Partnership for Advanced Computing in Europe

PRACE
Annual Report 2013

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

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PRACE Annual Report 2013

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PRACE and HPC usage in Europe: the sky is the limit?

With HPC becoming the tool of choice for more and more scientific and industrial researchers, PRACE is fulfilling its objective to provide world-class services and systems to the best European science, with scientific excellence as the principal criterion for awarding computing resources.

This Annual Report highlights some of the important achievements of PRACE in 2013, a few of which I will describe in short below.

The 5th PRACE Call for Proposals for Project Access served as the test-platform for an entirely new form of access to Europe’s top-level systems: PRACE Multi-Year Access. A limited group of 7 outstanding projects from academia and industry were awarded more than 175 million core hours for the first year of their research program, while an additional 175 million core hours were reserved for their second year, to be allocated after a mid-term review through the 7th Call. This two-step allocation procedure allowed the research teams to plan a 2-year scientific project, with guaranteed access to the resources assuming a positive mid-term evaluation.

The PRACE Scientific Steering Committee has evaluated the Multi-Year Access programme and has come to a unanimously positive conclusion, strongly advising the PRACE Council to continue similar forms of access in future Calls for Proposals.

More information on the Multi-Year Projects can be found on pages 33 to 35 of this Annual Report and I also encourage you to have a look at the full articles on each of these projects, published in PRACE Digest 1/2014 (www.prace-ri.eu/PRACE-Digest)

PRACE supports science and industry with world-class resources (6 Tier-0 systems in 4 countries), innovative and tailored access programmes (Multi-Year Access, SHAPE, Open R&D Access) and complementary Calls for Proposals (Project Access and Preparatory Access), but also with a wide and expanding range of HPC-related training and education services. Benefiting from the extensive cumulated expertise of all the PRACE partners, the PRACE Advanced Training Centres (6 centres across Europe) offer regular, free of charge training courses taught by the leading European HPC-experts and computer scientists. Additionally, the PRACE IP Projects, supported by the European Commission, offer 4 Seasonal Schools, an International Summer School – in co-operation with XSEDE (USA) and RIKEN (Japan) – Campus Schools, and specific placements for undergraduates and post-doc students (Summer of HPC).

Education and training is an important objective in PRACE, to present engineers and scientists to the new technologies and developments happening in the HPC environment; and to educate and train citizens with new skills and in new professions.

More information on the types of training that PRACE offers can be found on page 40 of this Annual Report.

PRACE is firmly rooted in the European HPC eco-system, with the 4 Hosting Members providing access to the top of the HPC pyramid, and the 21 General PRACE Members providing additional enabling services to Tier-1 resources via the DECI (Distributed European Computing Initiative) programme, and the common operation coordinated by the implementation-phase PRACE projects.

A further networking effort has started with the collaboration between ETP4HPC (European Technology Platform for High Performance Computing, an association of HPC vendors) and PRACE, for the development of a sustainable European HPC ecosystem.

The upcoming PRACE Scientific and Industrial Conference in Barcelona (PRACEdays14, see page 48) will allow scientists and industrial users to convene and connect on this and other recent developments.

With this, I invite you to browse through this edition of the PRACE Annual Report and read about these and other topics of interest to the HPC community. I hope the articles will provide you with food for thought as well as inspiration for 2014 and beyond.
The Industrial Advisory Committee

HPC for Innovation. Towards extended HPC usage for industry

Since its inception in 2010 PRACE has been steadily building relationships with industrial partners to adapt its offer of Tier-0 resources in Europe to the needs of both multinational companies and SMEs.

A milestone in this development was the creation of the PRACE Industrial Advisory Committee (IAC) in 2013, following the decision of the PRACE Council in October 2012.

The members of the IAC are all high-level industrial executives from various sectors and business types. The Committee held its inaugural meeting on 3 September in Brussels and has since then been providing advice and direction to the PRACE Council to improve the PRACE services targeted at industrial use of HPC. Topics of discussion include SME involvement, knowledge transfer, open innovation, training, and the needs of industry in Europe to grow its competitiveness.

Currently the IAC counts 8 full members and one observer from ETP4HPC. Two seats are still free for members representing Life Sciences and Finance. At the inaugural meeting, Mr. Jürgen Kohler, Head of NVH CAE and Vehicle Concepts at Daimler AG, was elected Chair, while Mr. Anders Rhod Gregersen, Senior Specialist at Vestas Wind Systems, took the position of Vice-Chair.

The IAC Chair will serve as the linking pin between the European Industrial community and the PRACE Council, a function taken up with serious interest by Mr. Kohler, who said that “HPC resources are vital for sustaining – and growing – European competitiveness in large-scale industry as well as in SMEs. I am already looking forward to the first PRACE Scientific and Industrial Conference in May next year, where the IAC will be hosted by PRACE alongside the PRACE Scientific Steering Committee and the PRACE User Forum. This event will provide excellent opportunities for science and industry to join hands – virtually and in reality.”

The IAC has been active on all levels since its creation: the PRACE SHAPE Programme (SME HPC Adoption Programme in Europe) has received input and guidance from IAC Members and the IAC Chair and Vice-Chair are members of the Organisation and Programme Committee (OPC) of the PRACE Scientific and Industrial Conference, which will be held for the first time in May 2014 in Barcelona (PRACEdays14). More information on both SHAPE and PRACEdays14 can be found on pages 8 and 48 of this Annual Report.

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<th>NAME</th>
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<tr>
<td>Peter Schoonjans</td>
<td>Airbus</td>
<td>Aeronautics/Aerospace</td>
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<td>Jürgen Kohler (Chair)</td>
<td>Daimler</td>
<td>Automotive/Transport</td>
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<td>Claire Waast-Richard</td>
<td>EDF</td>
<td>Energy</td>
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<td>Ricard Borrell</td>
<td>Thermo Fluids</td>
<td>Engineering/Manufacturing/SMEs</td>
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<td>Sergio Zazzera</td>
<td>ENI</td>
<td>Oil &amp; Gas</td>
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<td>Anders Rhod Gregersen (Vice-Chair)</td>
<td>Vestas</td>
<td>Renewable Energy</td>
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<td>Olli Hyynpa</td>
<td>NXP Semiconductors</td>
<td>Telecommunications/Electronics</td>
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<td>Lee Margetts</td>
<td>NAFEMS</td>
<td>ISV</td>
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<td>Jean-Francois Lavignon</td>
<td>ETP4HPC</td>
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PRACE Collaborations

PRACE is embedded in a tight network of collaborations with key players in the field of high performance computing in Europe and worldwide. These collaborations take many forms; e.g. as Memorandums of Understanding with the PRACE IP Project or with PRACE aisbl as a project partner or as a representative in advisory boards. Only with a strong link to the HPC ecosystem, the PRACE users, and other key players, can PRACE fulfil its mission.

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<td>EEF - European E-Infrastructure Forum</td>
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### PRACE IS REPRESENTED IN AN EXTERNAL BOARD OF:

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<td><img src="image1" alt="EGI" /></td>
<td>PRACE is represented in the European Grid Infrastructure (EGI)-InSPIRE External Advisory Committee.</td>
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<td><img src="image2" alt="e*nventory" /></td>
<td>PRACE is represented in the Advisory Board of e*nventory, an FP7 project dealing with impact assessment of eInfrastructures.</td>
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<tr>
<td><img src="image3" alt="eu gridpma" /></td>
<td>The European Policy Management Authority for Grid Authentication in e-Science is a body to establish requirements and best practices for grid identity providers. PRACE is represented as relying party.</td>
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<tr>
<td><img src="image4" alt="GÉANT" /></td>
<td>PRACE is using the GÉANT network services, the pan-European research and education network interconnecting Europe’s National Research and Education Networks. It is represented in the International User Advisory Committee.</td>
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<td><img src="image5" alt="ETP 4 HPC" /></td>
<td>PRACE is an observer in the European Technology Platform for High Performance Computing.</td>
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<td><img src="image6" alt="e-FISCAL" /></td>
<td>PRACE is represented in the advisory board of e-Fiscal, an FP7 project dealing with the assessment of costs of Research Infrastructures.</td>
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### PRACE HAS COLLABORATED IN OTHER WAYS WITH:

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<td><img src="image7" alt="XSEDE" /></td>
<td>PRACE and XSEDE jointly organise the EU-US HPC Summer School and work on the enhancement of interoperable services between PRACE and XSEDE through a joint call for request for support.</td>
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<tr>
<td><img src="image8" alt="RIKEN" /></td>
<td>RIKEN Advanced Institute for Computational Science (AICS) joined up with PRACE and XSEDE to organise the 4th “International Summer School on HPC Challenges on Computational Sciences”</td>
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<tr>
<td><img src="image9" alt="e-IRG" /></td>
<td>Within the e-InfraStructure Reflection group PRACE is a stakeholder in the provision of an ICT based Research Infrastructure.</td>
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<tr>
<td><img src="image10" alt="CoPoRI" /></td>
<td>PRACE participated in the Exchange of Experience group in the project for ESFRI: Communication and Policy development for Research Infrastructures in Europe.</td>
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<tr>
<td><img src="image11" alt="SCI (Security for Collaborating Infrastructures)" /></td>
<td>PRACE Security Forum is represented in the Security for Collaborating Infrastructures, a collaborative activity of security staff from several large-scale distributed computing infrastructures, including EGI, OSG, PRACE, wLCG, and XSEDE.</td>
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SHAPE

HPC to accelerate growth and innovation for European SMEs

SHAPE (SME HPC Adoption Programme in Europe) is a new PRACE-supported pan-European programme. It aims to raise awareness and provide European SMEs with the expertise necessary to take advantage of the innovation possibilities created by HPC, thus increasing their competitiveness.

In a “Russian doll” approach SHAPE will rely where possible on existing national initiatives to spread the word among SMEs and to amplify those initiatives at European level. Where such initiatives are not available at national level, SHAPE will provide a complete set of complementary services for SMEs; from information, training, and access to experts from academia (domain science as well as applied mathematics and HPC) to co-development of a concrete industrial project to be executed using PRACE HPC resources.

After their participation in SHAPE, companies will have a clear view of the potential of HPC: the investment needed to perform; the skills they need to hire; the software or methodologies to develop; and they have a choice to either continue to use PRACE services for Open R&D and/or to buy their own HPC facilities and/or to access remote HPC services on commercial Cloud platforms.

To better define and prove the viability and value of SHAPE, a SHAPE Pilot was initiated to refine the details of the programme and prepare its launch in a fully operational form. The pilot worked with a first set of SMEs and introduced HPC-based tools and techniques into their business, operational, or production environment. The mission is to help the selected SMEs to demonstrate a tangible Return on Investment (RoI) by assessing and adopting solutions supported by HPC, thus facilitating innovation and/or increased operational efficiency in their businesses.

The pilot started in June 2013 with an open Call for Applications to all European SMEs that have a business project that can be implemented using HPC. The call had a brilliant response, involving 14 SMEs, from 7 different Countries (Bulgaria, France, Germany, Ireland, Italy, Spain and the UK) and spanning across various industrial domains. The 10 selected SMEs received CPU and GPU hours via 15th cut-off of PRACE Preparatory Access.

Work Package 5 (WP5) of the EU-funded PRACE 3rd Implementation Project is developing a business model to make SHAPE a new permanent service within PRACE. The PRACE Council will decide in June 2014 on the next steps for SHAPE.

The upcoming PRACE Scientific and Industrial Conference (PRACE-days14) will feature a dedicated stream of presentations from successful SHAPE participants. See page 48 of this Annual Report for more information on PRACEdays14.
Albatern Ltd, UK – Numerical Simulation of Extremely Large Interconnected WaveNET Arrays
Albatern develops novel interconnected offshore marine renewable energy devices. The goal of the project is to develop and deploy a code to simulate a large scale WaveNET array using HPC parallel technology. The results of the simulations will contribute by mitigating risk and reduce overall development time and cost.

AMET s.r.l., Italy – Robustness in safety performances analysis
AMET is an Italian high-tech engineering company, active in the design and development of mechanic and mechatronic products and processes. The project aims to analyze state of the art simulation techniques to replace the standard deterministic approach, used to evaluate the passive safety performances of a vehicle, with a robust lean statistical approach.

Audionamix, France – Unmix Up
Audionamix is a French company developing innovative audio unmixing technologies, relying on computationally intensive optimization algorithms. The project will help Audionamix to explore the latest hardware and software solutions. The unmixing algorithms will be adapted to enable multi-GPU-based hardware configurations. The improvements in technology speed are expected to unveil new business opportunities in processing large audio material bases, accelerating R&D inside the company.

ENTARES Engineering / NExIO, France – CAPITOL-HPC+
ENTARES Engineering is a French SME developing electromagnetism simulation software to study the electromagnetic behavior of products during the design, before the manufacturing phase. This project aims to validate a quick and easy parallel simulation tool that can be operated at an early stage of system design, with a controlled level of accuracy. In addition, a commercial offer for this software environment, such as pay-per-use scheme, developing a partnership with a computing center to propose a service, will be investigated.

Juan Yacht Design, SL, (JYD), Spain – Testing LES turbulence models in race boat sail
Juan Yacht Design SL is a Spanish company specialized in the design of sail boats. The project aims at testing new methods for the design of racing boat sails using novel HPC simulation techniques, introducing competitive advantages that will allow JYD to become a world class leader in this segment.

Lapcos ScrL, Italy – Virtual Test Bench for Centrifugal Pump
Lapcos is an engineering firm which adopts virtual prototyping technologies. The proposed project is aimed at building, upon the OpenFOAM library for CFD, a custom, vertical product for automatically design centrifugal pumps, exploiting HPC resources.

MONOTRICAT S.r.l., Italy – CFD simulation of an innovative hull
Monotricat SRL is an Italian company that designs an innovative hull, characterized by hydrodynamic efficiency; the aim of the proposed project is to use CFD on HPC methodologies applied to its hull in order to optimize their R&D work flow.

NSilico Life Science Ltd, Ireland – High Performance Computation for Short Read Alignment
NSilico is a company based in Ireland, developing integrated molecular diagnostics and analytic tools for the life sciences and healthcare industries. The project aims at identify accurate data analytic applications for ribosomal RNA sequence analysis taking advantage of massively parallel architectures. This would not only provide a technical advantage but would also provide the developed solution with greater access to commercial markets.

OPTIMA pharma GmbH, Germany – Enhanced airflow simulations around filling machines in clean rooms
Optima pharma offers an immensely diversified and innovative range of filling and packing machines for pharmaceutical products, e.g. sterile liquids and powders, and will profit from airflow simulations in clean rooms which minimize trial and error cycles during innovative machine design and reduce expensive hardware tests.

THESAN S.p.A, Italy – Improvement of hydraulic turbine design through HPC
Thesan is an Italian SME involved in energy sustainability. The project aims to optimise the design of a volumetric machine (hydraulic turbine) currently being developed by Thesan, improving the overall performance by designing and realising rotating chambers where the fluid flows, drastically cutting down the time and resources needed to construct a physical prototype and actually building the preferred structure only.

