PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

PRACE
Annual Report 2014

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 agreement RI-312763.
# PRACE Annual Report 2014

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Making innovations into traditions

The PRACE Annual Report 2014 is already the third issue of a series that is promising to become a yearly highlight in the work of the Partnership for Advanced Computing in Europe. With more pages, more success stories, more articles and more highlights, this report sets the standard for the years to come.

While the report looks back on the past year as a successful one for PRACE as well as for HPC-driven science and industry in Europe, you will notice that some articles already carefully look forward to developments that we will be in the middle of when this report is published. This includes PRACE 2.0, about which you can find more information in the interview with Sanzio Bassini, Chair of the PRACE Council on pages 28 and 29.

PRACE is developing at high velocity; projects that apply for our support are larger in terms of core hours, wider in terms of international collaboration and support to large-scale instruments and European projects, and more numerous. Demand for world-class HPC resources still outnumbers the supply. The PRACE Key Performance Indicators and Peer Review Statistics are testimony to this; have a look on pages 30 through 34.

Of course PRACE couldn’t be PRACE without its members. On pages 6 to 9 our members voice their support for PRACE and their reasons for being a part of the European HPC Research Infrastructure.

With 25 HPC organisations in and beyond Europe, each with their own characteristics and specific expertise, PRACE is able to reach a scientific and industrial community that spans continents. That differences often give good sparks is underlined by the eight success stories you can find in the centre of this report. Two stories are about PRACE-supported projects directly linked to industry. They clearly show how European competitiveness can benefit from a cross-pollination between science and industry, aided by HPC.

But PRACE is much more than just the awarding of core hours to excellent projects. The PRACE IP Projects are active in many different ways, creating the necessary initiatives to support the development of HPC in Europe through events, training, code development, scaling, and much more. Have a look at pages 41 through 43 to find out more.

This Annual Report will be launched at PRACEdays15, which will be held from 26 to 28 May 2015 in Dublin, Ireland. And while this third edition of the PRACE Scientific and Industrial Conference is ongoing, the fourth edition and its future successors are already being planned. The highlights on this and other events on pages 44 through 47 will show you that PRACE is transforming its innovative initiatives into HPC traditions.

Dr. Sergi Girona
Chair of the PRACE Board of Directors
PRACE SHAPE gets European SMEs into HPC-shape

SHAPE, the SME HPC Adoption Programme in Europe, is a pan-European, PRACE-based programme supporting HPC adoption by small and medium-sized enterprises (SMEs). The programme aims to raise awareness and equip European SMEs with the expertise necessary to take advantage of the innovation possibilities opened up by High Performance Computing (HPC), thus increasing their competitiveness.

HPC is a powerful technology that can enable the development of new products or services, reduce time-to-market and cost of R&D, and increase quality. The opportunities opened up by HPC are vast and an increasing number of SMEs turn to HPC in order to create new business opportunities.

The Programme helps European SMEs overcome barriers to using HPC, such as cost of operation, lack of knowledge and lack of resources. It facilitates the process of defining a workable solution based on HPC and defining an appropriate business model. To better refine the SHAPE programme, a pilot was launched by the PRACE-3IP FP7 Project.

The SHAPE Pilot Call, which ran from June 2013 to May 2014, received submissions from 14 small and medium-sized companies (SMEs) from five countries and various industrial domains, including wave-energy, aerodynamics, audio processing, and safety. 10 projects were selected and the SMEs leading those projects were intensively supported by experts from PRACE SHAPE to develop their HPC solutions, providing them with knowledge that will allow them to make an informed decision on those solutions and plan future actions, while also considering the support of independent service providers at a later stage.

The success of the SHAPE Pilot Call was underlined by the IDC (International Data Corporation) which granted the HPC Innovation Excellence Award to two SMEs participating to the SHAPE Pilot: Thesan, on June 24th 2014 during the ISC 2014 conference in Leipzig, (www.prace-ri.eu/idc-nov14-nexio/). Furthermore SHAPE was presented the HPCwire Readers’ Choice Award for Best HPC Collaboration Between Government & Industry for the SHAPE Programme as a whole (www.prace-ri.eu/hpcwire-readerschoice-2014-winners/).

The results of the pilot were very encouraging and the PRACE Council therefore decided to make SHAPE a permanent service of PRACE. A second call was opened on 10 November 2014.

Future plans for SHAPE entail the inclusion of both Tier-0 and Tier-1 resources and further integration with other PRACE services, such as the HPC training offered through the PRACE Advanced Training Centres (PATCs).
## PRACE Members

As PRACE is about to end its first phase the PRACE members would like to give testimony on how being part of PRACE has benefitted their country.

