources

PRACE awards access to Europe’s six largest supercomputers to scientific and engineering projects through its peer review process. Scientific excellence is the most important criterion for awarding resources on one or more of the PRACE systems.

Today PRACE is one of the world’s leading providers of access to High Performance Computing (HPC) resources and expertise. Table 1 lists the PRACE systems portfolio including the hosting centre, the architecture and peak performance of each system. Detailed information on these systems can be found on www.prace-ri.eu/PRACE-Resources

<table>
<thead>
<tr>
<th>System Name</th>
<th>Hosting Centre</th>
<th>Architecture</th>
<th>Peak Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Curie</td>
<td>GECITEC, France</td>
<td>Bullx cluster</td>
<td>2 Petaflops/s*</td>
</tr>
<tr>
<td>Fermi</td>
<td>CINECA, Italy</td>
<td>BlueGene/Q</td>
<td>2 Petaflops/s</td>
</tr>
<tr>
<td>Hermit</td>
<td>GCS@HLRS, Germany</td>
<td>Cray XE6</td>
<td>1 Petaflops/s</td>
</tr>
<tr>
<td>JUQUEEN</td>
<td>GCS@FZJ, Germany</td>
<td>BlueGene/Q</td>
<td>5.9 Petaflops/s</td>
</tr>
<tr>
<td>MareNostrum</td>
<td>BSC, Spain</td>
<td>iDataPlex</td>
<td>1 Petaflops/s</td>
</tr>
<tr>
<td>SuperMUC</td>
<td>GCS@LRZ, Germany</td>
<td>iDataPlex</td>
<td>3.2 Petaflops/s</td>
</tr>
</tbody>
</table>

(*) Petaflops/s means a thousand trillion floating point operations per second.

PRACE Peer Review

The PRACE peer review process is based on the following principles:

- **Transparency** to all stakeholders.
- **Fairness**: Proposals are evaluated against the selection criteria published in the terms of reference of the call for proposals, reviews are done by experts in the scientific field of the proposal following a no-conflict-of-interest policy, and applicants have the right of appeal for the final decision.
- **Independence**: PRACE peer review constitutes a centralised exercise independent from similar exercises at member institutions.
- **Confidentiality**: Proposals will be treated in confidence by PRACE staff and reviewers. The identities of the reviewers shall not be disclosed.

The PRACE Peer review process includes two types of assessment: technical and scientific. The two assessments are carried out separately by different groups of experts.

- The technical review seeks to assure that the proposal is technically feasible for the intended platform. All proposals will undergo a technical assessment. This assessment is performed directly by the centres hosting the system to which access is requested.
- The scientific review follows the technical review. This assessment is performed by three internationally recognized experts from the relevant field of research. The experts have access to the results of the technical review. The applicant is informed on the outcome of both reviews and has the right to reply in order to provide information that supports the original proposal; information that changes the original proposal is not taken into account. The reviewer’s report will be made anonymous before being sent to applicants.

Both the reviews and the clarifications of the applicant are submitted to the PRACE Access Committee. This Committee meets in person to define the ranking order of the successful
projects, to identify those that have not passed the technical evaluation or are below the scientific threshold and to confirm the recommendations for reductions or increases of resources from the scientific reviewers. The Access Committee is composed of eminent scientists from across the remit of the PRACE scientific applications. The members will primarily be selected from PRACE partner countries, but scientists from other countries may also be chosen if necessary or desirable. The composition of the Access Committee is available at www.prace-ri.eu/Organisation

The ranked list of successful proposals is presented to the PRACE Board of Directors for a final decision on the allocation of the successful projects to one or more of the available computing resources. The proposal must respect the Access Committee’s recommendations in terms of:

- the ranking order of the successful proposals
- the recommendations on the reduction or increase of resources for each proposal
- the list of proposals rejected for technical reasons or below scientific threshold

In case the preferred system is already fully allocated, the PRACE Allocation Board, composed of representatives of each of the computing resource providers, can suggest a re-allocation of resources on a system with characteristics similar to those of the preferred system.

The projects successfully awarded in a given call are listed on the PRACE website (see www.prace-ri.eu/Regular-Access). The proposals that either have not passed the thresholds or could not be awarded resources are not disclosed and the contents of those proposals are kept confidential.

Eligibility criteria
Calls for proposals are open to applicants from academia and public research organisations as well as, since 17 January 2012, to commercial companies for open R&D activities.