For information on the SHAPE pilot, please visit the SHAPE website at www.prace-ri.eu/shape or contact shape@prace-ri.eu.
In 2013, three members of the PRACE Scientific Steering Committee (SSC) decided to step down: Prof. Risto Nieminen (Materials Science, Finland), Prof. Modesto Orozco (Life Sciences, Spain) and Prof. Thierry Poinso (Engineering, France). I am grateful for their contributions in ensuring the success of PRACE by providing valuable input on the needs of the scientific community. I am happy to welcome Prof. Dimitri Komatitsch (Computational Earth Sciences, France), Prof. Petros Koumoutsakos (Computational Sciences and Engineering, Switzerland) and Prof. Ignacio Pagonabarraga (Computational Physics, Spain) as new members of the SSC.

Based on requests from a wide range of user communities, a pilot for multi-year access was included in the 5th PRACE Call for Proposals for Project Access to PRACE computing resources. Several multi-year projects were approved in this Call; multi-year access being provided assuming a positive evaluation of the progress. This evaluation was performed by the PRACE Access Committee (AC) as part of the evaluation process for the 7th PRACE Call for Proposals for Project Access. All 7 projects that were granted multi-year access were invited to present their progress and the project to the access committee. The AC was very pleased with the progress in all of these projects and strongly supported their allocation for the second year.

The SSC has in 2013 analyzed this pilot call for multi-year access, finding the scheme a great success that meets the needs of Europe’s best research groups in computational modeling. The multi-year access scheme serves an important role in enabling world-class research. The SSC thus strongly recommended to the PRACE Council to make the multi-year access scheme a permanent instrument for access to PRACE resources. The SSC is happy see that this proposal was endorsed by the PRACE Council.

The SSC has in 2013 also analyzed the needs of the scientific community for storing large datasets that arise from large-scale simulations. Based on the responses of the scientific community on an open call for Expressions of Interest on Big Data, the SSC found that PRACE has an untapped potential for additional scientific discoveries and innovations in the large datasets obtained in many Tier-0 computations, going beyond the original goals of the simulation. Based on this analysis, the SSC urges the PRACE Council to develop a policy for handling access to such datasets and exploiting the scientific potential of these datasets. This will also contribute to the open-access policy of the European Commission.

The SSC is happy to note that there is an increasing demand for PRACE resources. At the same time, with the PRACE 1.0 project coming to an end and less Tier-0 resources being available, the SSC is also concerned that Europe will not be able to continue to provide the necessary computing resources to enable world-class research and innovation based on computer modeling. However, the SSC is glad to see the progress made in establishing PRACE 2.0, and that scientific excellence will remain the key criterion for access to PRACE resources also in PRACE 2.0. The evaluations made by the SSC of completed PRACE projects demonstrate that PRACE enables world-class research. A few of these projects are presented in this Annual Report, giving you a taste of the many achievements of PRACE.
Exploring methods for refining nanomaterials

The EU’s €10bn Graphene Flagship research initiative reflects the revolutionary potential that many experts believe the material holds. However, to fully exploit its exciting properties, the development of techniques that can manipulate individual atoms and change graphene morphology at nanoscale, thereby breaking up the homogeneity of its structure, is desirable. Undertaking computer simulations supported by PRACE, researchers have been exploring the possibility of using irradiation to fulfil this function.

An atom-thin layer of carbon, graphene possesses a number of remarkable features that render it a superlative prospect for the high-tech industries. Viewed microscopically, the material resembles a honeycomb lattice, or ‘chicken wire’ structure, but this simple appearance belies rare utility. It’s the thinnest compound known to man, whilst simultaneously the lightest, strongest, and most effective conductor of electricity yet known. Poised to bring about new types of flexible electronics, telecommunications and even paint, its potential applications are exciting and incredibly diverse. Encouragingly, although manufacturing the material was initially prohibitively expensive, recent studies have suggested new synthesis methods that could help to economise the process and make graphene available on the industrial scale.

And yet, fundamental challenges still remain. The types of graphene produced in lab environments frequently contain irregularities that detract from their functionality. Often grown on a metal substrate from which it is separated before use, graphene crystals formed using this experimental process often reveal flaws such as impurities, rippling and irregular orientation. Consequently, to meet its full commercial potential, there’s a pressing need for methods that can mitigate these physical inconsistencies, and impose uniformity at nanoscale.

Fortunately, when it comes to understanding how atoms interact at this level, supercomputing resources can offer invaluable assistance. “Simulations can significantly help researchers and divulge the attributes of materials through their astonishing predictive power,” says Dr Arkady Krasheninnikov, a senior scientist from the Department of Applied Physics at Aalto University and the University of Helsinki. “These models obtain data by considering solid structures as collections of atoms”. Using equations to determine their many properties without the use of computers would, he suggests, “pose a truly mind-boggling challenge.” Moreover, the accurate results of large-scale computer simulations may guide practical experiments and thus reduce their cost.

Whilst HPC modelling can divulge information about the physical characteristics of materials, including their electronic properties, it can also be used to predict their responses to external actions. Pressure is one of these, as is ion and electron irradiation, which was the subject of a recent investigation headed by Krasheninnikov. Concentrating on graphene, the study, titled “Effects of irradiation on nanostructures from first principles”, was granted eight months of access to PRACE facilities during 2012, and sought to answer a number of fundamental scientific questions.

“Graphene, despite all the accolades it has received, isn’t yet commercially viable, as techniques to create and manipulate it are still being developed,” says Krasheninnikov. Because of this, industrial heavyweights like Samsung are heavily investing in research to pioneer cost-effective manufacturing methods, and the €10bn “Graphene Flagship” program was recently launched in the EU. “For example, you can’t directly make a transistor from graphene, as it lacks electronic band gap due to its ‘chicken-wire’ atomic configuration,” says the scientist. “However,” he continues, “the initial product is malleable. By cultivating holes or purposeful defects, a regular nanomesh can be created throughout graphene structures. These uniform, periodic voids would be incredibly...
small – at nanometre scale – but could effectively open the gap in the material.”

“To achieve these modifications, we hypothesised that electron and ion irradiation could be used. Computer simulations enabled us to test this,” states Krasheninnikov. By processing scenarios in which single and multi layer, stacked graphene sheets were subjected to energetic ion bombardment, the researchers were able to determine various important aspects of this interaction. These included the stopping power of the energetic projectiles, and their energy deposition within the graphene’s structure. “Ion irradiation beams are ubiquitous, and found on production lines throughout the semiconductor industry. Theories and practice for irradiating 3D objects are, therefore, well advanced, but these models are inapplicable for 2D systems or products like graphene”.

“The experiments carried out by our coworkers demonstrate that if graphene is irradiated whilst on a metal substrate and then temperature is raised, vacancies within its structure will become mobile,” says Krasheninnikov. Small vacancies will then coalesce into larger regular holes in certain areas defined by the mismatch between the metal and graphene atomic structures, ultimately creating a standardised, evenly spaced nanomesh across the graphene sheet. This can help to achieve a regular, periodic structure, and our simulations provided microscopic insights into this process and helped to optimize the experimental parameters.

“A secondary objective of the project was to consider the damage inflicted by electron microscopes to the samples, due to the energetic electrons they use. This actually occurs in hundreds of laboratories throughout the world on a daily basis, and is a rather common problem,” adds Krasheninnikov. “Due to the energy deposited by the electron beam, the samples being studied can be altered, or damaged. This is similar to the way in which graphene is modified under ion irradiation. So, if we can begin to differentiate between native and induced defects, this could considerably improve the validity of research methodologies.”

“A further area we focused on was grain boundaries in graphene. If grown on metal surfaces like copper, it frequently nucleates in different parts,” says Krasheninnikov. “Like small islands, individual formations then coalesce to form a larger structure. But rather than a uniform graphene crystal arranged in perfect symmetry, the process often creates incongruous configurations of graphene. These possess different orientations giving rise to a variety of carbon rings at the borders between merged islands– including hexagons, pentagons and heptagons. The experiments showed the grain boundaries move under the electron beam and small grains can even disappear, completely ‘eaten’ by the larger. Our simulations showed that this happens by carbon bond rotations induced by impacts of energetic electrons”.

Using the PRACE French Tier-0 system (the CURIE supercomputing asset based in TGCC near Paris), Krasheninnikov and his collaborators were able to establish a number of exciting precedents and physical principles. “The research was quite fundamental. Our data can now help materials scientists, physicists and chemists to appreciate more about graphene and its behaviours.” Proudly acknowledging that the research was cutting edge, Krasheninnikov is adamant that it also meets immediate demands, and that its achievements will be widely utilised. “The knowledge we’ve obtained is something practical researchers actually need now,” he contends. “It could also be vital to devising future industrial applications. Producing defects and impurities in graphene in a regulated way is likely to be central to these processes.”

“Our results will have ramifications in economically and socially important areas, and, perhaps, could ultimately benefit the environment, if techniques for refining graphene can be optimized,” says Krasheninnikov. “Without the computational resources PRACE granted, however, this project would have been impossible.”

The scientist has recently applied for an ongoing collaboration with PRACE, which aims to consider further interactions between beams of energetic particles and graphene. These could further contribute towards the creation of bespoke, functionally structured nanomaterials fit for the future.

**Project title:** Effects of irradiation on nanostructures from first principles simulations  
**Project leader:** Dr. Arkady Krasheninnikov, Docent (Adjunct Professor) at the University of Helsinki  
**Project details:** This project was awarded 10,000,000 core hours on CURIE @ GENCI@CEA, France
Analysing cloud behaviours through HPC modelling

Clouds are dynamic structures, which interact with the air around them. However, analysing these processes is difficult for scientists, as they often occur at great height, defying easy observation. To understand their unusual physics, Italian researchers have used a detailed computer model, exploiting PRACE resources.

Although ‘cloud computing’ is now part of the technological mainstream, computing clouds requires highly specialised assets. Provided with a year of access to PRACE’s French CURIE supercomputer, an Italian team of researchers based at the Politecnico di Torino, Italy, sought to better understand what occurs within their nebulous, ethereal forms. Conducted between 2012 and 2013, the project was headed by Daniela Tordella, a professor of fluid dynamics in the university’s Department of Mechanical and Aerospace Engineering.

“We simulated some of the phenomena which occur inside clouds, using a model which replicates an area of about six metres by three metres by three metres,” she recalls. “This is, of course, only a tiny fraction of a cloud’s volume. However, successfully analysing what occurred within it necessitated one year of tests that relied on one of the most powerful computers in Europe.” Working alongside Tordella were members of the institution’s Philofluid Research Group, http://www.polito.it/philofluid, a collective that seeks to examine subjects including hypersonic jets and hydrodynamic stability. These interests fall within the discipline of fluid dynamics, a field seeking to explore the motion of liquids and gases. Because of their extremely varied, sometimes chaotic properties, scientists regard clouds as ‘turbulent’ environments for fluids, which function in physically complicated ways.

“This was our group’s first experience of a Tier-0 PRACE project. It was very positive, from the submission process onwards,” says Tordella. “The programme was clearly delineated, which was extremely helpful, and we were also able to fully explain the basic rationale for our research. The reviewers who assessed our proposal were highly scrupulous, and truly understood the science we presented. If there were any ambiguities, our group was permitted to clarify them. This was greatly beneficial and helped to resolve any misconceptions before a final decision had been reached.”

With approval came an allocation granting close to 30 million core hours on CURIE inside the 4th PRACE Call, which enabled the group to realise their plans. “We were able to witness the fluid dynamics of clouds at small scales, and also grasp how water vapour moves dynamically inside typical structures,” says Tordella. The group’s simulations looked at a process called turbulent mixing, which influences interactions between stratified flows of liquids and gases. Through considering these relationships, the researchers were able to obtain new insights on the causes of more overt phenomena, like water vapour transport. Particular attention was paid to the cloud/clean air interface - a region in which the cloud meets the surrounding sky. “Both top and bottom aspects of the cloud interface were studied,” says Tordella. “To model them, we used momentum and energy equations, and considered two different types of conditions – stable and unstable.”

“Clouds are very complex,” says Tordella, “but after analysing the simulations, we were able to formulate a number of novel principles which help to understand them. These include the ways in which energy and temperature interact around the periphery of clouds. For example, our results showed that a lot of kinetic energy...”

(Above) Visualization of the passive scalar field transported in two-dimensional and three-dimensional turbulent shear-less mixing generated by the interaction of two isotropic turbulent flows with different kinetic energy. The higher energy turbulent flow is on the left. The scalar is initially introduced only in the lower energy flow. The three sets of images represent the passive scalar concentration after 1, 5 and 10 initial eddy turnover times.
Overall objectives are discrete and explicit. Can help to ensure individual responsibilities and roles may become vague, PRACE’s cooperation in orienting their work can be very refreshing. Whereas in academic contexts, researchers coming from a university environment, the assistance PRACE can provide is critical to the collective future of research. For researchers entering the workplace, “one of the masters students who collaborated on the project has now obtained a very rewarding job post graduation, and another has successfully continued his research at PhD level.”

“We used 99 percent of our designated CURIE time,” Tordella states. “Typically, it’s not easy to maximise use of resources on HPC projects. Difficulties often arise, which may require modifications to important settings like time evolution parameters. However, user support provided by TGCC in Paris (where CURIE is located) was extremely responsive, helping us to overcome any issues when they occurred, which maximised usage of our allocation. Accessing the system was also easy, because we could connect to CURIE via desktop PCs located in different offices.”

“PRACE is a truly European research infrastructure, and from 2010-2015, four countries (France, Germany, Italy and Spain), EC and PRACE’s other members have invested around €500m of funding into it. How these resources are used, and made available to researchers, is critical to the collective future of research within the territory,” says Tordella. A notable benefit of PRACE in this regard, she perceives, is that it’s organised so that a clear focus is placed on important scientific questions. “Once initiated, the investigation proceeds in a very fluid way, and maintains fidelity to its initial objectives. For researchers coming from a university environment, the assistance PRACE can provide in orienting their work can be very refreshing,” she says. Whereas in academic contexts, individual roles may become vague, PRACE’s cooperation can help to ensure individual responsibilities and overall objectives are discrete and explicit.

Studying clouds has also provided a boost to the careers of junior researchers. “Many industries are beginning to use HPC resources extensively, so this type of experience can be invaluable when graduates enter the workplace,” reminds Tordella. “One of the masters students who collaborated on the project has now obtained a very rewarding job post graduation, and another has successfully continued his research at PhD level.”

Despite gleaning some exciting insights, the principles uncovered by the researchers may only hint at the full complexity of larger cloud systems. “I’ve submitted a new PRACE proposal, and we recently received the review report. The response was largely positive, so we’re hoping to obtain a further allocation,” reveals Tordella. “Within the remit of this project, we couldn’t study the formation of rain droplets, which is a very intricate physical and chemical process. However, we’re seeking to undertake future collaborations with scientists who can assist us in this analysis, from Imperial College London, the Max Planck Institute and the University of Warsaw. Supported by HPC services from PRACE, we hope this could form the basis of a further trans-European project. An additional dimension of this could involve collaborations with experts in telecommunications, since radar and satellites can also be used to monitor clouds.”

Project title: Fluid turbulence: self and passive scalar diffusion. Application to stably stratified flows
Project leader: Prof. Daniela Tordella, Associate Professor at the Politecnico di Torino
Project details: This project was awarded 2,440,500 core hours on CURIE Fat Nodes (FN) and 536,850 on CURIE Thin Nodes (TN), CURIE @ GENCI@CEA, France
Harnessing European HPC to improve nanomedicines

Drugs can be delivered to specific areas of the body and benignly dispensed, using nanomedicines, and mesoporous silica is a material which possesses the properties to fulfil this role. To enhance its utility and answer fundamental scientific questions, Italian scientists have been analysing how biological agents interact with it at molecular level.