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<td><strong>AUSTRIA</strong></td>
<td>Professor Dr. Wolfgang Schreiner, Associate Professor</td>
<td>Research Institute for Symbolic Computation (RISC) of the Johannes Kepler University Linz</td>
<td>“PRACE offers not only a world class computing infrastructure but also a vital platform for collaboration of European HPC users from various disciplines. Austrian scientists and researchers both contribute to and profit from its various facilities and activities.”</td>
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<td><strong>BELGIUM</strong></td>
<td>Serge Bogaerts, HPC &amp; Infrastructure Manager</td>
<td>Centre de Recherche en Aéronautique ASBL, in short ‘Cenaero’</td>
<td>“A recent member of PRACE, Belgium recognises that the organisation has been successful in providing an HPC infrastructure for European science and industry. Participating in PRACE initiatives is key to the development of scientific excellence and industrial competitiveness in Belgium.”</td>
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<td><strong>BULGARIA</strong></td>
<td>Hristo Hristov, Director of Information Technology</td>
<td>Ministry of Transport, Information Technology and Communications, Bulgaria</td>
<td>“PRACE has combined the capabilities of several European countries to develop a powerful HPC resource. Scientists and companies can form fruitful partnerships, working together in fields such as biochemistry, the development of new materials and the evaluation of crises.”</td>
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<td><strong>CYPRUS</strong></td>
<td>Professor Constantia Alexandrou, Institute Professor, Acting Director &amp; Professor</td>
<td>The Cyprus Institute, CaSToRC and University of Cyprus</td>
<td>“Our PRACE involvement has brought cutting-edge knowhow in HPC to Cyprus. It has also provided opportunities for Cypriot scientists to participate in PRACE training events and to have access to Tier-0 and Tier-1 resources through PRACE access calls.”</td>
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<td><strong>CZECH REPUBLIC</strong></td>
<td>Vit Vondrák, Head of Research Programme</td>
<td>IT4Innovations National Supercomputing Center at VSB</td>
<td>“Joining PRACE in 2010 was a great opportunity for the whole Czech HPC community. We have set up very fruitful relationships with many HPC centres from other European countries and our researchers regularly attend training events organised by PRACE.”</td>
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<td><strong>DENMARK</strong></td>
<td>DeIC – Danish e-Infrastructure Cooperation</td>
<td>DeIC – Danish e-Infrastructure Cooperation</td>
<td>“Denmark is a strong supporter of European HPC cooperation, including access to HPC at the local, national and international level. Denmark now looks forward to seeing PRACE progress to a truly joint European HPC infrastructure, based on cooperation within all aspects of HPC-based research.”</td>
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<td>FINLAND</td>
<td>Dr. Janne Ignatius, Project Director</td>
<td><em>Computing Research Infrastructures, CSC - IT Center for Science Ltd.</em></td>
<td>“Thanks to PRACE several Finnish computational research groups have achieved top quality results, the HPC training curriculum of PRACE is truly wonderful.”</td>
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<td>FRANCE</td>
<td>Catherine Rivière, CEO</td>
<td><em>GENCI (Grand Equipement National de Calcul Intensif)</em></td>
<td>“PRACE has helped demonstrate that a joint European effort is essential in order to compete with the US or Asia for giving access to world-class HPC capacities and services. Efforts of French research and industry teams provide a crucial contribution to our national competitiveness.”</td>
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<td>GERMANY</td>
<td>Prof. Dr. Arndt Bode, Member of the Board</td>
<td><em>Gauss Centre for Supercomputing (GCS e. V.)</em></td>
<td>“The first five years of PRACE have strongly supported the building of a European Science Ecosystem, which relies on the efficient use of numerical simulation for almost all areas of science. German scientists drive this development and are involved in this new European science culture.”</td>
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<td>GREECE</td>
<td>Ioannis Liabotis, Computer Infrastructure Project Manager</td>
<td><em>Greek Research and Technology Network - GRNET S.A.</em></td>
<td>“Greece has greatly benefited from PRACE since its inauguration in 2010. It has helped to strengthen the HPC expertise in the country by means of training and knowledge exchange with other European HPC centres, and has stimulated the funding of the national HPC infrastructure.”</td>
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<td>HUNGARY</td>
<td>Dr. Tamas Maray, Technical Director</td>
<td><em>NIIF Institute</em></td>
<td>“PRACE gives our scientists access to world-class HPC resources that a small country could not afford on its own. It also enables us to learn from and exchange knowledge with the leading HPC centres and specialists of Europe.”</td>
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<td>IRELAND</td>
<td>Prof. JC Despla, Director of ICHEC</td>
<td><em>Irish Centre for High-End Computing (ICHEC)</em></td>
<td>“Ireland can never and should never seek to have the largest computers in Europe, but thanks to the ambition of PRACE and European collaboration, Ireland's research community can compete for and secure this level of capability within Europe.”</td>
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<td>ISRAEL</td>
<td>Professor Shlomi Dolev, Chairman</td>
<td><em>Israel Inter-University Computation Center</em></td>
<td>“HPC is one of the most important tools for innovative research and since joining PRACE, a growing number of Israeli researchers have been awarded core hours. Membership to this pan-European effort helps us deliver high performance networking and new technologies to Israel.”</td>
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## PRACE Members