Eligibility criteria for academia and public research organisation
- The project leader is a senior researcher employed in a research organisation
- His employment contract should last at least 3 months after the end of the allocation period

Eligibility criteria for commercial companies
- The company has its head office and/or substantial R&D activity in Europe
- The project leader's employment contract should last at least 3 months after the end of the allocation period
- Access is requested for open R&D purposes only
- Commercial companies may apply on their own (as principal investigators: limited to a maximum of 5% of the total resources of a single PRACE system) or in collaboration with academia (as principal investigators or collaborators).

For commercial companies, access can only be awarded provided that the company commits to publish the results obtained in publicly available media.

PRACE hosting sites may put further restrictions on eligibility for use of the machines (for example, due to export rules or security measures). It is the responsibility of the applicant to ensure that they comply with the specific access criteria of each system.

Selection criteria
The applicant demonstrates the excellence of the project proposal based on 5 criteria. All the criteria presented below should be adequately addressed in the application:

1. Scientific excellence
- novelty and timeliness of the science proposed
- ambition and transformative potential of the proposal and expected advances
- appropriateness of the proposed methodology

2. Impact
- relevance of the research proposed in the context of developments in the domain in Europe or elsewhere
- possible commercial or societal application or transferability to other scientific disciplines
- appropriate plan and resources for dissemination and knowledge exchange (e.g. publications, presentations, collaborations with research peers, interactions with a different scientific discipline or general public)
- expected level of publications presenting the results obtained in the project

3. Relevance to the call
- level of scientific and technical maturity
- anticipated publication of results in one or more high quality journals
- focus on topics of major relevance for European research
- justification for the need to access Tier-0 resources

4. Applicant’s competence and skills
- appropriateness of the team’s track record
- competence and skills of the team presented in the application

5. Resources and management
- adequateness of the number of members of the team and their experience to deliver the goals of the project;
- plan commensurate with objectives
- adequateness of amount of resources requested to successfully complete the project

The PRACE website contains more information on the selection criteria at www.prace-ri.eu/prace-peer-review
**Facts and figures**

The first call for proposals opened in May 2010 marking the first opportunity for scientists and researchers to apply for resources on Europe’s largest supercomputers. Since then, 7 additional Regular Calls were opened, twice a year.

The spread of the allocations over the different research disciplines (chart 1) shows to be relatively even, although no pre-assigned quota exist(ed) per discipline or scientific area. Mathematics and Computer Sciences have the smallest slice of the pie, but are nevertheless well-represented among PRACE users. The low percentage is explained by the fact that the number of core hours requested per application is low compared with other disciplines.

The analysis of the total resource requests versus the total allocated resources per call (chart 2) shows that the resources requested vastly outnumber the resources available, even though the total amount of available resources has increased by one order of magnitude since the first call. This reveals the growing scientific need for HPC resources in Europe. The selectivity trend (ratio resources awarded per resources requested) is not observable yet since the full PRACE systems portfolio was only available since Call 5.

Dissemination activities to better advise applicants on how to submit proposals to PRACE Regular Calls have been scheduled in order to help potential applicants to apply.

PRACE statistics on the number of projects awarded per country are available at [www.prace-ri.eu/statistics](http://www.prace-ri.eu/statistics). The values for the number of awarded core hours depicted in Chart 2 below are normalised values based on the results of the Linpack benchmark for each system.

More details on the formula used for the normalisation can be found at [www.prace-ri.eu/statistics](http://www.prace-ri.eu/statistics).

**Useful contacts**

The PRACE Peer Review Team can answer your questions on PRACE Calls and the PRACE Peer Review Process. You can contact them via peer-review@prace-ri.eu. PRACE members can also coach applicants on how to apply to PRACE Calls.

For technical questions on the systems available, please contact directly the technical assistance of each of the Tier-0 centres, details of which can be found on [www.prace-ri.eu/PRACE-Resources](http://www.prace-ri.eu/PRACE-Resources). Requests for support from software experts on how to optimise an application code for a certain computing architecture should be addressed to the support working group at prace-optimization@fz-juelich.de.
To support the accelerated implementation of the Research Infrastructure established by the Partnership for Advanced Computing in Europe (PRACE) the European Commission issued three individual calls in 2009, 2010 and 2011, resulting in three distinct projects. In 2012 all three projects PRACE-1IP, PRACE-2IP and PRACE-3IP were running. The three projects have the mission to support the PRACE Research Infrastructure, and perform complementary or consecutive work towards this goal.