Analysis has been undertaken to determine how the drug moves within the pores, and how easily it can be washed out the mesoporous silica by the body fluids

“You can transport a drug by storing it in holes within certain materials,” explains Professor Piero Ugliengo of the University of Torino. One of these is mesoporous silica – a substance containing evenly spaced periodic voids into which medicinal molecules can be inserted. Providing spaces of between two nanometres to fifty nanometres in diameter, this class of silica can help protect and deliver several types of drug, including ibuprofen. “Analysis has been undertaken to determine how the drug moves within the pores, and how easily it can be washed out the mesoporous silica by the body fluids,” says Ugliengo. “Typically, these studies have been facilitated by experimental techniques like NMR (nuclear magnetic resonance spectroscopy), which help to illustrate the compound’s mobility.” Simultaneously biodegradable and biocompatible, silica’s medicinal potential is widely recognised.

However, little is known about the atomistic mechanisms that actually hold drugs in place within these minute, silica cages. “The walls of these molecular vessels are rather complicated. They’re basically amorphous,” explains Ugliengo. “A number of active sites, called silanol groups, exist on their surface at molecular level. Chemically, these help to form a hydrogen bond between the silica and the ‘passenger’ molecules that are the active clinical agents. This is basic chemistry, and fairly straightforward. But an important aspect of this relationship, and a
SUCCESS STORIES

topic of hot debate within the physics community, is the role of dispersion interactions, or London forces, and assessing how ‘free’ the confined molecules actually are”.

Together with a number of associates, including Roberto Dovesi (in charge of the CRYSTAL development and implementation on HPC machines), Massimo Delle Piane, Marta Corno and Alfonso Pedone of the Modena and Reggio Emilia University, Ugliengo has led a one-year study to explore this phenomenon. Titled ‘Mesoporous silica for drug delivery: a quantum mechanical simulation’, the investigation utilised the impressive processing power of the SuperMUC facility. The installation contains one of Europe’s fastest supercomputers, and is located in the Leibniz Supercomputing Centre near Munich.

“Thanks to the approval of PRACE, we were able to increase the size and complexity of our pre-existing model. The improved, more elaborate version enabled us to replicate real-life conditions and study a commonly used drug, the anti-inflammatory medicine ibuprofen”

Using quantum mechanical methods, the team initially began their work in the field independently, by undertaking small-scale HPC simulations on their own systems. “Thanks to the approval of PRACE, we were able to increase the size and complexity of our pre-existing model,” reports Ugliengo. “The improved, more elaborate version enabled us to replicate real-life conditions and study a commonly used drug, the anti-inflammatory medicine ibuprofen. The capacity of the model was actually enlarged to between 900-1000 atoms, which is currently the state of the art for ab initio simulations of this kind. One important part of our analysis consisted of docking an ibuprofen molecule at six internal walls of the pores. Thanks to recent developments in density functional theory, we were able to gain a far better understanding of specific interactions here. The generous amount of access granted by PRACE on SuperMUC – around 20 million hours – meant that we could fully explore this approach, and obtained some unprecedented, and highly detailed insights. We think these are very significant developments.”

Using CRYSTAL code as a simulation tool originally co-authored by the group of Professor Roberto Dovesi at Torino University, the researchers were able to assess the trajectory of implanted drug molecules and where they ultimately became embedded within the silica structure. The adsorption of ibuprofen is exergonic due to hydrogen bond and dispersive interactions with the wall surface. These interactions are large enough to cause significant deformation of the pore walls, which need to adapt in order to accommodate the medicine. This is at variance with respect to other oxides, like MgO, which are much more rigid upon molecule adsorption. “The team were actually able to study the attachment all the way up to the mono-layer, which occurs when a void created by a pore has been completely filled by the guest ibuprofen molecule,” says Ugliengo. “Crucially, we were also able to predict both the vibrational spectrum of the molecule as well as its NMR spectrum (the latter by using Quantum Espresso code developed at SISSA in Trieste), as a result of perturbation at the silica walls. This was a valuable observation, because we could compare our simulation against real-world experiments. The comparison revealed a significant
correspondence between them. This validated the data we obtained from our models.”

“One of the major issues we wanted to consider was whether the interaction energy between the drug and silica is partly coverage dependent. It was unknown whether this would increase or decrease, dependent on the number of ibuprofen molecules being inserted,” says Ugliengo. “Surprisingly, we found that their adsorption is only mildly co-dependent, and that each site is almost equivalent. Every adsorption event occurs, and behaves, almost independently of the others when dispersion interactions are not taken into account in a quasi Langmuirian fashion. Even though ibuprofen is not a simple molecule, and the silica surface is not at all flat and rigid, these fundamental principles still apply.” A later stage of the project, carried out using the open source CP2K code, examined the stability of silica under a ‘high load’ of ibuprofen at room temperature. This enabled a consideration of its likely behaviour and mobility within the pores. Encouragingly, the tests showed that in these conditions, molecules obtained an additional degree of rotational mobility, but retained their bonds with the silica surface, close to their original positions. Their stability and, hence, utility were retained, rendering them excellent platforms for future nanomedicines.

“The opportunities extended to us by PRACE permitted a real breakthrough to occur, both in terms of results and methodology,” concludes Ugliengo. “This is because, crucially, the availability of vast HPC resources compelled us to fine-tune the CRYSTAL code, and prove its scalability in larger environments. This is also a great achievement.” For other physico-chemical disciplines, the Italian group’s progress could provide a valuable boost. By demonstrating that the density functional theory approach is applicable to larger systems, the project may act as a paradigm, illustrating the effectiveness of tools that could solve conundrums in related fields. Moreover, because the insights gleaned suggest ways of modulating the relationship between drugs and their carrier, the project could also prove a vital milestone in the conception of practical nanomedicines.

**Project title:** Mesoporous silica for drug delivery: a quantum mechanical simulation  
**Project leader:** Prof. Piero Ugliengo, Associate Professor at the Università di Torino  
**Project details:** This project was awarded 20,000,000 core hours on SuperMUC @ GCS@LRZ
Star formation modelling: the next generation

Star formation is integral to cosmology and astrophysics, their spectacular lifecycle both subtle and complex, and spanning aeons. To comprehensively understand this process, scientists have accessed PRACE resources to create computer simulations offering unprecedented levels of detail.

Although space is often considered a dark, static void, within it, kinetic physical forces are constantly at work. Several of these, scientists suggest, regulate the formation of stars. The elements that help to create them ultimately affect several other important features of galaxies, because stars are a dominant energy source, and also control galactic chemical enrichment. But understanding these interactions poses significant challenges. The duration of a star’s lifecycle – from birth until its spectacular demise as a supernova – stretches across millions of years. Moreover, numerous physical factors need to be considered, including magnetic fields, gravity and supersonic turbulence.

“Trying to understand star formation using limited computer simulations, which might exclude some of these agents, is a methodology that has fundamental drawbacks,” explains Paolo Padoan, a professor at the Institute of Cosmos Sciences at the University of Barcelona (ICCUB). “Due to their complexity, star simulations are often conducted at three different scales. They may look at the genesis of individual stars, the molecular clouds that form them, or at an even vaster scale, such as a galaxy, to try and understand their evolution. However, the scales are somewhat estranged in terms of fidelity. Using most contemporary techniques, if you attempted to model a galaxy, for example, the stars within that simulation would lose resolution. Conversely, a model of an individual star could reveal significant detail, but the simulation might omit forces present around it. Unless all of these factors are assessed, in sufficient detail, you’re not modelling star formation correctly”.

To develop a rigorous alternative, Padoan requested a PRACE allocation. “I wanted to reconcile the three different scales,” he says. “This approach to simulation is numerically gigantic, in terms of the data it creates. So, inevitably, it entails some compromise. It doesn’t look at a galaxy, at its largest scale, but allows us to replicate a section of it. This is sufficient to consider some of the more expansive processes at work. So, by using such
In association with colleagues based at the Universities of Copenhagen and Helsinki, Padoan was able to create simulations on far greater scales than orthodox simulations, using a version of a code called Ramses. The model contained an area 1000 parsecs by 1000 parsecs (a parsec is approximately equivalent to 3.25 light years). “The largest, giant molecular clouds are around 10-50 parsecs in size,” explains Padoan. “To properly analyse them, we’ve refined the Ramses code by adding new modules to it, and improving overall performance to enhance scalability. Because of this, we could replicate several such clouds within the simulation. Several stellar clusters could potentially form within each cloud, and each of these might contain hundreds of stars. So, overall, we’re considering thousands of new stars.”

Allocated 25 million core hours of access to SuperMUC, sited at the Leibniz Supercomputing Centre, the researchers were able to produce around 20 terabytes of data, which will be interpreted by them for a year. Initial analysis of their findings enabled the scientists to observe more clearly the ‘lifecycle’ of different stars, which interact with interstellar space, also referred to as the ‘interstellar medium’. Known as the ‘galactic fountain’, this phenomenon is a form of recycling, and has often been observed in disc-shaped galaxies. As massive stars explode in supernova events, they propel hot gas out of the disc into its surrounding halo, where it cools and condenses. This gas eventually falls back into the originating disc galaxy, contributing to the formation of new stars within it. “Stars have an important role in the diffraction of different types of gases – cold neutral gas, warm neutral gas and hot ionised gas – in the interstellar medium around them,” explains Padoan. “These dynamic thermal processes may also help form new stars.”

“In this project, we’ve been able to carry out the first simulations which comprehensively describe the operations of the galactic fountain, whilst simultaneously resolving the formation of specific stars. The resources we were allocated permitted us to consider scales of unprecedented magnitude,” reports Padoan. “We can now resolve isolated molecular clouds, their internal structures and, within them, the collapse of individual stars. Overall, we’ve shown that a process of self regulation is at work.”

Another major aim of the venture, Padoan continues, was to determine whether feedback from supernovae explosions could explain the observed velocity and dispersion of cold gas. “We know that in molecular clouds, where stars are formed, cloud gas is highly turbulent. Our simulations demonstrated that numerous supernovae explosions were collectively responsible for these velocities, and the pervasive turbulence that has been observed by scientists. These phenomena have actually been caused by the overlapping of supernovae remnants, over long periods of time”.

“Using the simulation has enabled us to verify the conclusions of other scientists,” reveals Padoan. “Our findings aren’t necessarily new discoveries, but nevertheless corroborate the accuracy of our model. Essentially, our simulations have convincingly shown that supernovae feedback is a primary agent that modulates forces contributing to star formations. In fact, the experiments indicate that, when certain densities or amounts of gas are present in the interstellar medium, star formation rates are correspondingly influenced”.

HPC resources are also essential to analyse the vast amounts of data generated by the project, which will also be offered online to other researchers. Padoan’s group currently have plans for several follow-up simulations, which are similarly dependent on powerful IT assets. One of their latest simulations is incredibly long, covering millions of years, and will also produce large volumes of information-rich data for the researchers to review. What renders this particular model state of the art is that it monitors not only one stellar lifecycle, but also successive eras of stars, all of which are precipitated by supernovae and created within the simulation. “By viewing stars in this way, we’re taking things to the next level,” says Padoan. The subjects of the model will eventually become totally self contained, and subject to the feedback created by exploding stars – just as in nature.”

**Project title:** Extreme Star-Formation Modeling: From the Galactic Fountain to Single Stars in One Run  
**Project leader:** Prof. Paolo Padoan from Catalan Institute for Research and Advanced Studies (ICREA) and University of Barcelona  
**Project details:** This project was awarded 16,875,000 core hours on SuperMUC @ GCS@LRZ
Simulating turbulent airflows to inform energy-saving engine designs and pioneer surgical technologies

Combustion engines contain passages through which gases are channelled. By developing tools to accurately simulate these flows, scientists can consider ways of enhancing their efficiency. Application of this methodology to the human nose can also provide insights on the effectiveness of surgical procedures.

Energy demands, and increasing CO₂ emissions are widely proclaimed by scientists as some of the largest challenges facing society today. In response, the German federal and state government has funded an inter-disciplinary research initiative, “Tailor-Made Fuels from Biomass”. Its objective is to effectively obtain energy from renewable, organic sources, which are typically combusted to generate power. Developing efficient, clean engines to facilitate this process is therefore an integral part of its work.

Important foundational work to help stimulate the design of new engines was recently undertaken at the Institute of Aerodynamics in RWTH Aachen University, Germany. Titled “Direct Numerical Simulation of the Flow in an Internal Combustion Engine”, the primary objectives of the project were to develop and apply simulations that could examine the flow field of gases within an engine in real conditions. Undertaken between May 2012 and May 2013, the project team was granted PRACE access to HERMIT, a CRAY XE6 supercomputer sited at the High Performance Computing Centre, Stuttgart.

A formidable initial challenge faced by the scientists was to develop a fast, accurate algorithm that would underpin their simulations. “Our main objective here was to devise a general solution, applicable to different geometries. This is because, within an engine, various types of cylinder are essential components,” says Professor Wolfgang Schröder. Because the mechanical environment simulated was complex, replicating the intake and compression strokes of a four-valve, single cylinder system, running at typical speed, testing it required intensive computations. Schröder, an expert in fluid dynamics who also led the project, elaborates that “introducing a new algorithm can introduce a higher rate of conversion, which improves the speed of calculations.”

Initially, the team performed high-resolution, large eddy simulations (LES) to obtain basic data on turbulent structures, scales and intensities. Following this phase, they planned to conduct more detailed tests and, ultimately, to show the mixing within the engine’s turbulent flow. They theorised that such processes interacted with the engine’s flame, where energy-releasing combustion occurs. If flows influence flame behaviours, adjusting properties such as their areas, propagation speeds and stability can impact on the overall performance of engines.

“When scientists want to investigate complex physical behaviours using simulations, they often look at techniques which can offer discrete solutions. These are frequently based on certain types of structured mesh,” says Schröder. By separating three-dimensional space into discrete units, or blocks, it becomes far easier to predict and trace the trajectories of gases within a simulated environment. “One common example is a pipe-shaped mesh, which is often applied to cylinders like those we’ve been studying. However, because we were looking at moving systems – involving pistons and valves – the complex geometry made this approach difficult to use.”

The team developed a mesh generator that can be applied to the unique nasal cavities of different patients
Instead, the researchers decided to exploit an alternative framework – a Cartesian mesh. “This is markedly different from a cylindrical mesh. In fact, it resembles a number of stacked, equally sized Lego bricks,” illustrates Schröder. Because the mesh calculates boundaries in a mathematically efficient way, rather than using prescribed or defined settings, it retains high fidelity. Described as “simple, but very flexible, and rather fast”, the system was successfully applied to various geometries. Using multiple-level functions, the LES simulations were able to record flows within different engine components, including cylinder heads, engine heads, valves and pistons. “The code is currently experimental, but could potentially be made commercially available in five to ten years time,” suggests Schröder. “Our experiments have shown that it can deliver improvements in computation times, ranging from 10 to 100 per cent”.