### ITALY
Francesca Garofalo, Responsible of Coordination and Project Management Office  
*SuperComputing Applications and Innovation Department (SCAI), CINECA*  
“PRACE has helped the Italian scientific community gain great benefits from the access to the most advanced, powerful and integrated digital resources and services for scientific discovery, to becoming themselves actors of the big challenge to push Italian and European competitiveness forward.”  
[www.hpc.cineca.it](http://www.hpc.cineca.it)

### NETHERLANDS
Professor. Dr. Anwar Osseyran, Managing Director  
*SURFsara BV*  
“PRACE has enabled scientists from the Netherlands to get access to large capability systems at the top of the HPC pyramid, which has allowed them to scale up their scientific challenges. Access to the PRACE systems has also been a driving force in further improvement of the national HPC infrastructure in the Netherlands, including industrial interest, as the scientific results of PRACE stimulate scientists to grow and extend their models.”  
[www.surfsara.nl](http://www.surfsara.nl)

### NORWAY
Arild Halsetrønning, Managing Director  
*UNINETT Sigma*  
“Norway in isolation does not have sufficient critical mass and funding to develop and maintain an agile production computing infrastructure that at any time entirely fulfils our needs. However, as a member country in PRACE, Norwegian scientists have access to HPC systems with a capacity or an architecture which are not available at a national level.”  
[www.uninett.no/Sigma](http://www.uninett.no/Sigma)

### POLAND
Dr. Norbert Meyer, Head of HPC Department  
*Poznan Supercomputing and Networking Center*  
“Poland as a country is a PRACE partner from the very beginning and member (PSNC) of PRACE AISBL. All of these actions were related to our plans to give the Polish scientific community an alternative solution to use PFlops machines in Europe for those who have critical HPC applications from the area of grand challenges. In addition, there is a unique opportunity to participate in training and request for assistance of qualified personnel to optimise the applications source code.”  
[www.man.poznan.pl](http://www.man.poznan.pl)

### PORTUGAL
Professor Pedro Almeida Vieira Alberto, Professor of Physics and Coordinator  
*Laboratory for Advanced Computing of the University of Coimbra (UC-LCA)*  
“The success of PRACE as a European HPC infrastructure is measured by its continuing effective support of European Science and Technology which rely on large scale numerical simulations. PRACE has supported leading edge research by Portuguese scientists and has stimulated the development of the HPC infrastructure in Portugal which in turn will enhance the international competitiveness of national researchers and companies.”  
[www.uc.pt/lca](http://www.uc.pt/lca)
SLOVAKIA
Professor Dr. Jozef Noga, Coordinator & Professor of Chemical Physics
Computing Centre of the Slovak Academy of Sciences
“After a long time gap, two years ago our country restarted investments into high performance computing. This facility has been successfully exploited in diverse areas of our research. Being an adhering member of PRACE since 2014, we expect new opportunities in HPC for our scientists, far beyond the capacity that our small country can allow.”
www.vs.sav.sk

SLOVENIA
Professor Dr. Jožef Duhovnik, Laboratory Head
“Membership in PRACE is a great recognition for the University of Ljubljana and also a great challenge. We have to justify the trust of the Slovenian country and the European partners, not only in terms of technological development, but above all, through promoting and facilitating the use of supercomputing in education and industry.”
www.fs.uni-lj.si

SPAIN
Francesc Subirada, Associate Director
BSC (Barcelona Supercomputing Center)
“PRACE has proved its importance so far as regards the future of science in Europe, and also for its own cohesion. It is an honour for Spain to be one of the countries that has contributed to the infrastructure, and we hope to continue on the same path in the future. Also, we are well aware that it is really important to achieve a more significant participation of companies in the PRACE infrastructure.”
www.bsc.es

SWEDEN
Dr. Jacko Koster, Director
Swedish National Infrastructure for Computing (SNIC)
“Access to PRACE resources provides Swedish scientists with access to resources not available nationally. The participation of SNIC in PRACE represents a long-term collaboration of SNIC with major European centres to help understand and tackle technical and policy challenges that are inherent to HPC infrastructure.”
www.snic.se

SWITZERLAND
Dr. Maria Grazia Giuffreda, Head of user Engagement & Support
ETH Zurich/Swiss National Supercomputing Centre, CSCS
“In its first five years, PRACE aimed at creating a European Science Ecosystem that, by bypassing geographical borders, attempts to support and enable high impact scientific research. Swiss science has enthusiastically contributed to the ecosystem by being at the forefront of development worldwide.”
www.cscs.ch