The First Implementation Phase project (PRACE-1IP) started in July 2010 and focused on the deployment and operation of the European Tier-0 infrastructure; on the related enabling and petascaling of applications; on establishing relations with academic and industrial users; on advanced training for HPC users; on technology watch and prototyping of promising architectures; and on components and software for future multi-Petaflop/s systems. Most activities of PRACE-1IP were successfully completed in June 2012. Work on the prototypes continues until the end of 2013, in order to evaluate the latest hardware components installed in those systems.

The Second Implementation Phase project (PRACE-2IP) started on 1st September 2011. The objectives of PRACE-2IP are: Integration of Tier-1 systems both on the technical and operational level and the support for the European-wide calls for Tier-1 resources as part of the Distributed European Computing Initiative (DECI); identifying best practices for HPC system commissioning and prototyping new architectures, components, and concepts; scaling of new applications for Tier-1 and Tier-0 systems and working with selected communities. Moreover, Dissemination and Training is intensified including the establishment of PRACE Advanced Training Centres (PATCs) and the deployment of the PRACE training portal, both concepts developed already during PRACE-1IP.

The Third Implementation Phase project (PRACE-3IP) started on 1st July 2012 with partners from 25 PRACE countries. During the combined PRACE-2IP all-hands meeting and PRACE-3IP kick-off 180 researchers met in Paris from 5 - 7 September 2012 to plan and synchronise the details of the project work. The objectives of PRACE-3IP are:

- Continue and expand outreach and training; scaling and optimisation of application codes, exploitation of new tools and techniques for HPC; operation coordination of Tier-0 and Tier-1 ecosystem including support for SMEs and industrial users.
- A completely new undertaking will be a pilot in Pre-Commercial Procurement (PCP) in HPC. This will be the first of its kind in Europe. Due to the nature of PCP this part of the project is planned to run for 48 months, whereas all other project work will be completed within two years.

Below, some of the project highlights are explained in detail.

### Ecosystem and operation

**Continuing the successful DECI programme: DECI calls and projects**

Up to December 2012, the PRACE-2IP project has launched two DECI (Distributed European Computing Initiative) calls, and continued a call which was launched before the PRACE-2IP project started. These have continued the successful DECI programme which allows researchers across Europe to access the top national HPC resources of European countries. The DECI projects give researchers the possibility to have one-year access to high-level computational facilities. It boosts the collaboration between research groups in different European countries; it is also possible to apply for a whole range of HPC architectures. The DECI programme is based on an extensive collaboration between the PRACE partners. Therefore, the DECI calls have attracted a large number of proposals for HPC resources: in total 233 proposals were received, from over 20 countries. From the proposals, PRACE has been able to accept over 130 DECI projects which represent diverse areas of science: from material sciences to astrophysics and plasma physics with applications in fusion research, from bio sciences to chemistry and engineering with applications in fluid dynamics. The DECI projects have been allocated over 200 million core-hours of computer time in 2012.

### PRACE Infrastructure and operations

The core infrastructure is formed by the most powerful supercomputer systems available currently for the European research community. PRACE-2IP partners complemented the core infrastructure with a wide range of national systems. These latter systems provide users with the opportunity to run projects which uses fewer cycles or scale to a smaller number of processors. They can also use them to prepare their codes to run on larger systems. To enable the sharing of work on different systems or the migration of work and data from one system to another as seamless as possible the systems are tightly linked by a private high bandwidth...
network provided by the European research network infrastructure of GEANT. Several services are implemented to further integrate the systems.

Dedicated network
The dedicated network has a star topology with its centre in Frankfurt, Germany. It allows up to 10 Gb/s communication throughput between the partners’ supercomputer systems and servers. The network allows unconstrained and undisturbed use of the predefined communication bandwidth. This simplifies the detection of bottlenecks and the investigation of the interaction between the involved supercomputer systems, applications and the network itself. Each site agrees not to connect any other systems to the PRACE backbone and not to route any other traffic via this infrastructure. With this policy a “Net of Trust” was established and this allows for application traffic between the systems, which would not be allowed otherwise.

Access to resources and data transfer
PRACE-2IP enhanced the UNICORE software enabling users to submit jobs to any PRACE system in a uniform way and assisted its deployment at new partner sites. It complemented GridFTP by deploying and tuning G-transfer to improve multi-petabyte data transfers. PRACE-2IP supports the operation of the distributed PRACE resources through a consistent administration and a one-shop user support.