“The results we’ve obtained, with PRACE’s assistance, have formed an important foundation for future developments in the field of turbulent airflow research”

Unexpected algorithmic problems encountered whilst preparing high-resolution direct numerical simulations prevented the team from obtaining all of the data they had intended within their PRACE allocation. However, the researchers were able to use the latter part of their period of access to HERMIT to progress on a related study endorsed by the German Research Foundation. The project, ‘Rhinomodel’, applies similar principles to flow studies of engines, and attempts to examine the movement of air through the human nasal cavity.

“This project is based around the concept of computer aided surgery,” says Schröder. “The idea is to develop technology which can be used by physicians to assess the effectiveness of surgical procedures before they’re performed. Widening of the nasal cavity is an operation that is often carried out if a patient has difficulties inhaling. The object of this is to reduce their loss of air and improve oxygen flow within the nose. Our simulations could help doctors to safely understand the effects of potential modifications to the nose on airflow, and appreciate related factors such as moisturisation.”

To meet this challenge, the team developed a mesh generator that can be applied to the unique nasal cavities of different patients. “Over the past few years, we’ve been able to pioneer a system which, instead of taking days or weeks, produces a usable framework within a couple of seconds. In hospitals, this would be based on computerised tomography (CT) scans. Algorithms would then process this information, generating data which can be used to understand the new airflow,” comments Schröder. Number-crunching challenges must be overcome before such a system is deployed in hospitals, however. Although the mesh itself can be rapidly created, computations can still take up to a day complete. To hasten this important stage of the process, refined algorithms, and the creation of high-resolution simulations fit for clinical purposes must be realised.

“The results we’ve obtained, with PRACE’s assistance, have formed an important foundation for future developments in the field of turbulent airflow research,” says Schröder. “In the Rhinomodel and biomass projects, the use of HERMIT was absolutely essential to developing models within reasonable timescales, which we hope will be practically applied in the future. We also intend to use additional HPC resources imminently, in order to complete our analysis of turbulent engine flows. RWTH has a significant need for ongoing access to these facilities, not only to complete our current work looking at combustion of biomass, but also to make progress in related fields. These include controlling combustion instabilities, and several aeroacoustic investigations, such as considering how to reduce airframe noise”.

**Project title:** Direct Numerical Simulation of the Flow in an Internal Combustion Engine  
**Project leader:** Prof. Dr.-Ing. Wolfgang Schröder at RWTH Aachen University  
**Project details:** This project was awarded 72,700,000 core hours on Hermit @ GCS@HLRS, Germany
Creating end-user systems to calculate real world physical phenomena

Mathematically calculating the behaviour of physical phenomena using equations requires scientists to consider multiple variables. Computers can assist them, but, for non-initiates, this method may prove challenging. To aid potential users, researchers accessed PRACE facilities to realise a new system that automatically completes several parts of the simulation process.

There's invariably more to the physical world than meets the eye. For example, the way in which water flows is often perceived as so natural, that it's easy for observers to overlook less conspicuous factors that determine its properties. For scientists, however, all of these considerations must be scrutinised. To accurately obtain a mathematical understanding of a physical subject, various parameters influencing it, such as temperature and pressure, must be comprehensively and precisely calculated.

Partial differential equations (PDEs) are a common tool employed to solve physical problems, and can accommodate these different factors. Unlike other types of equation, they allow scientists to work out how several continuous, changing variables affect others, and hence contribute towards the result of the equation. Higher temperatures, for example, might increase the elasticity of a particular material. This method is applicable to various subjects, including sound, heat, electrostatics and even the field of quantum mechanics.

Between May 2012 and April 2013, a French team located in Nice, Paris and Strasbourg embarked on a project designed to help non-specialists execute PDEs. Titled “High Performance Computing with Generic Solvers for Partial Differential Equations (HPC-PDE)”, the researchers connected to the Paris-based CURIE supercomputer asset, which was used to test and continuously enhance new software designed to streamline the complex equations.

“Our project initially concentrated on an open source software programme, FreeFem++,” explains Professor Frederic Nataf, a participant in the project from the Laboratoire Jacques-Louis Lions, Paris. “It’s often used globally for teaching purposes, and also by companies who need to conduct numerical simulations. If they use a computer for this purpose, however, it creates significant demand for CPU time.” The programme possesses a fundamental benefit which was highly attractive to the researchers – it is fully scalable, and can hence be run on desktop PCs, as well as HPC clusters, thus making it an ideal foundation for their work. “We wanted to enhance this software, and enable end users to solve large scale PDE easily, without worrying about difficult parallel implementation problems,” adds Nataf.

To improve the software’s performance, the group used CURIE to explore how domain decomposition methods could help it to solve equations. The principle behind this approach is essentially ‘divide and conquer’ – that is, to split a difficult problem into smaller problems, or ‘domains’, which can be independently undertaken and, once completed, are jointly co-ordinated to produce solutions. This concept has proven especially apt for parallel computing, in which different calculations are completed...
within different processors on the same machine, or across different computers.

“We intended to design efficient domain decomposition solvers for various problems,” explains Nataf. “These could include, for example, how solid objects deform, and become internally stressed due to prescribed loading conditions. If objects are made of materials with different properties, like steel and rubber, traditional IT tools tend to perform poorly, whilst computing them – creating a clear need for an improved methodology”.

“Our ultimate goal was to ensure that an end user, who might not possess specific knowledge of this area, which is very technical, could nevertheless use the system effectively,” says Nataf. “These operators might include physicists or engineers, who we hoped would be able to run the software via parallel machines. This particular aspect of our work was highly original, as most PRACE projects are actually aimed at specialists.”

On many contemporary systems, he says, domain decomposition methods are non-scalable. This means that when a problem is split, increasing the number of processes and computer subdomains, it actually becomes more difficult for a machine to compute. “This is very common if ‘one level’ domain decomposition methods are used” he comments. “However, it is possible to address this issue, by using a modified ‘two level’ approach. This alternative functions either by solving an auxiliary problem, known as a ‘coarse space problem’ that is constructed around geometric considerations, or by solving other local problems”.

“Using CURIE, we carried out various simulations in solid mechanics, which examined difficult problems with our new software” elaborates Nataf. “Part of these trials involved replicating a geometry corresponding to a solid object, and exploiting a mesh or grid to map it in 3D. This was used to numerically solve various equations. After the model is created, almost every subsequent stage of the process is automatic. Ultimately, you’ll generate a solution you can plot and visualise. Between defining the problem and obtaining a result, the software takes all the information entered into it (including the mesh), then builds an approximate mathematical model. This corresponds to building a large linear system across parallel machines, offering many, many cores.” Beginning their work on CURIE using a linear solver, which attempted to complete equations in chronological sequence, the group gradually introduced a series of improvements to their system. Following the addition of C++ code and incremental removal of any bugs which were encountered, the revised software is now more flexible, and fully compatible with parallel solving methods.

“CURIE enabled us to test different parallel numerical algorithms, and we’ve found this method extremely successful” Nataf reflects. “It can solve very large problems with billions of unknowns, using something like 8000 cores to realise a parallel computing methodology. The rendering time for equations is only around one or two minutes. Compared to other software, our system performs faster, and is extremely robust.” The software was also tested on the CEA supercomputer Titane, and the IDRIS HPC asset Babel, where it demonstrated what the researchers characterise as a ‘super linear speedup’. To improve ease of access, the software will be fully downloadable from the internet, and has recently been highlighted at SC’13 – an annual supercomputing conference. “The paper we submitted at this event was very well received” emphasises Nataf. “Out of 92 other texts in contention, ours was nominated for the best paper award by the technical program committee.”

The team’s initial PRACE collaboration was an unequivocal success. “Overall, the experience was quite straightforward” comments Pierre Jolivet, a PhD candidate at the Laboratoire Jacques-Louis Lions, who also contributed to the project. “Using large scale computers was a significant help for us, and both the technicians and offline staff who assisted our team were very responsive. Because of our access to HPC, we actually changed a lot of the software architecture as our work progressed. Processing at larger scales, computational simulation work can encounter bottlenecks which just aren’t present when you’re using less powerful platforms. Consequently, the opportunity to work with PRACE was extremely beneficial for our research. There are many exciting opportunities for applying HPC in this area, which we hope to continue working on with the organisation”.

**Project title:** High Performance Computing with Gener-ic Solvers for Partial Differential Equations (HPC-PDE)  
**Project leader:** Dr. Frederic Nataf, Senior scientist at CNRS  
**Project details:** This project was awarded 1,000,000 hours on CURIE @ GENCI@CEA, France
Investigating the structure of atmospheric turbulent flows

Turbulence and fog pose significant hazards for civil aviation. To understand the meteorological processes that create them, researchers have performed HPC simulations offering unprecedented detail. Their findings may help to inform safer practices within the aircraft industry and also establish a number of exciting scientific firsts.

Regardless of their technical virtuosity, many of our most advanced mechanical devices ultimately fail when faced with extreme weather. Because of aircraft’s susceptibility to these hostile conditions, passengers are regularly marooned in the no-man’s land of airport departure lounges. Such delays are often ascribed to “turbulence” or “fog”. Consequently, understanding the causes and propagation of these conditions is a scientific challenge that could offer practical benefits for jet-setters and airline companies alike.

Between March and November 2012, a team of researchers from Toulouse seized this opportunity, using a PRACE allocation to investigate specific types of turbulence that can jeopardise aircraft operations. To ensure that the project had the necessary computing, aeronautic and climate modelling expertise, the group was assembled from three local institutions. The project’s co-ordinator, Dr Roberto Paoli, was based at CERFACS (the European Centre for Research and Advanced Training in Scientific Computing), and associates drawn from Météo France (the French national meteorological service) and the University of Toulouse’s Laboratoire d’Aérologie.

“Our fundamental concept was to use PRACE’s computational resources to examine the problem of stratified atmospheric turbulence and its connection to the aviation sector. Specifically, turbulence located in the upper troposphere to lower stratosphere at altitudes between ten and eleven kilometres, and turbulence developing in the vicinity of airport taxiways and runaways,” explains Paoli. Because these are regions which aircraft regularly navigate or taxi during ground operations, such conditions can adversely affect their performance and safety procedures. “These events are not only dangerous, but also have an impact on the efficiency of flight operations due to re-routing and delays in takeoffs and landings.” Unlike convective turbulence – which is often linked to other extreme weather such as thunderstorms, downdrafts or lightning – stratified turbulence has less spectacular harbingers, making it harder to predict. Its manifestations include clear-air turbulence (triggered by wind shear, mountain waves and the jet stream), and heavy fog, which can perilously decrease visibility.

“It’s also important to remember that these forces also have an important environmental significance,” notes Paoli. “Turbulence controls the dispersion of gaseous and particulate emissions from aircraft engines, and so influences the composition of our atmosphere. As air traffic volumes continue to grow, this impact will eventually become increasingly more important”.

The group considered three different manifestations of stratified turbulence. Their first objective was to obtain a general understanding of turbulent structures, followed by experiments that would examine more specific phenomena in detail. These latter phases of the project sought to examine turbulence generated by mountain waves, and examine the contribution of turbulence to radiative fog.

Using CURIE, a French Tier-0 asset located near Paris and operated by CEA, the researchers were able to conduct simulations that achieved impressive scales of resolution. “If you want to capture features of turbulence accurately, you need to employ models which offer sufficient detail. In terms of computational resources, this requires many, many processors. Consequently, we couldn’t host these experiments on our own clusters. The project demanded a supercomputer” says Paoli. The researchers carried out three-dimensional Direct Numerical Simulations (DNS) and Long-range Eddy Simulations (LES), which used a code named Méso-NH, developed by Météo France. To accurately capture complex turbulent behaviours, an expansive simulation area, extending for four kilometres in all directions, was employed.

“Turbulence controls the dispersion of gaseous and particulate emissions from aircraft engines, and so influences the composition of our atmosphere”
A three-dimensional grid was used to monitor processes occurring within this virtual cube, with sampling points spaced at two metre intervals. This meant that, in total, the model contained 8 billion such grid points.

Initial simulations enabled the team, as they had planned, to scrutinise general features of atmospheric turbulence. “We actually carried out the first LES which characterises atmospheric turbulence at sub-kilometre scales, and also demonstrated how this phenomena influences the dispersal of aircraft emissions,” explains Paoli. The simulations revealed that turbulence is not vertically aligned, but organised in large horizontal eddies, or ‘pancakes’. As they develop, such formations lead to the creation of local shear layers, which gradually separate and transfer energy to smaller scales.

The group’s secondary objective – to analyse turbulence generated by mountain waves – gleaned less data than anticipated, but nonetheless established several helpful precedents. “When wind heats a high mountain, it creates ‘rollers’ which break up and generate fine scale turbulence or fluctuations. These can propagate outwards to such an extent that they eventually become a hazard for aeroplanes,” says Paoli. Due to the complexities of modelling mountains and their surrounds, however, the team found that their Meso-NH based framework was ultimately too coarse for the task. “This experience will however prove very useful to our peers,” suggests Paoli. “Before our experiment, nobody could have anticipated the difficulties we encountered. We learnt that to understand these processes, grid resolution needs to be increased to a level which is likely unattainable for the present generation of supercomputers. Because of this, the progress we’ve made can help to define, and improve future modelling strategies”.

Meso-NH proved far more apt for analysing fog, the third subject proposed by the researchers. “Fog begins as a surface problem caused by the condensation of water vapour at ground level, but can spread to higher altitudes,” says Paoli. To analyse this gradual process, the Toulouse-based team used Charles de Gaulle airport in Paris as the basis for their HPC model. By comparing one simulation that included real airport structures like control towers and terminals with another in which all buildings were removed, the scientists were able to discern that local architecture influences fog propagation. “We found that the presence of buildings increases turbulence due to wind,” states Paoli. “This initially delays the formation and spread of fog to an extent. But, once it forms and thickens, this turbulence actually increases the vertical development of the fog, causing it to rise higher.”

“The experience of collaborating with PRACE was excellent,” reports Paoli. “Interaction with central management, with whom we established the project, was great. Operationally, we faced an initial challenge, in that we had to modify our code to ensure its compatibility with CURIE at the start of the project. Fortunately, the technical staff based at the HPC centre offered us considerable support. Once the code was installed and established, the performance of the supercomputer was extremely impressive. We were able to use all of the 21 million CPU hours we were granted during this project, and will be applying for a further allocation this year.”

**Project title:** Large-eddy simulations of stratified atmospheric turbulent flows with Meso-NH: application to safety in meteorology and environmental impact of aviation

**Project leader:** Dr. Roberto Paoli, Research scientist CERFACS

**Project details:** This project was awarded 21.5 million core hours on CURIE @ GENCI@CEA, France
Understanding how collisionless shocks behave within plasma is a fundamental scientific question. Exploiting the power of HPC to examine these phenomena has enabled scientists to create detailed models of them, revealing new facets of their behaviour. Findings from the study promise to deliver a significant theoretical legacy, and may also contribute to the development of new medicinal therapies.

Luis Silva, a professor of physics at the Instituto Superior Técnico (IST) in Lisbon, is a member of a group pursuing laser and plasma research. To assist their investigations, the team recently received a PRACE allocation to utilise the JUQUEEN Tier-0 system, located in Jülich, Germany, between November 2012 and April 2013. In addition to staff at IST, Professor Warren Mori from UCLA in the United States and Dr Raoul Trines at the Rutherford Appleton Laboratory in the UK also collaborated in the venture. “Our joint aim in this project, titled “Shock Acceleration in the Laboratory with Ultraintense Lasers”, was to look at the formation of shockwave structures which resemble a sonic boom but actually occur within a plasma,” he explains.