TURKEY
Ertugrul Karacuha, Director
National HPC Center (UHeM)
“The PRACE infrastructure project has definitely made an invaluable contribution to the science community and to science itself. The Turkish scientists working on the relevant subjects had great opportunities to collaborate with European colleagues through PRACE.”
www.uhem.itu.edu.tr

UNITED KINGDOM
Dr. Susan Morrell, Head of Research Infrastructure
EPSRC
“The UK’s world-leading computational scientists and engineers require equally world-leading computing infrastructure to carry out their research, and the PRACE infrastructure has played a key role in enabling some exciting and innovative research projects to be carried out, which would not have been possible using national facilities.”
www.epsrc.ac.uk
The last year has been very busy for the Scientific Steering Committee (SSC) with a great deal of attention being paid to ensuring that the future needs of European science and innovation can be met with PRACE 2.0, the next step in the evolution of the PRACE research infrastructure. In shaping PRACE 2.0, it has been a great pleasure as chairman of the Scientific Steering Committee (SSC) to note the strong commitment all PRACE partners have on science and scientific excellence as key to the success of PRACE. This makes me confident that PRACE will continue to be a success, fostering scientific and innovation excellence in Europe by providing world-class computing facilities and services. By providing training through the PRACE Advanced Training Centres (PATC), PRACE will also transform European science and industry into the more computationally driven approach that will characterise science and innovation in the future.

Data is becoming increasingly important in many areas of science. The computations made on PRACE resources provide a wealth of data that can contain the seed for new scientific discoveries, and it is important that these opportunities are being fully exploited. Following the recommendation of the SSC based on an expression of interest on big data across scientific communities, the Council of PRACE approved a pilot call for joint data storage services and resources, now part of the 11th call for PRACE access, in order to help maximise the scientific value of the calculations performed on PRACE resources.

With the fast pace in the evolution of computational hardware towards exascale and new scientific needs in terms of computing and storage solutions, there is a growing recognition that software maximising the utilisation of computational hardware is essential for making breakthroughs in computational science. This is recognised by the European Commission in their recent call for the establishment of Centres of Excellence for computing application. PRACE supports this initiative and will provide the selected Centres of the Excellence with access to its world-class resources and services in order to enable computational applications that can serve the scientific community.

The SSC has been carefully monitoring the quality of the science produced using PRACE resources. We are happy to note the high standards of our peer-review process, and that this enables us to support the best European research. PRACE currently provides computational resources to more than 50 research projects funded by the European Research Council, totalling more than 800 million core hours. The science produced has a high impact and includes several papers in high-ranking journals such as Nature.

My term as Chairman of the Scientific Steering Committee has come to an end. It has been a great privilege to contribute to PRACE aisbl and help position European science at the forefront in the use of computational science for enabling scientific discovery and innovation in international research. I would like to acknowledge the important contributions of Prof. Richard Kenway who is now stepping down as past Chair of the SSC. As the first Chair of the SSC, he was instrumental in making the SSC a key partner for PRACE and for defining the high scientific standards that now characterise the PRACE research infrastructure.

I welcome Dr. Sylvie Joussaume as the new Chair of the SSC and Prof. Petros Komoutsakos as the new Vice Chair. Under their leadership, the SSC will continue to be an important contributor to ensure European excellence in science and innovation through the computational resources made available through the PRACE research infrastructure following a rigorous centralised peer review processes.
Caught and caged: the future of drug delivery

DNANANO is bringing the frontiers of nanotechnology to the heart of biomedicine. With innovative new designs for a more stable and effective breed of nanodevice, the emerging field of nano-biomedicine could soon welcome in a new era of targeted drug delivery.

In the current science and technology landscape, nanoscience promises huge advances for a variety of fields that are otherwise reaching their technological limitations. One area in which nanoscience holds special excitement is in the field of biomedicine where its potential to revolutionise targeted drug delivery is eagerly anticipated.

To enable such advances a major focus for nanoscience is in meeting the demand for new bottom-up methods of self-assembling nanodevices which, thanks to strict properties of self-recognition, have their ideal ingredient in DNA. However, the routine use of synthetic oligonucleotides and techniques such as cryogenic transmission electron microscopy (Cryo-TEM) and small-angle x-ray scattering (SAXS) make the construction and experimentation of 3D-DNA nanostructures a costly, low yield procedure.

To reduce these expenses, the DNANANO project is running long-time atomistic simulations using the Curie supercomputer in France. By predicting the likelihood of successful self-assembly of DNA nanostructures and their structural properties, the costly trial and error element can be eliminated, ultimately allowing for more robust and accurate designs of DNA nanostructures.

Figure A: Original truncated octahedron nanocage composed by twelve B-DNA helices forming the hexagonal faces and six square shaped faces made up of four single-strand linkers.