Operational services – available and monitored
Operational services guarantee a high level of availability and reliability of the supporting services. The supported services are tested at each site on a regular basis by a network of agents reporting the status of services to a central monitoring server. The PRACE operational staff through a web interface in addition to local monitoring facilities can view the results.

Monitoring the services, taking actions on and escalating open problems is shared among partners on a weekly basis. Problems reported by users are handled by a separate task group.

New service developments
Before new services or major changes in existing services are proposed for production an extensive evaluation takes place. In the past year evaluations took place for among other things job submission facilities, data management facilities and improvements of the facility for the submission and processing of project calls.

New Technology
Market watch and HPC centre infrastructures
Twice a year a market watch report is delivered to the PRACE community. The focus of the watch is on petascale systems worldwide from Top500, SC and ISC conferences, and other web or vendor sources, but also on some global trends watch on HPC systems components. It eventually watches the global evolution of PRACE resources w.r.t. other continents, the general trends in Tier-0 programming environments, Tier-0 usage within PRACE, as well as how the whole European HPC landscape is moving.

HPC centre infrastructures are also important, in relation with HPC systems, when delivering globally efficient solutions in terms of performance, energy and eventually cost is at stake. White papers were released on various aspects of HPC centre design and operations, and a bi-annual European Workshop on HPC Centre Infrastructures is organized to go on sharing experience of all stakeholders from technology suppliers to computing centres.

Evaluation of accelerator technology
The prototypes developed in PRACE-1IP and PRACE-2IP allow for the investigation of future HPC specific technologies. Additionally PRACE-2IP will assess application performance in terms of porting effort involved and raw performance.

The focus of the PRACE-2IP prototypes is the evaluation of the usefulness and usability of each current accelerator technology, e.g. Intel Many Integrated Cores (MIC), Nvidia GPU and AMD GPU, coupled with innovative cooling technologies and possible alternatives to InfiniBand, which should help to leverage the computing power provided by accelerators for more applications. The Scalable Hybrid prototype (CSC, CSCS, SARA,) will consist of 256 nodes with 128 NVIDIA Kepler K20 GPU’s and 128 Intel PHI’s. Phase one of the prototype which is currently deployed consists of 10 T-Platforms V-200 blades (Dual Xeon E5-2640, 32GB 1600MHz DDR3 RAM, Mellanox FDR InfiniBand) air-cooled nodes and five NVIDIA Kepler K20 cards and five Intel Xeon Phi cards.

The EURORA prototype (CINECA, GRNET, IPB, NCSA), an evolution of the AURORA rack was developed by Eurotech. It is a direct liquid-cooled system. The EURORA system has 64 compute cards, each of which has 2 Intel Xeon processors, a 90GB SSD, 1 FPGA and 2x accelerator cards - K20 (currently) and Intel Xeon Phi.
Scalable Hybrid and EURORA also assess the usefulness of hot-water cooling (“free cooling”) in northern and in southern Europe in contrast to the first hot-water cooled prototype which was installed at the Leibniz Rechenzentrum (LRZ) in Germany as part of the PRACE-1IP prototypes. Preliminary results showed that in comparison to standard air cooled systems hot-water cooling can save a significant amount of energy in central European climates by using free cooling (no water chillers only outside heat exchangers). All systems will incorporate energy efficiency assessments and measurements.

The CPU/GPU prototype (PSNC, WCNS, Cyfronet), investigates AMD APU’s as compute node alternatives. It consists of 40 nodes with 2x6-core Xeon 2GHz E5 processors; non-GPU nodes have 32GB memory whereas GPU-nodes have 64GB memory. Each node has a SSD local drive and QDR Infiniband. The 12 GPU-nodes will feature an AMD W9000 GPU (1Tflop/s Double-precision performance, OpenCL 1.2 support and 6GB of ECC DDR5 memory). All electronics are submerged in liquid (Iceotope system). PowerDAM (Power Data Acquisition Monitor developed at BADW-LRZ) will be deployed which will be an easy way of accessing information about power consumed by individual jobs.

**Application enabling**

**Scaling Applications for Tier-0 and Tier-1 Users**

PRACE-2IP provides medium-term petascaling and optimisation support for European HPC applications to ensure that they can make effective use of both Tier-0 and Tier-1 systems. This extends the work of PRACE-1IP to include Tier-1 systems complementing the Community Code Scaling activity, which is developing longer-term collaborations with communities.