Gases transform into plasmas when heat, or other energies cause atoms to release some of their electrons. In this state, the residual atoms retain a positive charge, whilst the separated electrons are liberated to move freely – a condition known as ionisation. When sufficient atoms are ionised and significantly affect the electrical properties of the gas, it is deemed to have become plasma.

“A certain type of event involving plasma, called a ‘collisionless shock’, can be stimulated under controlled conditions,” says Silva. “These phenomena share some similarities to a shock wave - the blasts produced by supersonic aircraft that propagate in the air. This is caused when the vehicle travels at speeds higher than sound, causing a perturbation and non-linear shockwave.”

Collisionless shocks occur when particles emit and absorb collective excitations, or plasma waves, which energise them. These interactions frequently occur at cosmic scales and, scientists theorise, could help to explain how supernovae interact with the matter existing in space between star systems, known as the interstellar medium. Indeed, plasma – the so-called ‘fourth state of matter’ – constitutes perhaps 99 percent of the visible universe, illustrating both its ubiquity and the scientific importance of comprehending it.

Within extreme conditions, Silva details, the processes that generate collisionless shocks “are highly non-linear”. Hence, the only way to analyse them is via computationally intensive, rigorous models. “Our simulations tried to follow the dynamics of individual protons, electrons and positrons evolving in such a system. This is why PRACE became involved in our research, because we’re using a specific type of numerical model that, although it was created in the sixties, is highly scaleable. Because of this attribute, it’s very apt for utilisation on a large machine.”

“To achieve an impact in the field, our work has actually pursued two parallel, but interrelated strands, over the past twenty years,” continues Silva. “One seeks to improve the modelling code we use – to upgrade, and improve the performance of the algorithm. The other is to ensure it can be used effectively, on new generations of machines.” Employing a state-of-the-art code used for plasma simulations known as OSIRIS, and co-developed by IST, adapting these tools to take advantage of the
powerful resources offered by PRACE was an important early part of the research. “It’s vital for us to check if we can run and compile the code on different HPC devices, because, despite possessing a number of standardised features, each machine will have different types of interconnects, networks and processors. Consequently, we may spend up to a month refining our code so that, dependent on the specifics of the latest HPC hardware available to us, overall performance can be maximised. It’s rather like racing a Formula 1 car. To ensure it’s fast and reliable, you need to fine-tune it to make sure it performs optimally on a specific track.”

One of the most important research questions addressed by the group is the hypothesis that cosmic rays are accelerated due to non-collisional shocks. Hitherto, assessments of this notion have been limited to the theoretic realm. “What we’ve been trying to achieve is modelling these relationships, and including all the physics from first principles onwards,” Silva says. “We wanted to recreate actual physical conditions as closely as possible, and identify the catalysts which generate shockwaves, using lasers or particle beams. Once discovered, we hoped to learn of ways to artificially accelerate particles, in the same way as cosmic rays.” The team exploited 2D and 3D particle-in-cell (PIC) simulations, which demonstrated both the formation of collisionless shocks, and particle acceleration stimulated by shocks in a laboratory context.

“This was an exciting spin-off from our main study. Recently, considerable efforts have been directed towards understanding how lasers can accelerate protons. The main driver behind this is the need to build compact proton accelerators, which could, for example, prove helpful for the treatment deep-seated cancer tumours. Lately, there has been a considerable pursuit of this objective in several facilities. If this technique can be harnessed, it could become integral to new medical applications. To viably serve this function, the protons would need to be accelerated to energies close to 200MeV,” explains Silva.

The group’s findings indicate that, under certain conditions, collisional shockwaves can accelerate protons in potentially useful ways. According to their data, high-velocity plasma flows, driven by laser-plasma interactions, could generate strong magnetic fields that ultimately create the desired collisionless shock effect. Moreover, by modulating conditions such as laser polarity and plasma density, they also found that it was possible to control velocity and field structure of shocks. Another possible means of instigating shocks, using lasers to heat and create plasma to accelerate ions (thereby precipitating an electrostatic shock), was also proven viable. Encouragingly, these theoretical techniques could be practically realised, using current laser systems.

PRACE’s assistance, Silva reflects, considerably helped the project to realise its goals. “For researchers, in countries which don’t possess major HPC assets, the intervention of PRACE has been life-changing. Previously, we had to use machines in the US, which at times relegated us into a secondary position. With PRACE, we can actually take the lead, and develop projects independently. It’s a vital resource for those outside affluent western European nations that maintain their own HPC infrastructures. Thanks to the several grants we’ve received, facilitating access to some of Europe’s elite facilities, we’ve moved ahead and attained a leading position in this fascinating field.”

Project title: Shock Acceleration in the Laboratory with Ultraintense Lasers: from astrophysics to ion acceleration for medical applications
Project leader: Prof. Luis Silva, Professor at Instituto Superior Técnico
Project details: This project was awarded 37,000,000 core hours on JUQUEEN @ GCS@Jülich, Germany
**Q&A**

Interview with Robert-Jan Smits, Director-General, DG Research and Innovation, European Commission

- **Horizon 2020 will be the most open Framework Programme for Research and Innovation in the world. Can you elaborate on what this openness will entail?**

  **Robert-Jan Smits:** Indeed, Horizon 2020 is open to everyone. As more research and innovation is performed in international partner countries and the societal challenges we are facing are global, it is crucial that European researchers are able to work together with the best researchers and research centres worldwide.

- **How will Horizon 2020 address HPC?**

  **RJS:** High-performance computing has been recognised as a strategic and crucial asset for the EU’s innovation capacity. We have called on Member States, industry and the scientific communities to step up joint efforts to ensure European leadership in the supply and use of HPC systems and services. From our side we have planned numerous activities related to HPC in the current work programme for research infrastructures. And there are many more areas – beyond research infrastructures – ranging from micro-electronics to climate simulation, where HPC features as an essential component.

- **What is the role of ESFRI?**

  **RJS:** The mission of ESFRI is to support a coherent and strategy-led approach to policy-making with regard to research infrastructures in Europe, and to facilitate multilateral initiatives leading to the better use and development of research infrastructures, at EU and international level. The open access to high quality Research Infrastructures (e.g. in the area of HPC) supports and benchmarks the quality of the activities of European
scientists, and attracts and retains the best researchers from around the world. PRACE – one of the most successful ESFRI initiatives – is strategic for HPC in Europe. The high-end computing systems of PRACE provide access to advanced computing resources for scientists from across Europe.

The mission of PRACE is very much along the same lines: to develop the policies for HPC in Europe, and foster the establishment of a multilateral HPC ecosystem for science and research across Europe.

**How do you see the role of PRACE in supporting the goals of the European HPC strategy in Horizon 2020? What challenges do you see ahead?**

RJS: PRACE has already defined its central role in a European HPC strategy under the Seventh Framework Programme for Research and Technological Development (FP7). I expect PRACE to continue this leadership function under Horizon 2020. Certainly, there are challenges if you look around the globe and witness the rapid growth of the HPC capacities in Asia. Across Europe we have to ensure that the Member States follow up on their commitments concerning HPC, as expressed in the Council Conclusions of May 2013.

**How important is an association such as PRACE in supercomputing, in terms of ensuring European innovation and competitiveness in both academia and industry?**

RJS: PRACE has already demonstrated through its close relationship with industry (by allowing to more than 20 companies including SMEs to use its resources or assessing prototypes with suppliers) that it has a catalysing role both across Europe and in spearheading global HPC developments such as the operation of the most power-efficient HPC system. PRACE has also delivered more than 8 billion computing cycles to researchers enabling them to make fundamental contributions to global challenges ranging from cell biology to climate change. I expect PRACE to continue to be a focal point for scientific computing across Europe.

**How important is training delivered by Research Infrastructures across Europe and internationally?**

RJS: Academic and industrial usage of HPC and numerical simulation will grow only if Europe offers the dedicated training necessary to optimise the usage of the next generation of supercomputers. PRACE is involved in developing curricula to train the next generation of computational scientists, e.g. through its 6 PRACE Advanced Training Centres (PATCs). PRACE has also enlarged its international cooperation through the International Summer School on HPC Challenges in Computational Sciences by co-organising it with XSEDE (USA), RIKEN (Japan) and Compute Canada in 2014.

The work PRACE is doing in the area of training and related international cooperation is therefore truly exemplary. This activity is helping to structure HPC training efforts across Europe and, through the various summer-school actions, excellent global cooperation in this field has been established. These training efforts and curricula should lead to a broader awareness and more expertise in this crucial field so that in the end innovation is fostered through it.

**“PRACE has also delivered more than 8 billion computing cycles to researchers enabling them to make fundamental contributions to global challenges ranging from cell biology to climate change”**

**How do you see the future of PRACE on the research and innovation landscape in Europe?**

RJS: The sustainability of PRACE is a key issue – as it is for any ESFRI initiative. But PRACE is special in some ways as it requires constant renewal, unlike research infrastructures made of bricks and mortar. This constant renewal process – necessary to stay at the forefront of technology – is the basis for providing an HPC service to the European research and innovation community. This, in turn, enables them to do world-leading research. And this makes PRACE a key transverse component for the European research community.

In FP7, PRACE demonstrated its broad and very positive impact on the European R&I scene. To maintain and expand this impact, it is necessary that the various Member States concerned keep, and even go beyond, their commitments to provide world-class computing resources. For a Research Infrastructure like PRACE to continue to be successful, the explicit and concrete support of all Member States and their HPC centres or agencies is essential. Only in a joint and united effort will Europe be able to continue to provide the vitally needed HPC resources for its science and innovation communities.
PRACE supported projects on the rise

PRACE provides HPC resources to researchers from academia and industry through 2 complementary forms of access: Preparatory Access dedicated to code scaling and optimization and Project Access for large-scale, computationally intensive open research projects.

Since PRACE’s inception in 2010, PRACE Calls for Proposals for both Project Access (also referred to as Regular Access – RA) and Preparatory Access (PA) are more popular every year. While the Early Access Call for Proposals for Project Access (EAC) mid-2010 received 65 applications, the 7th Call in 2013 received 118 project proposals; in 3 years, the number of proposals almost doubled. Not only in terms of applications did the PRACE Calls do well over the years; starting with 1 machine in EAC, PRACE allocated 350 million core hours to 10 projects. The number of machines increased to 6 for the 4th Call and by the 7th Call 42 projects were accepted, receiving a total of 1.3 billion core hours; an almost 4-fold increase in allocated core hours over less than 4 years. As of the 5th Call, industrial projects became eligible for PRACE resources, under the Open R&D programme.

Although the number of core hours made available to PRACE Calls for Proposals steadily increases, demand still outnumbers supply by a factor of 3. The number of project applications increases, but also the number of core hours requested per project. Prof. Janka from the Max Planck Institute for Astrophysics in Garching, Germany, for instance, researches the birth mechanisms of supernovae. He received 97.8 million core hours on CURIE @ GENCI@CEA, France and 48.9 million core hours on SuperMUC @ GCS@LRZ, Germany through the 4th Call and the same allocation again under the 7th Call. This makes for a total award of close to 300 million core hours!
All applications to PRACE Calls for Proposals for Project Access are technically and scientifically reviewed and then prioritised on the basis of their scientific excellence: resources are awarded starting from the highest-ranked, down the list until the available resources run out or until there are no more projects that have passed the scientific threshold. The pie chart above shows that the scientific or industrial domain to which the project belongs is not a criterion in the selection process.

From the EAC up to and including the 7th Call for Proposals for Project Access PRACE has allocated a cumulated amount of 6.8 billion core hours to 259 projects, supported by researchers coming from 38 countries and fostered collaborations in Europe as well as with USA, Russia, Japan and China.

PRACE has increased its support to European industrial competitiveness with the first Open R&D projects and to large scale scientific instruments and Flagships, awarding resources to projects linked to ITER, the Human Brain Project and Graphene, to name but a few.

**Preparatory Access fuels Project Access**
Preparatory Access is not called Preparatory Access for nothing: it gives scientists and researchers a chance to develop, test and scale out their modelling programmes to be eligible for and successful on the highest class of supercomputers. Scalability of the code is a requirement for access to Tier-0 systems.

Preparatory Access comes in 3 flavours:
- Type A for code scalability tests,
- Type B for code development and optimisation, and
- Type C for code development and optimisation with the support of PRACE experts.

PRACE Preparatory Access is a continuous Call for Proposals with a cut-off date every 3 months. The procedure to receive an allocation via Preparatory Access is lighter than that of Project Access, as it only entails a technical assessment.

A comparison between awarded projects under Preparatory Access (1st through 11th cut-off) and under Project Access (2nd through 7th) revealed that for every Project Call 25% of awarded projects were developed with the support of a previous PA project allocation.

Researchers use Preparatory Access Type B and Type C for the continuous development of their applications and the access to large-scale configurations for validation of their codes. This type of HPC
PEER REVIEW PROCESS

access benefits entire scientific communities, as codes are developed and shared to improve existing models and research methodologies.

For Preparatory Access as such a significant growth over the years can be seen. Between the 1st cut-off in 2010 and the 15th cut-off in 2013 the number of applications has risen 16-fold (from 3 to 50). The number of awarded projects has kept pace and rose 20-fold from the 1st to the 15th cut-off (from 2 to 41).

Also, over the years, more machines have been included in Preparatory Access: 2 systems were available for the 1st cut-off, while nowadays 10 systems offer time and support. Those 10 systems offered 60 million compute hours in 2013.

The growth of Preparatory Access combined with the number of projects that pass from Preparatory Access to Project Access clearly shows the need for HPC resources to be made available for European scientific communities, as well as the need for support in scaling and porting applications for HPC-usage in research and science.

Preparatory Access was also the point of entry for the 10 SME-led projects accepted under the SHAPE programme. More on that can be found on page 8 of this Annual Report.

Multi-year projects

Multi-year access was awarded as a pilot in the 5th Call: A select group of seven excellent scientific proposals were allocated core hours in the first year, while resources were reserved for the second year of their project, to be awarded through a mid-term hearing before the PRACE Access Committee, with the objective to allow planning of long-term execution on the same HPC system(s) via projects that undergo only a single peer review process. The PRACE Scientific Steering Committee (SSC) has completed the intermediate evaluation process of the multi-year access and came to a very positive conclusion. The SSC will make a proposal to the PRACE Council to adequately decide on the possible future continuation of this form of access to PRACE resources.

On page 33 of this Annual Report a summary of 7 multi-year projects is included. Full articles of each of these projects can be found in PRACE Digest 1/2014 (www.prace-ri.eu/PRACE-Digest).