**“The seven million core hours on the Tier-0 system awarded to the team – led by Professor Mattia Falconi – under the PRACE 6th Call for Proposals has been essential for their operations”**
Taking their cue from a nanocage published prior to DNANANO, Professor Falconi and the team are looking to produce the first example of a preassembled DNA nanocage capable of a reversible controlled encapsulation and release of cargo. The original nanocage is a truncated octahedron composed of twelve B-DNA helices forming the hexagonal faces and six square shaped ‘corners’ made up of four single-strand linkers. “We are modifying one face of this polyhedron, one square face, by introducing hairpins,” explains Professor Falconi. In other words, four single-strand linkers making up one of the corners are replaced with these hairpins, structures known to open when subjected to increasing temperatures (Figure 1 A, B).

At 37°C, the original nanocage is unable to hold a cargo of the enzyme horseradish peroxidase (HRP) because its hexagonal faces are too small to afford the HRP entry. With its new hairpins, however, simulations of the modified nanocage at 37°C show that it undergoes sufficient fluctuations and deformation to allow the HRP molecule access. Furthermore, at 4°C these effects are no longer observed, meaning that the introduction of hairpins affects a specific type of change whereby the protein can enter, reside and leave the nanocage depending on the temperature (Figure 2). This then, is indeed one of the first examples of a preassembled DNA nanocage capable of a reversible controlled encapsulation and release of its cargo. In a cellular context this mechanism of encapsulation cannot feasibly be used in full for biomedical applications but it does provide a remarkably strong proof-of-concept.

Meanwhile, another series of similar octahedral nanocages has helped Professor Falconi to gain important insights into the factors influencing their stability and dynamical properties. In three cages, the double helices are connected with different single-strand linkers - either thymidines, adenines or a mixture of the two - to determine their impact. Surprisingly, classical MD techniques have shown that different linkers do little to alter the stability and dynamical properties of the nanocages, which can instead be attributed primarily to the geometry of the nanostructures themselves.

Though these nanocages are hardly affected by the differences between single-strand linkers, a change is altogether more apparent when they are replaced by double helices. Having experimentally assembled a nanocage entirely with double-strand linkers, MD analysis shows that the structure is much stronger and more stable than its single-strand predecessors.
Increase in stability brings with it the possibility of more robust designs, a useful tool for the general advancement of nanostructure functionalities. This wholly double-stranded DNA nanocage, for example, could potentially be employed as a building block for higher order structures.

Although a solely temperature stimulated nanocage carrier is not entirely practical, as a proof-of-concept it has provided the stimulus to pursue what DNANANO started. “Now we are working on a new kind of mechanism for opening and closing our structure,” explains Professor Falconi. The idea is to introduce a programmable pH-triggered nano-switch into their nanocage by replacing two of the linkers in just one corner with two DNA triple helices or with two mismatched hairpins. The pH-dependency of these replacement triple helices can be tweaked with precision over more than five units to act as a gate while the two mismatched hairpins take care of the temperature dependence.

With these controllable gates, it should be possible produce a DNA nanocage that can transport and release its cargo under very specific pH/temperature conditions.

“We are collaborating with groups who are experts in DNA design, assembly and spectroscopic characterisation,” states Professor Falconi, “and with colleagues from Tor Vergata’s Department of Chemistry we will investigate the pH we need to open the gates.” Looking to use PRACE assigned facilities once again, the combined expertise of these groups aims to provide them with a holistic understanding of the project and insights that allow a continual refinement of the proposed mechanism. If they can pull it off, this innovative DNA nanocage will mark a decisive step forward for nano-bio-medicine.

**Project title:** DNANANO Molecular dynamics simulation and experimental characterization of a DNA nanocage family.

**Project leader:** Prof. Mattia Falconi, Structural Biology Group, Department of Biology, University of Rome Tor Vergata, Italy

**Project details:** Awarded 7 million core hours on CURIE Fat Nodes (FN) @ GENCI @ CEA, France
**TRASFER: a new direction for spintronics**

The physics behind spin transfer electronics (spintronics) has helped a host of electrical devices become successively smaller, more efficient and cheaper. Now, Dr Paolo Barone aims to merge the fields of Rashba physics and ferroelectrics to explore its potential application in spintronic devices.

Since its emergence in the 1980s, the field of spintronics has garnered a great deal of interest for its potential to revolutionise the development of electrical devices. Rather than using the charge of electrons to carry information, spintronics aims to exploit spin-degrees of freedom and cut out the loss of energy that occurs through friction and heat, thereby achieving an unparalleled efficiency.

Recently, attention has begun to focus on spin-orbit interactions as an intrinsic mechanism for linking an electron’s spin with its motion. Particularly appealing is the relativistic spin-orbit interaction at the heart of the Rashba effect that can be found in most noncentrosymmetric materials. While this effect alone is of great interest, coupling it with the properties of ferroelectric materials may soon take spintronics in a new direction of exciting new functionalities.