The Scaling Application activity identifies applications-enabling projects by various calls. The approach was developed already in PRACE-1IP. Many scientific areas are covered by the application work, and include theoretical chemistry, materials science, computational fluid dynamics, earth sciences, climatology, engineering, energy, and life sciences.

**Architecture expertise and best practice guides**

The Scaling Application activity has developed specific expertise on most, if not all, of the architectures that make up Tier-0 and Tier-1 of the European HPC system. PRACE-1IP provides best practice guides on PRACE Tier-0 systems that cover programming techniques, compilers, tools and libraries. PRACE-2IP supplements these with best practice guides for other architectures that are important at Tier-1 to allow European researchers to make efficient use of these systems.

**A unified benchmark suite**

The project created a single HPC benchmark suite based on earlier work by DEISA and PRACE that can be used by European HPC centres in procurements.

**Petascaling of applications**

The PRACE project enabled over 50 applications to exploit the capabilities of the PRACE Tier-0 systems. One example is CP2K, a key application for European materials scientists. Recent work in PRACE-2IP has led to a 50% performance improvements using mixed-mode MPI and OpenMP. Previous enabling work in PRACE-1IP showed strong scaling of small problems up to 8192 cores on BlueGene/P and delivered further incremental speedups of up to 35% depending on the type of calculation. Freely available CP2K program contains a wide range of methods including classical potentials, Density Functional Theory, QM/MM, Hartree-Fock and MP2. CP2K is deployed and widely used on the PRACE Research Infrastructure at both Tier-0 and Tier-1.

**Sustainable application co-development of community scientific applications**

The Community Code Scaling activity initiates a sustainable program in application development for supercomputing applications targeted at problems of high scientific impact that require High Performance Computing (HPC) for their solution. The application development program was accomplished by involving a number of scientific communities in the process of enabling a few of their most relevant simulation codes to innovative supercomputing architectures. This process relies on a close synergy between scientists, code developers and HPC experts.

**Performance modelling approach**

A number of codes have been analysed, their performance evaluated, their suitability to the refactoring program investigated, adopting the performance modelling approach. This methodology relies on the analytic modelling of the main algorithms and on the performance analysis, based on the usage of performance tools. It allows for studying the current behaviour of a code, emphasising...
performance and bottlenecks. But it is also a predictive tool, allowing the estimation of the code’s behaviour on different computing architectures, and identifying the most promising areas for performance improvement. The methodology is cross-domains, codes independent and provides an objective and quantitative way of evaluating applications.

As a result a number of codes were selected from five different scientific domains: astrophysics, material science, climate, engineering and particle physics. Specific groups were formed to work on each of the selected codes. Many project partners and community members have been involved on the work for each code. Due to the different features, needs and targets of the codes, each group adopted their own working methodology, strategy and schedules in order to reach the objectives.

A typical example of the work accomplished is given by RAMSES, an important astrophysics code describing the behaviour matter in the universe via a combined hydrodynamics+Nbody approach. AMR makes it possible to get high spatial resolution only where this is actually required, thus ensuring a minimal memory usage and computational effort. Our performance modelling approach identified the two kernels that could benefit most from a mixed CPU GPU re-implementation. Different approaches splitting the work between CPUs and GPUs using a hybrid OpenMP+MPI model were evaluated. Our solution allows solving larger problems and reduces MIP communication.

**Industry Application enabling**

Today many open source codes used by industries are unable to exploit massive parallelism, furthermore, other open source applications with an high potential impact on industrial research and innovation are not ready for industrial production on powerful HPC systems. Therefore, it is important to enable and petascale these codes, allowing industrial users to access petascale resources and to be competitive through high-end simulation. PRACE-2IP addressed in its activity “Industrial Application Support” two important actions in this direction: to focus on petascaling open source codes of interest for the industrial communities and to enable for emerging industry relevant open source codes for HPC systems.

Enabling three open source codes for the PRACE Tier-0 and Tier-1 systems: three well known Open Source applications in Computational Fluids Dynamics (OpenFoam), structural mechanics (Elmer) and Hydrodynamics (Delft3D, a modelling suite to investigate hydrodynamics, sediment transport and morphology and water quality for fluvial, estuarine and coastal environments) were selected. These applications are well known in different Industrial fields, and the open source scheme adopted for these applications, allows avoiding the use of competitor codes with expensive licenses.