Full deployment of 6 Tier-0 machines

As of the 4th PRACE Call for Proposals for Project Access, all 6 PRACE Tier-0 resources were available:

- IBM Blue Gene/Q “JUQUEEN” (GCS@Jülich, Germany)
- Bull Bullx cluster “CURIE” (GENCI@CEA, France)
- Cray XE6 “HERMIT” (GCS@HLRS, Germany)
- IBM System X iDataplex “SuperMUC” (GCS@LRZ, Germany)
- IBM System X iDataplex “MareNostrum” (BSC, Spain)
- IBM Blue Gene/Q “FERMI” (CINECA, Italy)

“Starting mid-2014, PRACE 2.0 will come into life, continuing and increasing the access to Europe’s largest and most capable systems through a single peer-review process”

With their full deployment, the PRACE 1.0 phase was fulfilled, offering access to 6 world-class Tier-0 systems with complementary architectures and delivering a cumulated peak performance of more than 15 PFlops/s. This level of performance and diversity of architectures, unattainable for a single country, exemplifies the goal of PRACE, to unite European efforts in order to sustain European competitiveness.

Starting mid-2014, PRACE 2.0 will come into life, continuing and increasing the access to Europe’s largest and most capable systems through a single peer-review process.
PRACE wraps up the evaluation of a multi-year allocation pilot to encourage and support long-term execution of vital research

As Europe's premier HPC Research Infrastructure, PRACE is always looking forward, singly focused on future discovery and innovation. That is behind PRACE’s mission of continuously improving access to the research infrastructure that makes such discovery and innovation possible. By tailoring access to the needs of the scientific and industrial communities, and enabling emerging communities to take advantage of HPC, PRACE plays a vital role in leveraging the inherent value of today’s science and turning it into the discoveries and inventions of tomorrow.

A pioneering initiative in this regard was the recent assessment of multi-year access in the 5th Call for Proposals. A select group of seven excellent scientific proposals were awarded a one-year allocation while resources were reserved for the second year of their project, to be awarded through a mid-term hearing before the PRACE Access Committee.

The objective of this multi-year access is to allow planning of long-term execution on the same HPC system(s) via projects that undergo only a single peer review process. While the multi-year access is a pilot and still under review, initial results and feedback indicate that the model has the potential to offer significant benefits.

To date, all seven projects awarded multi-year access from academia and industry were confirmed for their second year of access.

- Under the watchful eye of Principal Investigator Dr. Alexandros Alexakis, the Non-universal statistics in Magnetohydrodynamic turbulence (MHD Turb) project is studying the behaviour of turbulent flow coupled with magnetic fields, focused on Magnetohydrodynamic (MHD) turbulence. This project was awarded 8.5 million core hours on JUQUEEN @ GCS@Jülich, Germany for its first year and another 18.5 million on the same system for its second year.

- A research group led by Prof. Chris Allton from University of Swansea is currently gathering new insights into strong interaction by developing reliable simulations of how matter behaves in the elusive quark-gluon plasma phase, chipping away at the intricacies of physical matter itself by pushing the boundaries of matter. Their project Pushing the Strong Interaction past its Breaking Point Phase II: Towards Quantitative Understanding of the Quark-Gluon Plasma was awarded 17.5 million core hours on Fermi @ CINECA, Italy in both its first and second years.

- The advanced modelling of turbulence currently being studied by the Argo research team in Cenaero, Belgium may lead to the development of counter-rotating open rotor (CROR) engines, a promising technology discovered in the 1980s but hindered by the excessive noise. The ambitious project led by Dr. Koen Hillewaert at Cenaero focuses on the development of new computational methods for industrial applications, with special emphasis on jet engines and propulsion, and further potential uses in wind turbine and machine design. His project PADLES - p-Adaptive Discretisations for LES in turbomachinery was awarded 14.25 million core hours on JUQUEEN @ GCS@Jülich, Germany for its first year and another 12 million on the same system for its second year.

Thinking ahead

The data for quark-gluon plasma research was gathered using the ATLAS detector system in CERN's Large Hadron Collider. Copyright: CERN 2012
Dr. Mounir Tarek and his team at the Université de Lorraine in France are using PRACE resources to study ion channels, small gateways in the membranes of cells that allow the flow of electricity through the brain. Dr. Tarek believes that research on one of the most fundamental elements of brain function will play a key role in revolutionizing understanding of the brain and shed light on the mechanisms behind behaviour and cognition, assist with the diagnosis and treatment of brain disease, and even use the way brain cells communicate with each other to develop the next generation of supercomputers. His project Electrophysiology - Atomistic modeling was awarded 28 million core hours on CURIE @ GÉNCI@CEA, France and 42 million core hours on SuperMUC @ GCS@LRZ, Germany in both its first and second years.

This project led by Dr. Tarek is linked to the Human Brain Project (www.humanbrainproject.eu) a major multidisciplinary European initiative – one of the 2 EU flagships FET projects – to gain profound insights into what makes us human, develop new treatments for brain disease and build revolutionary new computing technologies.

The discovery of the Higgs Boson was greeted with great celebration in March 2013, signifying an essential milestone in particle physics. Huge amounts of research continue to examine the interaction of elementary particles. Dr. Karl Jansen and his German-based team are delving deeper into the interactions between these elementary particles, specifically, the interaction of quarks and gluons, described theoretically as quantum chromodynamics (QCD), in the hope of gaining greater understanding of the events immediately following the Big Bang. Dr. Jansen's project Next generation lattice QCD simulations of the first two quark generations at the physical point was executed on three Tier-0 systems simultaneously in its first year with 7.5 million core hours on Fermi @ CINECA, Italy; 17.5 million on JUQUEEN @ GCS@Jülich, Germany; and 5 million on SuperMUC @ GSC@LRZ, Germany. For the second year another 7.5 million on Fermi and 17.5 million on JUQUEEN were allocated.

Heading up a 10-strong team of researchers, Dr. Sébastien Masson is intent on advancing the field of climate modelling by using three experimental models of climate simulation in the PULSATION project (Peta scale mULTigridS ocean-
This project is advancing progress by producing more precise models of the climate with special emphasis on how smaller areas, or “zooms” within the model, can have an effect on the large scale. The use of PRACE supercomputers has also enabled interaction with the World Research and Forecasting (WRF) application community. The project received 22.5 million core hours on CURIE @ GENCI@ CEA, France for its first year and another 12 million on the same system for its second year.

The research team of Dr. Francois Willaime at CEA (Commissariat à l’Energie Atomique et aux énergies alternatives; Alternative Energies and Atomic Energy Commission) are providing invaluable insights into how transition metals that are employed for their great strength and ability to bear loads, behave at the atomic level, focusing on predicting how they will perform on the large scale. This research entitled DIMAIM - Dislocations in Metals using Ab Initio Methods has broad practical applications in engineering – from bridges to nuclear power plants. It received 20 million core hours on MareNostrum @ BSC, Spain in both its first and second years.

“The discovery of the Higgs Boson was greeted with great celebration in March 2013, signifying an essential milestone in particle physics”

These multi-year projects have been outlined in more detail in the 1/2014 issue of the PRACE Digest: [www.prace-ri.eu/PRACE-Digest](http://www.prace-ri.eu/PRACE-Digest)

The PRACE Access Committee, in charge of allocating PRACE resources to the most outstanding projects, has transferred the results of these multi-year projects to the PRACE Scientific Steering Committee (SSC) for evaluation. The SSC has recommended to the PRACE Council that this new type of access continues and the PRACE Council has accepted that recommendation. PRACE now envisages to plan for longer term projects, led not only by individual scientists (primary investigators, PIs), but also by research groups and consortia.
Catherine Rivière, CEO of GENCI, is Chair of the PRACE Council until June 2014. We spoke to her about some of the ways in which the organisation has moved forward during her time in the position, as well as how she intends to extend the reach of its HPC resources beyond the world of traditional academic users.

▶ Ms. Rivière, could you tell us about some of the major achievements of PRACE over the last year?

Catherine Rivière. First of all I’d like to point out that, thanks to PRACE and its 25 members, Europe has, for the first time in its history, made world-class HPC resources available to its researchers. It is a vital contribution for Europe’s competitiveness, especially because of the high scientific value of the projects awarded and the results obtained.

PRACE, which was just a dream five years ago, has become a successful ESFRI e-infrastructure. 2013 was the first year we had all the 6 PRACE machines fully in operation at the same time, providing a computing power of more than 15 Pflops to all European scientists and representing 80% of the European HPC capacity for civil research.

Since 2010, 7 billion hours in total have been granted to the best European Science, enabling 259 scientific projects to use HPC high-level resources from academia and industry. And the demand is increasing in each call: for the sole 7th Call that was open from February to March 2013, we were asked to provide close to 3 times the computing time available! This means that PRACE is now well integrated in the European HPC ecosystem and plays a key role for computational science.

As an example, let’s talk about the 150 million core hours awarded through the 7th PRACE Call on CURIE and SuperMUC to a German team from Max Planck Institute for Astrophysics that will make three-dimensional simulations of supernovae explosions of massive stars, applying neutrino hydrodynamics. The same amount of core hours, unreachable with national resources, had already been granted to this team through the 4th PRACE Call. This kind of follow-up action demonstrates that PRACE is a strong support for stimulating high-impact science.

Another example is the HiResClim (High resolution Ensemble Climate modeling) project which received over 50 million core hours on MareNostrum and is expected to substantially contribute in the field of the climate prediction, in link with the ENES (European Network for Earth System Modeling) community. Its contribution to developing next generation high resolution climate models and ensembles will participate in the next phase of the Coupled Model Intercomparison Project (CMIP6), led by the Intergovernmental Panel on Climate Change (IPCC).

Because training and retaining competences represents an important issue for Europe, PRACE has provided more than 300 training days to nearly 3000 attendees since the creation of the 6 PRACE Advanced Training Centres (PRACE) in 2012. Europe clearly needs well-trained young researchers in both science and numerical applications.

Beyond all these achievements, the strategic role of PRACE has been recognised by European institutions. Following the EC’s communication in 2012 called “High Performance Computing: Europe’s place in a global race “, acknowledging the role of HPC in enabling scientific discoveries and innovation for both research and industry, the Competitiveness Council went in the same direction in 2013 by adopting conclusions on HPC. It was the first time that such conclusions on HPC were adopted both by Member States and European Commission.
You opened the services of PRACE to industry in 2012. Has this been a success?

CR. It is the other part of our success! PRACE is one of the most attractive infrastructures in the world for industrials. Since the inception of the Open R&D mid 2012 by the PRACE Council, more than 20 companies (from large to small and medium sized companies) have already benefited from our resources to shorten development cycles and improve the reliability of their products. Offering the opportunity for the best industrial researchers to develop open research is essential to foster innovation in Europe.

In 2013, French car company Renault was awarded 42 million core hours on CURIE, to improve their crash optimisation models. This will increase car safety and would have been impossible to perform using Renault’s own HPC facilities. This is a great example of how PRACE is giving large computing capacity to a company to anticipate future European EURONCAP safety rules and in consequence increasing its competitiveness.

PRACE also awarded core hours to SMEs, a good example of which is HydrOcean, who were granted more than 13 million core hours to perform massive computational fluid dynamics (CFD) simulations based on Smooth Particle Hydrodynamics (SPH) methods. These simulations will have applications in ship survivability under wave impact as well as aquaplaning in automobiles. And, as a positive side-effect, HydrOcean won, in 2013, the “HPC Innovation Excellence Award” attributed by IDC, an American market research, analysis and advisory firm specializing in information and consumer technologies.

To get more SMEs to use HPC, the pilot phase of our SHAPE programme (SME HPC Adoption Programme in Europe) was launched in September 2013 in the field of the PRACE-3IP project supported by EC. A total of 30 SMEs, from 6 European countries and working in various domains from CFD to life science and digital media, were selected: we help them to assess the full potential of HPC, and equip them with the expertise necessary to take advantage of the innovation possibilities opened up by HPC. Following its results SHAPE is expected to become a full PRACE programme in June 2014.

Are there any areas of research that are as yet untouched by the benefits of supercomputing but could potentially be revolutionised by it?

CR. In Horizon 2020, the European Commission asks for a collaborative approach to tackle Grand Challenges such as climate change, sustainable energy and personalized medicine. HPC, and therefore PRACE, will be necessary to take up these challenges, to deal with big data, develop models and simulations, and manage multi-disciplinary research projects. PRACE already served resources to high impact projects in these fields and recently awarded million core hours to first projects issued from the Human Brain Project and the Graphene EC Flagships.

How do you ensure the continued success of PRACE?

CR. Creating PRACE in 2010 was a real challenge at the time, but after two years we had defined our roadmap, and today PRACE is the only persistent European e-Infrastructure on the so-called ESFRI list. It now supports a pan-European infrastructure that is an example for how pooling resources can make European research and industry stronger!

Working together with all 25 PRACE Members is not always easy, but I think we are starting to develop a common PRACE culture, especially in the Implementation Projects, and I am very happy about this.

PRACE’s ecosystem is strong and a key factor for its success. However, much remains to be done to guarantee Europe’s position in the supercomputer league, to increase the adoption of high performance computing across all scientific and industrial communities and to ensure sustainability of the infrastructure for the future. This requires regular contact with decision makers at the highest European political level to make sure they will understand our needs.

That’s the reason why we are putting our best foot forward to communicate on the benefits of supercomputing and to reach new scientific and industrial communities; in September 2013 we released a publication called “Supercomputers for all” for this very reason and organized a social event for EC directorates to make the case for PRACE, and for HPC in general, as a driver for innovation and growth throughout Europe.

My message is this: PRACE is a strong player to ensure Europe’s competitiveness in a worldwide HPC race with US, China, Japan, South Korea and Russia, but also a key ingredient for Europe’s competitiveness in general.

“PRACE is one of the most attractive infrastructures in the world for industrials”
PRACE started offering Open R&D access to industry in the 5th Call for Proposals for Project Access (November 2012). Open R&D access means that industrial researchers, from European companies or companies having a significant R&D activity in Europe, can be awarded core hours on PRACE Tier-0 systems via the same peer-review process as academic scientists with the condition that the results of the project need to be made public after the end of the allocation period.

After just 18 months, PRACE Open R&D access is already successful in Europe with HPC resources awarded to projects from more than 20 businesses, both large corporations and SMEs from various European countries. The economic sectors represented by these businesses are varied: more traditional industries such as energy, automotive and aeronautics are present, but also enterprises developing renewable energies or micro-electronics see the advantages of HPC. Even insurance companies that need to assess risks for their coverage offers have found their way to PRACE Calls for Proposals.

PRACE Open R&D access has been successful in Europe: 8 projects were accepted under the 5th, 6th and 7th Project Access Calls of which 1 was a multi-year project that started in the 5th Call and received its second year under the 7th Call. Under the Preparatory Access 8th through 13th cut-off, 12 projects were accepted from 11 companies from around Europe. Other projects, both under Project Access and under Preparatory Access count industrial partners among their collaborators.

PRACE Open R&D has already attracted attention and interest from various other initiatives or countries around the world, most notably INCITE (Innovative and Novel Computational Impact on Theory and Experiment from US DoE) and UIUI (University of Illinois at Urbana-Champaign) from the USA, and RIST (Research Organization for Information Science and Technology) from Japan.

This PRACE support to European industries in not limited to the provision of HPC resources, it also allows industries to benefit from high-value services provided by PRACE in terms of information, training and expertise.

So far, PRACE has organised 5 Industrial Seminars around Europe, attracting high-level executives and researchers from large industrial companies as well as from dynamic and innovative SMEs. The PRACE Industrial Seminars provided a platform for dissemination of results obtained with PRACE support, networking between participants as well as knowledge transfer and promotion of best practices. In 2014 the PRACE Industrial Seminar will be combined with the PRACE Scientific Conference, forming the first edition of the PRACE Scientific and Industrial Conference: PRACEdays14. See page 48 in this Annual Report for more information on this event.