Research at the SPIN institute of Italy’s National Research Council (CNR-SPIN) is dedicated to exploring and applying innovative materials in the electronics and energy fields. Heading up the TRASFER project, CNR-SPIN researcher Dr Paolo Barone is investigating candidate materials among known semiconductor ferroelectrics and new transition-metal oxide hetero-structures in which Rashba-like effects and the permanent switchable polarisation of ferroelectricity may coexist.

“Ferroelectric materials have been used for a long time in memory storage,” explains Barone, “but a ferroelectric Rashba system would imply that a single material could be used for both memory and logic applications.”

It’s one thing to grasp the fundamental physics involved when merging the ferroelectric and spintronic fields but quite another to identify new materials. But as Barone relates, it helps to spend over four million core hours on the MareNostrum at the Barcelona Supercomputing Centre (BSC):

“It was definitely needed. When you theoretically characterise a ferroelectric material it’s not just a one shot calculation, and to find new materials you need to perform lots of calculations.”

In noncentrosymmetric single crystals, the lack of inversion symmetry elicits something known as the Dresselhaus effect, which is similar to the Rashba effect. Running calculations on a perfect single crystal of the ferroelectric semiconductor germanium telluride (GeTe), it was theoretically predicted to display a large Rashba-like spin-splitting effect with switchable spin-polarisation. “Originally we thought ‘okay, we have a Rashba ferroelectric semiconductor that we can use in a modified spin-transistor with a built-in memory functionality’, states Barone, “but then we realised that there are complications in the real material.” Finding GeTe in a perfect crystal structure can be a challenge and are often host to distortions and intrinsic vacancies that affect its properties. Until ongoing collaborations with experimentalists can verify what happens in real GeTe systems, it remains to see whether it can serve as a Rashba ferroelectric semiconductor.

“When you theoretically characterise a ferroelectric material it’s not just a one shot calculation, and to find new materials you need to perform lots of calculations”
However, there is another relationship that is equally intriguing. Noncentrosymmetric materials that display Rashba effects and topological insulators are both observed to have similar spin-polarised states, implying a close relationship between the different classes of materials. By probing the topological properties of electronic structures, Barone hopes to gain a more profound understanding of the possible link that exists between topological order and Rashba physics.

In order to assess the topological properties of a range of materials, the team used post-local density approximations. “Specifically, we often used hybrid functionals that are computationally very consuming,” explains Barone, “so it would have been very difficult to perform these calculations without access to PRACE resources like MareNostrum.” Due to their ability to support surface states that are perfectly metallic, their conductivity and a spin-momentum locking similar to that of the Rashba effect, topological insulators are potentially very interesting in terms of applications. In principal one could achieve perfect conductance for highly performing devices. Here, access to BSC’s supercomputing facilities again proved essential for studying the surface states as Barone states: “In density functional theory you need to construct large supercells containing hundreds of atoms which would not have been possible without access.”

A good candidate for exploring the relationship between Rashba physics and topological order, tin telluride (SnTe) was recently proposed as the first example of a new kind of material: a topological crystalline insulator (TCI). Despite the structural similarities to GeTe, its ability to undergo ferroelectric transition at low temperature is not shared by SnTe. However, SnTe looks like an even more promising candidate as a ferroelectric Rashba semiconductor. From these investigations, Barone has unearthed the microscopic mechanisms that lead to topological transition not only in SnTe but in lead (Pb) related materials too: “By applying strain, we predict that you can have topological transitions in the whole class of Pb chalcogenides and that you can control these properties in SnTe under strain.”

While experimental collaborations continue to explore GeTe, members from the TRASFER team are already targeting it for use in next-generation electronic devices. For a successful high performance spintronic device like a modified spin polarised field effect transistor (Spin-FET), you need a good conduction material. Ferroelectric materials are good insulators, so in order to successfully merge the ferroelectric and spintronic fields a compromise is needed. “Though its theoretically possible to do something with GeTe there is still a lot of work to do,” says Barone. Since ferroelectrics typically belong to a class of transition metal oxides, it would be desirable to find some other materials in order to implement its properties.

Taking a slightly different approach, Barone is currently planning to initiate an investigation into the relativistic electronic properties of such transition metal oxides, though instead of single crystal forms, he will be looking into heterostructures. Potentially, one may in some way be able to control the material’s insulating properties and induce a transition toward semiconductance. If Barone can achieve the desired compromise between ferroelectrics and semiconducting materials for novel functionalities, then his next project just might usher in the next generation of spintronic devices.