Enabling six selected emerging application codes making them mature for effective industrial usage: The emerging applications cover different industrial fields: computational mechanics (ALYA-SolidZ), fracturing and granular flows (NUMFRAC), system complexity (Ontonix), risk and uncertainties analysis (SPEED and URANIE), viscoelastic fluid flow (VISCOSOLVE). Results example: SPEED has increased scalability on BG/Q Tier-0 System from 1.024 up to more than 16,000 cores on an industrial test case. The industry which provided the benchmark data-set is now applying for Access Tier-0 resources in an Open R&D scheme.
Events of interest to the HPC community

ISC13
16 – 20 June 2013
With over 170 exhibitors from research and industries representing supercomputing, storage and networking, this will be the largest HPC exhibition in Europe in 2013. About 2,500 attendees are expected and the ISC Conference is famous for its world-class program, with more than 300 academia and industry leaders tackling the most important issues of High Performance Computing. PRACE will be present with a booth and will host a BoF on services to Industry. www.isc-events.com/isc13/#

International Summer School on HPC Challenges in Computational Sciences
23 – 28 June 2013, New York City, United States
Leading American, European and Japanese computational scientists and high-performance computing technologists will offer instruction on a variety of topics, including Access to EU, US, and Japanese cyber-infrastructures; HPC challenges by discipline (e.g., bioinformatics, computer science, chemistry, and physics); HPC programming proficiencies; Performance analysis & profiling; Algorithmic approaches & numerical libraries; Data-intensive computing; Scientific Visualization. www.prace-ri.eu/International-Summer-School-2013

SC13
17 – 22 November 2013, Denver, United States
SC13 will feature one of the largest exhibitions in conference history, with nearly 400 exhibitors from industry and research institutions around the world. PRACE will be present with a booth to highlight its activities, achievements and advancements. www.sc13.supercomputing.org/

PRACE Industrial Executive Seminar
PRACE held its 5th Industrial Executive Seminar on 15 and 16 April 2013 in Bad Boll near Stuttgart. The 2014 edition is foreseen to be hosted in Barcelona, Spain. Keep an eye on www.prace-ri.eu/PRACE-Industrial-Seminars for more details in the coming months.

PRACE Advanced Training Courses
Six PRACE member sites host PATC courses: the Barcelona Supercomputing Center (Spain), CINECA - Consorzio Interuniversitario (Italy), CSC - IT Center for Science Ltd (Finland), EPCC at the University of Edinburgh (UK), the Gauss Centre for Supercomputing (Germany) and the Maison de la Simulation (France) are the first PRACE Advanced Training Centres. The PATCs will provide top-class education and training opportunities for computational scientists in Europe. Upcoming PATCs can be found here: www.prace-ri.eu/PRACE-Advanced-Training-Centres

International Conference on Scientific Computing 2013
3 - 6 December 2013, Pafos, Cyprus
This major event on scientific computing is co-organised by PRACE and the LinkSCEEM-2 project. It brings together an international community of HPC researchers from Europe and the Eastern Mediterranean to present and debate new methods and results covering a diverse range of topics. For more information: www.cyprusconferences.org/csc2013/index.php
PRACE welcomed SC12 visitors to the PRACE booth in Salt Lake City, 12–15 November 2012

PRACE was present at SC12 to exhibit the 6 Tier-O systems to which scientists and researchers can gain access through the PRACE peer review process. PRACE Prototypes were discussed at a BoF session and this year’s edition of the PRACE Treasure Hunt gave everyone a chance to win a brand-new Samsung Galaxy Tab!

The PRACE USB key, containing the latest news of PRACE, was again popular with both press and visitors.

(Below) PRACE Booth Team at SC12. PRACE dedicated staff was present to answer all questions about PRACE, the PRACE Projects, the Tier-O systems and the peer review process.
EVENTS

BoF: PRACE Future Technologies Evaluation Results
Furthermore, the PRACE Projects informed visitors about their prototypes through a “Birds of a Feather” (BoF) session on Wednesday 14 November.

(Left) PRACE BoF Team at SC12
Sean Delaney, Torsten Wilde, Gilbert Netzer, Alex Ramirez and Radek Januszewski after a successful BoF session at SC12, Salt Lake City

PRACE Treasure Hunt
On Wednesday 14 November PRACE staff drew the name of the winner of the PRACE Treasure Hunt out of more than 130 contestants. Vikas Aggarwal of Oracle received a Samsung Galaxy Tab2!

HPCwire 2012 Readers’ Choice Awards
PRACE Partners have received well-deserved recognition in the HPCwire’s Readers’ and Editors’ Choice Awards at SC12: www.prace-ri.eu/HP-Cwire-Award-Winners-2012