Part of the PRACE policy to offer more services to industry is the opening-up of the wide HPC curriculum provided by the 6 PATCs (PRACE Advanced Training Centres) to industrial participants. Training and retaining skills and talent is a core-issue for all businesses and the PATCs provide part of the solution by offering additional tailored courses for industry, e.g. on uncertainties quantification or use of open-source software (e.g. OpenFoam and Elmer).

Finally, as raising awareness and supporting SMEs in using HPC is a key challenge for improving European competitiveness, PRACE added a tailored service towards SMEs called SHAPE: the SME HPC Adoption Programme in Europe which launched a Pilot Call under the 15th PRACE Preparatory Access cut-off and awarded the maximum of 10 pilot-projects headed by European SMEs (see for a description of those projects on page X of this Annual Report). The projects are currently underway, and will run until August 2014. The SHAPE Pilot has generated already a lot of interest from future users. SHAPE serves as a conduit for SMEs to access HPC expertise and find their way into the HPC eco-system.

While Open R&D and SHAPE are successful in their first days, PRACE is continuing to update and upgrade its offering of HPC access.

One form of future industrial access currently under scrutiny by the PRACE Board of Directors (BoD) is pre-competitive R&D. This would be the next step in the development of PRACE Open R&D and would allow industrial researchers to postpone publication of the results obtained with the support of PRACE with one or two years, allowing the entrepreneur involved to exploit the results first and gaining some competitive advantage. The IAC supports the BoD in assessing new procedures that would allow for such an arrangement.
**HIGHLIGHT HYDROPLANING**

Hydroplaning simulation with 16,800,000 particles: the tire speed is 130km/h and the thickness of the water layer is 1 cm.

HydrOcéan, a French SME working on Naval and offshore numerical hydrodynamics, was awarded the IDC Innovation Excellence Award in November 2013 for the use of HPC applied to their SPH-Flow code. After a first allocation on Hermit @ GCS @ HLRS under the 5th PRACE Call for Proposals for research on ship survivability under extreme wave impacts, HydrOcéan was again awarded under the PRACE 6th Call for Proposals for Project Access with 8.2 million core hours on CURIE @ GENCI@CEA, France, for further research on hydroplaning using SPH-Flow:

“Even though the external aerodynamics of vehicles are now relatively well understood thanks to numerical models, problems of external hydrodynamics for automobile exhibit characteristics that make them very difficult to take into account with traditional numerical methods. Thanks to an innovative code, SPH-Flow, based on the meshless scheme SPH (Smoothed Particle Hydrodynamics) these limitations can now be removed. The objective of our project “External hydrodynamic for automobile” is to demonstrate that it is now possible to simulate external hydrodynamic flows in automotive industry and thus accurately predict the risks caused by water. To this end, two issues will be addressed in this project: hydroplaning and river crossing. To accurately simulate the physical phenomena involved in this type of flow, significant computing resources are required. The access to several million hours of computing time through the PRACE resources enabled the realization of this type of calculation launched on thousands of cores. This enabled to achieve unprecedented accuracy in this type of application,” says Dr. Matthieu de Leffe of HydrOcéan.

HydrOcéan’s project supported by PRACE also allowed this French SME to gain wider international visibility. “We are currently considering opening a new office abroad,” added Dr. de Leffe.

**HIGHLIGHT SEISMIC RISKS**

Munich Re, a German insurance and reinsurance provider, and one of the world’s leading companies in this domain, used PRACE-awarded resources on Fermi @ CINECA, Italy (40 million core hours under the 7th Call) to study the seismic risks in Santiago de Chile.

“The main objectives of our project are: (a) the generation of massive 3D deterministic scenarios apt to fully describe the seismic hazard in Santiago de Chile (including crustal, subduction, inter- and intraplate events), and (b) inclusion, for a selected set of earthquake rupture scenarios, of the 3D description of middle rise and high rise buildings in the city of Santiago, in order to assess the importance of the Dynamic Soil-Structure and Site-City Interaction (DSSI and SCI, respectively) effects. Santiago de Chile was chosen on two criteria: 1) the high population level (more than one third of the total Chilean population lives in the great Santiago region) together with the high concentration of value at risk during a major seismic event, and 2) the large amount of detailed information regarding the geophysical model of the Santiago basin and the building stock, as collected during reconnaissance surveys after the Maule earthquake on 27 February 2010,” says Dr. Marco Stupazzini of Munich Re.

“PRACE OpenR&D made it possible to access the right HPC architecture capable of coping with the challenge of physical-based 3D scenario simulations. SPEED (Spectral Elements in Elastodynamics with Discontinuous Galerkin) was optimized for IBM Tier-0 architecture, with the support of CINECA’s technical staff. Thanks to the high-parallel efficiency of SPEED - the possibility to run simulations on a Tier-0 machine - the execution time was drastically reduced and such deterministic simulations were feasible, producing reliable “real-time” results,” he added.

Dr. Marco Stupazzini of Munich Re
PRACE continues to train the next generation of HPC experts

Since the establishment of six PRACE Advanced Training Centres (PATCs) in March 2012, their operations have significantly boosted the impact of the PRACE training programme implemented by the projects.

BSC – Barcelona Supercomputing Center (Spain), CINECA - Consorzio Interuniversitario (Italy), CSC - IT Center for Science Ltd (Finland), EPCC at the University of Edinburgh (UK), Gauss Centre for Supercomputing (Germany) and Maison de la Simulation (France) are the current PRACE Advanced Training Centres.

In the 2012-13 academic year, they have together provided 71 courses (spanning a wide range of domains including programming languages and models, use of PRACE systems, numerical libraries, open source software, pre and post processing, visualisation, ...) attended by 2,059 participants who have consistently given high quality ratings (8.5 out of 10 on average) for the courses. This highly successful pilot phase of the PATCs, along with valuable lessons learnt during their implementation, have since laid the foundation of a plan (as described in the PRACE-3IP deliverable D4.1: Continuity Plan for the PATCs) to transform the PATCs into a permanent service under the PRACE Research Infrastructure.

The PATCs will jointly deliver a total of about 79 courses in the 2013-14 academic year, with 24 of these already having been held in 2013. A significant development has been the addition of PATC courses that are targeted towards industry (e.g. HPC Packages for CFD, Modelling and Analysis, Uncertainty Quantification, ...). The yearly PATC curriculum is evaluated by a panel of external international experts from various scientific domains.

Apart from PATC activities, the PRACE projects also oversaw four Seasonal Schools in 2014, held in Ireland, Sweden, Czech Republic and Slovenia, as well as the International HPC Summer School (see above). The PRACE Training Portal continues to host a wide range of course material from PRACE training events, and a number of video tutorials have been created by PRACE and made available for distance learning purposes.

Looking forward to 2014, another extensive and wide-ranging programme of training awaits, including ~55 PATC courses, two Seasonal Schools (Tel Aviv, Israel in February and Hagenberg/Linz, Austria in April) and the International HPC Summer School 2014 in Budapest, Hungary in June (see above). For information on all PRACE training activities, please visit the PRACE Training Portal at: www.training.prace-ri.eu
International Summer School on HPC Challenges in Computational Sciences

Success in 2013 leads to further co-operation in 2014

More than 70 graduate students and postdocs from Europe, Japan and the United States participated in the Fourth Annual International Summer School on HPC Challenges in Computational Sciences held on 23 – 28 June 2013, in New York City. It marked the first time that Japan, represented by the RIKEN Advanced Institute of Computational Science, has entered into a formerly bilateral collaboration between Europe (DEISA and PRACE) and the U.S. (Teragrid and XSEDE) in organising this annual series of schools. Feedback was overwhelmingly positive from everyone who attended the school that promoted knowledge of HPC and its applications in different domains through a mix of lectures and hands-on exercises, instructed by leading scientists and technologists from European, Japanese and the U.S. By bringing together participants and presenters from institutions representing 15 countries, the event also encouraged international collaborations and friendships.

In 2014, the International HPC Summer School will take place in Budapest, Hungary on 1-6 June. The collaboration welcomes Compute/Calcul Canada as a new partner in organising this event which will host participants from Canada, Japan, Europe and the U.S.

More information is available at: www.prace-ri.eu/International-Summer-School-2014

PRACE Summer of HPC

The PRACE Summer of HPC (SoHPC) is an outreach programme targeting undergraduate and postgraduate students. In 2013 it offered twenty-four top students the opportunity to spend two months at one of ten HPC centres around Europe.

The programme kicked off with an engaging, instructive and team-building training week at EPCC in Edinburgh on 30 June 2013. Students undertook training in outreach, MPI, OpenMP and visualisation. After training the SoHPC participants departed to their host sites around Europe and began work on their projects. Each student worked with a mentor and produced a visualisation or video based on PRACE technical or industrial work.

(Above) SoHPC students at their training week in Edinburgh

(Left) Dinosaur Racing by Antoine Dewilde ©PRACE aisbl

(Right) Ocean temperature by Antonios Karkatsoulis ©PRACE aisbl
In the final week, each participant presented their work to the other participants and mentors and those presentations are available to view on the SoHPC YouTube channel at www.youtube.com/summerofhpc. In keeping with the outreach aim of the programme, the participants also blogged about their experiences during the SoHPC and attracted over 13,000 unique visitors in 112 different countries. You can find out more at www.summerofhpc.prace-ri.eu.

SoHPC 2013 came to a close on 30 August with the participants departing to their home countries. Two outstanding students were chosen to receive awards in recognition of their contribution to the SoHPC. On 2 December 2013, Dr. Sergi Girona, chair of the PRACE Board of Directors presented the award for Best Visualisation to Niki Loppi and the award for PRACE HPC Ambassador to Vito Simonka.

The Summer of HPC has encouraged the participants in their path to become the next generation of HPC users, software developers, system administrators and data visualisation experts, forged friendships and created a community of young enthusiasts and their peers, family and friends. The results of the projects have also provided important outreach and dissemination material, which has been used in outreach events such as the British Science Festival and the EU Contest for Young Scientists and will be a resource for many events in the future.

More information:
www.summerofhpc.prace-ri.eu
www.facebook.com/summerofhpc
www.twitter.com/summerofhpc
www.youtube.com/summerofhpc
The PRACE User Forum

In 2013 the PRACE User Forum held its first full General Meeting, kindly facilitated by the organisers of CSC2013 (www.cyprusconferences.org/csc2013/index.php) (see page 51 of this Annual Report for a report on that event). The meeting attracted over 80 participants.

Arising out of feedback from the User Community, the Forum entered into a fruitful dialogue with PRACE on various issues such as:
- Heterogeneous access to PRACE compute resources, for example coupling access to Tier-0 and Tier-1 systems;
- Extending data storage times in order to facilitate the lengthy data analysis necessary to gain the most from today’s complex simulations.

The Forum also discussed topics for future co-operation with PRACE, including:
- If the PRACE policy regarding international access to PRACE resources is significantly impacting any research community;
- If PRACE Letters of Offer should contain information on the approximate financial value of the award for use by the Users with their own institutional information gathering exercises.

The User Forum regularly informs the PRACE Board of Directors (BoD) of the outcomes of their discussions. The PRACE BoD will then take those topics and suggestions into consideration for possible new or adjusted policies.

To keep communications with the User Community transparent and efficient, the Programme Committee decided that best use of resources would be to maintain a social media presence on LinkedIn and Twitter.

The Forum can be found at www.linkedin.com/groups/PRACE-User-Forum-4793989 on LinkedIn and at @PRACEUserForum on Twitter. The LinkedIn group contains, for example, details of the discussions at the User Forum General Meeting at CSC2013 and is open to contributions from any PRACE Users, or prospective users.

Finally, the Committee gained a new Chair and Vice-Chair: Gustavo Yepes (from Universidad Autónoma de Madrid, Spain) and Koen Hillewaert (from Cenaero, Belgium), respectively. Turlough Downes stays on the Committee as the outgoing Chair. Further nominations to the Programme Committee of the User Forum are now sought.

In 2014 PRACE supports the User Forum by hosting their General Meeting at the PRACE Scientific and Industrial Conference (PRACE-days14), which will be held from 20 to 22 May 2014 in Barcelona. The User Forum will meet on Tuesday 20 May in the afternoon before the official opening of the conference. For more information, go to: www.prace-ri.eu/pracedays14
PRACE Projects support the Research Infrastructure

In 2013, all three PRACE Implementation Phase (IP) Projects were running in parallel supporting the implementation of the PRACE Research Infrastructure. Some highlights of the work of the PRACE IP Projects are reported in detail in other parts of this annual report. This is the case especially of the extensive training activities of the PRACE Advanced Training Centres, the SHAPE pilot or the dissemination actions like the presence of PRACE at numerous HPC exhibitions and events.

The 1st Implementation Project (PRACE-1IP) was extended until 31 December 2013 after 48 months intensive and effective project work. The final eight months were dedicated to application scaling for capability science projects on the Intel MIC architecture available on CINECA's EURORA prototype and BSC's MareNostrum. The results of that work are reported in 18 White Papers available on the PRACE website.

The 2nd Implementation Project (PRACE-2IP) was extended by 12 months in order to 1) evaluate the latest hardware components installed in the previously selected prototypes, 2) extend the community code enabling support, and 3) continue the best practice for HPC system commissioning and novel programming techniques. The PRACE-2IP project successfully passed its periodic review by the European Commission.

The 3rd Implementation Project (PRACE-3IP) is the successor of the PRACE-1IP project and continues many of its activities. In addition, the Pre-Commercial Procurement pilot explained in detail below was prepared. An important milestone was reached, with the publication of the tender notice on 22 November 2013 after a very thorough legal check and several focused EC reviews. Moreover, PRACE-3IP received the highest possible rating in the first periodic project review with all activities of the project being rated as excellent.

Ecosystem and Operation

DECI Calls and Projects
During 2013, two sets of DECI (Distributed European Computing Initiative) projects were completed and two new calls were issued, following the now well-established six month cycle of DECI projects which provides computational scientists with access to a large range of Tier-1 resources for one year. Support for projects already running successfully was transferred from PRACE-2IP to PRACE-3IP. The DECI-10 call received 85 proposals and the DECI-11 call had a record of 115 proposals. Together these calls resulted in 89 successful DECI projects. In total, almost 400 million hours of compute time were awarded to projects in a diverse set of scientific disciplines. Two DECI mini-symposia took place showcasing the work performed under DECI at ParCo2013 and the International Conference on Scientific Computing 2013.

PRACE Infrastructure and Operations
The operations team is responsible for the set of common services which integrates the PRACE Tier-0 and Tier-1 systems into one infrastructure. The basis of this integrated infrastructure is a dedicated network which connects the systems in a star topology. In 2013 three new Tier-1 systems have been connected using a 1Gbps IPsec setup and one new Tier-1 system has been connected with 1 Gbps through the new GÉANT plus service. This dedicated network is used among others for high throughput data transfers with GridFTP between PRACE systems.