**Project title:** TRASFER - integrating Topological order and RAShba-like effects in FERoelectrics  
**Project leader:** Dr. Paolo Barone, CNR-SPIN, Consiglio Nazionale delle Ricerche, Italy  
**Project details:** This project was awarded 4.4 million core hours on MareNostrum @ BSC-CNS , Spain
Calculating the cosmos

Simulations of galaxy evolution have consistently come up short against the problem of feedback, a complex set of mechanisms that directly impact on galaxy formation. Professor Joop Schaye and Dr Rob Crain of Leiden University have been untangling feedback on the frontline of efforts to construct the first accurate virtual universe.

By pointing a telescope into space one can learn a lot about the universe, but until the human lifespan can stretch over billions of years, direct observations aren’t going to yield much variation in the properties of individual galaxies. Determining the precise physical conditions that drive galaxy formation and evolution requires powerful numerical simulations that allow us to witness the lives of these star systems from their birth to the present day in a matter of minutes.

Time and again, however, such simulations have failed to produce a picture that matches the view on the other side of the telescope. Now, thanks to the team behind the Evolution and Assembly of Galaxies and their Environments (EAGLE), we have the first simulation to accurately reproduce the stellar mass function as it is seen in the present day.

With its members hailing from thirteen institutes representing Australia, Belgium, Denmark, Germany, the Netherlands, Spain and the UK, the EAGLE team is as big as its members’ ambition. Working with their colleagues from Durham University, Leiden University’s Professor Joop Schaye and Dr Rob Crain (now at Liverpool John...
Moores University) have emerged from the numerical difficulties besetting earlier attempts with the right parameters for their cosmological simulations. This is in no small part thanks to the access awarded by PRACE to the Curie supercomputer in France, the second Tier-0 system open to scientists in Europe. “In my opinion,” states Crain, “our allocation of just under 40,000,000 core hours CPU time was instrumental to the project’s success.”

In lieu of an experimental side to the discipline, simulations make it possible to tinker around with the physics that are thought to control the formation and evolution of galaxies. “We can, for example, make gravity stronger or weaker. We can turn the knobs of the experiment,” explains Schaye. With the desired alterations, a simulation is run to the present day to see if it matches up with the observation.

Gravity as a force is thought to be understood relatively well. What is not well understood is a process known as feedback, a combination of mechanisms impacting the interstellar gas that forms the fuel supply to galaxies. While its importance has long been known, feedback has consistently thrown a spanner in the works for cosmological simulations, as Schaye explains: “Without having the feedback sorted out, galaxies were too massive, too compact and too spherical. Galactic winds and outflows were typically not strong enough in those previous simulations.”

The time afforded with the Curie supercomputer has been crucial to solving the issue, enabling EAGLE’s team to conclude what the specific feedback problem was. “People can get the wrong impression and think ‘why didn’t you just turn the dial up on the strengths of the winds’?, but it was the ability to use these supercomputing facilities that enabled us to figure out that it was a problem which needed addressing both numerically and physically,” says Crain.

In EAGLE’s simulations, feedback is driven by two main processes: one associated with the formation of stars and another concerning the growth of black holes lying at the centre of galaxies. Without these processes properly configured, virtual galaxies grow too soon in the cosmic history and too massive. “Really what we’re trying to do with these physical mechanisms,” Crain explains, “is to find a way of putting the galaxies on a diet.” By running lots of simulations, the team were finally able to see how these processes needed to be linked to the formation and evolution of galaxies in order to produce the right growth history (by realising that the galactic winds and outflows had been too weak, and then working out how to strengthen them). The end result: a stellar mass function that looks as it is seen through a telescope.

Typically, it is much easier to gain access to facilities like Curie in order to carry out production runs than it is for time-consuming experimentation, and here the PRACE award has proved invaluable to EAGLE. Shorter time allocations can tempt research groups to cram as many production runs into their schedule as possible but with the luxury of time, the EAGLE team were free to concentrate on experimentation and learn a lot more. Ultimately, the project’s final production run took only a fraction of the allocated time. “Testing,” states Schaye, “can require two, often five, times more than the amount needed for the run. Without the time to do that we would not have been able to do the project.”

“For EAGLE, this huge step is just the beginning. Now, a thorough analysis of the simulations can begin in earnest which, as prior experience has taught Schaye and Crain, means a flurry of published papers and some years to digest their findings. But this is all part and parcel of a process that promises to offer exciting new discoveries about our universe. Already, these simulations have opened up new avenues of research and spin off simulation projects. Now that a representative volume of space (that’s an area comprising around 10,000 Milky Way sized galaxies or bigger) has successfully been reconstructed, they want to develop simulations that can zoom in on individual objects at a much higher resolution.

The representative simulation EAGLE has achieved means it is possible to delve further than ever before into the physics of galactic construction. One can ask, for instance, what factors have caused the diversity of properties in the galaxies that are observed in the universe? Some galaxies are large, some are spiral and others elliptical; some galaxies are forming stars efficiently while some are not forming stars at all. “Now that we have a simulation that reproduces this diversity,” explains Schaye, “we can use it to look for the physical causes and see why this is the case.” No less than a virtual time machine, EAGLE’s simulations will afford the greatest insight yet into the processes that have led to and continue to affect our own Milky Way and the universe around us.