“The operations team is responsible for the set of common services which integrates the PRACE Tier-0 and Tier-1 systems into one infrastructure”

PRACE Network
The status of services is monitored and the results are used by the Operator on Duty to signal and report problems. The operational team also monitors if problems are handled in a timely manner and takes action if needed. A common helpdesk is provided, which can be used by centres’ staff to report and resolve problems with PRACE services and systems. A change management process guarantees the reliability of services.

The security of the infrastructure must be guaranteed and requires a close collaboration between all partners. The Security Forum, with representatives of all partner sites, coordinates both the handling of security incidents as well as the development of common policies and procedures and risk assessments of services. The Security Forum also collaborates with other larger infrastructures, like EGI and EUDAT in Europe and XSEDE and OSG in US regarding the exchange of information about security incidents and the development of high level security policies. The latter enable the interoperability among these infrastructures. In 2013 also a common security training event was organized with EGI and EUDAT.

New Technology

Technology Watch and HPC Centre Infrastructures
Technological watch is an ongoing activity that delivers its results to the PRACE community on a regular basis. It focuses on petascale systems worldwide and analyses information from Top500, SC and ISC conferences, and other web or vendor sources.
It also encompasses watching global trends on HPC systems components, like InfiniBand, GPGPU, MIC or advanced cooling techniques. It assesses the global evolution of PRACE resources with respect to other continents, and analyses how the European HPC landscape is moving.

HPC centre infrastructures are becoming more and more important, in relation with HPC systems. Delivering globally efficient solutions in terms of performance, energy consumption and consequently cost is at stake. Besides complementing the series of “HPC Centre White Papers” previously produced the 4th European Workshop on HPC Centre Infrastructures was organized by CEA, CSCS and LRZ in April 2013.

Prototypes
In PRACE-2IP, new HPC technologies were evaluated; establishing and fostering ties with hardware vendors; providing early guidance on upcoming changes in programming paradigms and techniques; and offering recommendations for future Tier-0 and Tier-1 systems. On the current prototypes PRACE is investigating the latest accelerators, new interconnects, and the different cooling technologies.

For example, one prototype developed at Poznan Supercomputing and Networking Center (PSNC) is evaluating immersive liquid cooling, an innovative supercomputing cooling technology, and AMD APUs and GPUs.

Some results have shown that performance improvement was matched with the corresponding improvements in energy efficiency, indicating that proper software optimisation for performance should be a priority also for saving energy in a HPC context. Also, by now it is clear that the GPGPU accelerator technology is gaining wider acceptance. The main drawback to employing this technology is the need for new programming languages and a switch to different programming techniques. The newly developed Intel Xeon Phi on the other hand promises the use of an accelerator without major application changes. These different accelerators are being investigated by the project partners CINECA and CSC. In addition, the AMD APUs and GPUs are becoming more sophisticated and promise the ability to run standard languages.

Pre-Commercial Procurement
The PRACE-3IP project is running a joint Pre-Commercial Procurement (PCP) pilot targeting “Whole System Design for Energy Efficient HPC”.

The process that PRACE PCP pilot follow is divided in two stages:
- The Tendering Stage for selecting and awarding the suppliers;
- The Execution Stage is composed of three phases during which the selected suppliers provide the R&D services described in their offers.

The key event was the publication of the call for tender for the PCP on 22 November 2013, which was the starting date of the Tendering Stage.

A set of technical requirements was designed to present an achievable challenge to the vendors in order to encourage as many bids as possible, whilst still presenting a research and development challenge for the companies. Any solution proposed by a vendor must target energy efficiency in whole system design. The evaluation of improvements in energy efficiency will be verified by real production applications codes in use by PRACE today, as well as by the HPL (High Performance Linpack) benchmark.

An Expert Committee was set-up for answering questions from interested vendors. A Benchmark Code Owners group is in place whose task is to prepare the benchmarks defined in the tendering documents. The definition of the organisation, framework and tasks needed to perform the evaluation of the PRACE-3IP PCP results has been completed.

This PCP pilot, performed for the first time in the context of HPC by a pan-European group of procurers, posed many new legal, financial, and technical challenges. They were met through very thorough consultations with technical expert and lawyers ensuring that the PCP can be completed successfully.

Application enabling
Scaling Applications for Tier-0 and Tier-1 Users
The aim of the applications enabling activity is to support European researchers to ensure that there is a broad range of important applications that can run efficiently on state-of-the-art supercomputers. The long-standing core activities are collaborating with users to ensure that they can effectively exploit both Tier-0 and Tier-1 systems. During 2013, around 50 such collaborative projects were enabled and to another 100
projects advice was provided. In addition, the work on enabling applications to address key socio-economic challenges from the “PRACE Scientific Case for HPC in Europe” started. A broad range of important programming models, tools, libraries, algorithms and I/O techniques is documented in deliverable “HPC Tools and Techniques”. In the next year, the most promising tools and techniques to benefit real applications will be exploited. A key achievement was the combining of the existing PRACE and DEISA benchmark suites to produce the Unified European Applications Benchmark Suite (UEABS). The applications and data sets from UEABS are published on the web to provide a resource for procurements and performance data useful for prospective users. To ensure that the expertise of the PRACE partners is beneficial to the European HPC community, dissemination through White Papers and Best Practice Guides was continued; there are now well over 100 White Papers and around 15 Best Practice Guides.

The efficient usage of Tier-0 architectures places high demands on the used software packages and in many cases advanced optimisation work has to be applied to the codes to make best use of the provided supercomputers. Consequently, there is a high need for Preparatory Access (PA) giving the opportunity to analyse and optimise codes prior to applying for resources through the PRACE Calls for Proposals for Project Access. The complexity of supercomputers requires a high level of experience and advanced knowledge of different kinds of concepts regarding programming techniques, parallelisation strategies, etc. Such demands often cannot be covered by the applicants themselves, but special assistance of supercomputing experts is needed. PRACE offers such a service through Preparatory Access type C for optimisation work with support from PRACE experts. In 2013 14 PA type C projects were approved, that might apply for future Regular Calls. By December 2013, already 11 former PA type C projects successfully applied for PRACE Regular Call. These numbers prove the enormous success of the work done in the field of application enabling. The results of the PA type C projects together with the enabling work done are documented in White Papers, available on the PRACE website.

One of the recent projects dealt with the performance investigation and the improvement of the multiple biological sequence alignment software MSA_BG on the BlueGene/Q supercomputer JUQUEEN at Forschungszentrum Jülich, Germany. Multiple Sequence Alignment (MSA) plays an important role for biological sequences analysis and allows the study of evolutionary relationships between the considered sequences. The implementation of OpenMP in addition to MPI considerably improved the performance of MSA_BG.

The graph above shows the results of the Multiple Sequence Alignment (MSA) method applied to 149 sequences with a maximum length of 1036 nucleotides. While the blue line shows the scaling behavior of the hybrid MPI/OpenMP version of MSA_BG, the red line represents the performance of the original version of the code. These scaling plots clearly reflect the performance benefit which results from the applied optimisation work.

The number of MPI tasks and OpenMP threads respectively is chosen in such a way that all nodes involved in the simulation work to full capacity. This condition allows for direct performance comparison between the pure MPI version and the hybrid version of the code.

Community Code Scaling

Seventeen scientific simulation codes have been enabled for the coming generations of High Performance Computing architectures by the PRACE-2IP project. This was accomplished with a strong contribution from the scientific communities, building a close and effective synergy between researchers and code developers and HPC experts. The first contribute with their deep comprehension of the research subjects and the algorithms, the latter provide the necessary skills and competencies on novel hardware architectures, programming models and software solutions resulting in a refactoring program to optimally map applications to emerging supercomputing architectures.

During 2013, codes from five different scientific domains (Astrophysics, Material Science, Climate, Engineering and Particle Physics) have been re-designed and re-implemented according to the performance models defined during the early stage of the project. Excellent results were obtained for many of the constituent applications, addressing a broad spectrum of issues like scalability on huge numbers of cores, exploitation of hybrid systems equipped with accelerators, adoption of high performance numerical libraries.

Further improvements are being accomplished by further exploiting the experience, expertise, technological instruments and collaboration acquired and built along the work package life span, in the one year extension the work is focused on 13 success stories to further enhance the quality, the effectiveness and the efficiency of the developed software and its readiness for the new HPC architectures that the PRACE-RI will deploy as Tier-0 or Tier-1 systems.

Support for Industrial Users

Industry Application Enabling

PRACE focused both on petascale open source codes of importance to industry and the enabling of emerging industry relevant open source codes for HPC systems.

This activity, started in PRACE-2IP, produced valuable results in PRACE-3IP allowing some industries to use the enabled application codes to apply for R&D access in the regular PRACE Tier-0 calls. An example is the Speed code (open-source code for the simulation of seismic wave propagation problems) which increased its scalability on the BlueGene/Q Tier-0 System from 1.024 to more than 16.000 cores on an industrial test case (see Highlight: Seismic risks on page 39). The company that provided the benchmark data-set has now applied for access to Tier-0 resources in the Open R&D scheme. The application is related to seismic risk assessment in large urban areas for an insurance company.

Seminar for Industrial Users

PRACE strengthened also its working relations with industry during the 5th PRACE Executive Industrial Seminar held on 14–16 April 2013 in Stuttgart region.

This forum has already become a well-known tradition in the European HPC landscape. Since the start five years ago about 140 different companies from Europe and the USA have been attracted to these events which included topics such as HPC use in industry, HPC technology and applications and support provided by PRACE.

The main focus of the 2013 meeting was on “HPC Changing Europe’s Industrial Landscape”. An additional major topic has been the launch of the SHAPE pilot, a PRACE-supported HPC adoption programme for small and medium sized enterprises (see page 8). Representatives of 18 SMEs and about 40 corporations attended the seminar and were informed about PRACE future plans and offers in the range of industrial relations.

The Winner of the second round of the PRACE Competition for the Most Innovative HPC Industrial Application was CERFACS from France.

In 2014 the PRACE Executive Industrial Seminar will be merged with the PRACE Scientific Conference to form the PRACE Scientific and Industrial Conference. The first edition of that event will be held from 20 to 22 May 2014 in Barcelona (PRACEdays14 - see page 48).

More information

PRACE website: www.prace-ri.eu
PRACE White Papers: www.prace-ri.eu/white-papers
PRACE Best Practice Guides: www.prace-ri.eu/Best-Practice-Guides
PRACEdays14: www.prace-ri.eu/pracedays14
In 2014, PRACE will organise its first Scientific and Industrial Conference – under the motto: ‘HPC for Innovation – when Science meets Industry’. The conference combines the previously separate PRACE Scientific Conferences and PRACE Industrial Seminars and will bring together experts from academia and industry who will present their advancements in HPC-supported science and engineering.

The PRACE days will be held in Barcelona at the Universitat Politécnica de Catalunya (UPC) campus from Tuesday 20 to Thursday 22 May 2014.
PRACE will present its Scientific and Industrial Awards as well as a prize for Best Poster

A satellite event will be organised on Monday 19 and Tuesday 20 May:
**Workshop on exascale and PRACE Prototypes**

The PRACE User Forum will meet on Tuesday 20 May, in the afternoon.

On Wednesday 21 May, parallel sessions on Computer Science, Life Sciences, Chemistry & Materials

On Tuesday 20 May, in the afternoon.

On Thursday 22 May a panel of experts will discuss the “Economic and scientific impact of collaboration between science and industry.”

Science, Environmental Sciences, Automotive & Engineering, Astrophysics, and Mathematics will include presentations on some of the most outstanding projects using PRACE resources in these fields.

A special parallel track is reserved for the first results of the PRACE SHAPE Programme for SME access to HPC.

The attendance fee is €60. Travel and accommodation will not be reimbursed.

For more information: [www.prace-ri.eu/pracedays14](http://www.prace-ri.eu/pracedays14)

#PRACEdays14 @PRACE_RI

PRACE is looking forward to making this event a tradition for the European HPC communities!

PRACEdays15 will be held from 26 to 28 May 2015 at the Aviva Stadium in Dublin, Ireland.
Past PRACE Events

PRACE @ ISC

At ISC13, PRACE had a strong presence at the event, with the booth attracting 500 visitors through mini-presentations on “PRACE 2.0 strategy”, “Industrial applications” and “PRACE training opportunities and Advanced Training Centers”; a Treasure Hunt; a video game; various publications; and the always popular PRACE T-shirts and give-aways.

PRACE also hosted a Birds-of-a-feather session on “PRACE&HPC Services for Industry”. This session presented initiatives for industry and industrial applications.

At ISC14, which will be held from 22 to 26 June 2014 in Leipzig, Germany, The Chair of the PRACE Board of Directors will lead a session to analyse the European HPC ecosystem from the angle of technology, service, and applications. Of course PRACE staff will welcome visitors to the PRACE booth, #932.

PRACE @ ICT2013

The European Commission organized the ICT2013 – Create Connect Grow event in Vilnius Lithuania from 6 to 8 November 2013 where over 5000 people attended. In the exhibitor area PRACE showcased its globally competitive HPC ecosystem that encourages and supports in achieving pan-European industrial competitiveness.

A networking session entitled “PRACE and EUDAT tackle the Big Data Challenge” was jointly organised by PRACE and EUDAT to disseminate ways in which the two research infrastructure projects collaborate to provide state-of-the-art solutions in the big data age.
PRACE and LinkSCEEM host scientific community in Cyprus

The Conference on Scientific Computing 2013 (CSC 2013) jointly organized by PRACE and the FP7 infrastructure project Linking Scientific Computing in Europe and the Eastern Mediterranean (LinkSCEEM) was held in Paphos, Cyprus from 3 to 6 December 2013.

CSC 2013 brought together 120 international computational scientists and conference speakers from 28 countries who presented highlights of their scientific work performed using PRACE and LinkSCEEM computational resources.

PRACE provided 18 fellowships for young scientists from 12 PRACE member countries to come and present posters at the conference. Similarly, LinkSCEEM provided funding for 27 fellows from 7 Eastern Mediterranean countries.

PRACE also provided funding for the prizes awarded to the 3 best posters as voted by participants of the conference. One of these prizes was awarded to a poster from SESAME, Jordan, with the topic of the poster being on Synchrotron radiation applications. A PRACE fellow from Sabanci University, Turkey was also amongst the winners with the topic of the poster being on molecular dynamics simulations on a human iron binding protein. The final poster prize was awarded to a LinkSCEEM fellow from The Cyprus Institute with the topic of the poster being Lattice Quantum Chromodynamics. Each poster prize included a statue of Aphrodite and €350 to enable the winner to attend a scientific conference in his/her field. The prizes were awarded by Professor C. Lang, member of the PRACE Scientific Steering Committee.

During the conference, the PRACE Scientific Steering Committee (SSC) and the PRACE User Forum also held their annual meetings.

PRACE @ SC

PRACE once again presented their on-going achievements at an engaging and informative booth at SC13, which was hosted in Denver, Colorado from 18 to 21 November 2013.

Over 600 visitors stopped by the striking booth to speak to PRACE representatives, attend mini presentations, and participate in PRACE competitions.

PRACE, together with XSEDE (US) and RIKEN AICS (Japan) organised a Birds-of-a-feather session at SC13 on HPC training perspectives and collaborations from PRACE, XSEDE and RIKEN AICS, which resulted in the sharing of training materials, discussion of lessons learned, and steps towards further potential collaborations.

PRACE will be present again at SC14 in New Orleans, Louisiana, USA, from 17 to 20 November 2014.