**Project title:** EAGLE - Evolution and Assembly of GaLaxies and their Environments  
**Project leader:** Prof Joop Schaye, Leiden Observatory, Leiden University, Netherlands  
**Project details:** Awarded 39.8 million core hours on CURIE Thin Nodes (TN) @ GENCI @ CEA, France
Conventional particle accelerators are huge. Reaching a colossal seventeen miles in circumference and bridging the border between France and Switzerland, the Large Hadron Collider (LHC) at CERN stands as the world’s largest single machine. The LHC and accelerators like the Relativistic Heavy Ion Collider (RHIC) and Fermilab’s Tevatron, however, are beginning to reach the limits of their technology and with it our ability to grasp fundamental physics. In place of these conventional techniques, plasma based acceleration is emerging as an attractive alternative that could potentially lead to machines an order of magnitude smaller.

As an assistant researcher at the University of Lisbon’s Instituto Superior Técnico (IST), Dr. Jorge Vieira mixes theory with high performance computing to tackle a wide range of issues in the field of plasma physics. The properties of ultrarelativistic-beam plasma interactions have the potential to revolutionise conventional technologies, but to understand them one needs to run intensely powerful, computationally demanding simulations. “Access to SuperMUC was absolutely critical for the project,” states Vieira. Awarded 45 million core hours by PRACE, the facilities at the Leibniz Supercomputing Centre (LRZ) in Germany make it possible to guide theoretical development and efficiently explore all the angles of plasma physics.

A plasma accelerator can be thought of as a type of energy converter: It transforms the energy from a driver to the energy of plasma waves that is then converted into the energy of an accelerated beam. In plasma accelerators, the driver is usually an intense electron or laser pulse that is used to excite relativistic plasma waves, and inside these waves particles can be trapped and accelerated. “By increasing the energy of the driver,” Vieira explains, “in principle you will also be able to increase the energy of the particles that will be accelerated.”

Before plasma-based accelerators can enjoy widespread scientific and industrial deployment, however, a few issues need to be resolved. Large amplitude plasma waves are perfect for electron acceleration, but their use in positron acceleration has been a longstanding challenge. This is because the background plasma ions in large amplitude plasma waves exert a defocusing effect on positrons. The total distance, or total time, for acceleration would therefore be relative to the typical distance or time that the positron beam takes to become defocused. In this scenario, energy gains would simply be too small.

With the SuperMUC computer, however, Vieira has been able to run simulations that paint a different picture for positron acceleration. As a driver, an intense Laguerre-Gaussian laser - shaped like a doughnut - is able to generate large amplitude plasma waves ideal for high-energy positron acceleration. These capabilities are integral to the viability of plasma acceleration as an alternative to the conventional methods. Successful simulations of positron acceleration in large amplitude plasma waves like these provide the basis for future designs of plasma-based linear colliders.
Plasma acceleration also holds great promise for the future of imaging. When relativistic charged particles accelerate in a plasma wave they can also emit intense bursts of X-rays. Since their typical energy is dependent on both the total energy of the relativistic particles and their trajectory while accelerating, SuperMUC supercomputing resources were critical for looking into ways to control these trajectories and enhance X-ray emission. This was done in collaboration with Dr Marija Vranic and Dr Joana Martins from the same research team at IST. Firstly, an ultrarelativistic electron beam was generated from a wakefield accelerator. Against this beam, an intense laser pulse was collided to produce a counter propagating effect. Under the influence of the laser pulse, the wriggling and the motion of the electron beam successfully led to enhanced X-ray emission. Such enhancement, as Vieira illustrates, could mean a new generation of compact like sources: “Any application, from medicine to material science, related to the imaging of small micrometric structures could potentially benefit from the X-rays emitted in plasma accelerators.”

Figure 3: Three-dimensional simulation of a plasma wakefield excited by a donut shaped laser. Green surfaces represent regions of constant plasma density.

In 2009 a bold idea concerning proton driven plasma acceleration was published in Nature Physics. It described how a proton beam could drive a plasma wave so intense that in a single plasma stage electrons would be accelerated to energies far greater than conventional accelerators can manage today. As drivers, the proton bunches at CERN are the most energetic beams of any kind currently available and could potentially accelerate electrons and positrons beyond the energy frontier.

It’s a daunting task, however, as the concept of proton driven plasma acceleration rests on the assumption that CERN’s proton bunches can be dramatically compressed, a difficult thing to achieve with conventional technology. Gearing up to carry out the world’s first proof-of-principle experiment is the AWAKE project, a large-scale collaborative effort that aims to begin injecting the first proton beams into a plasma cell in 2016.

In preparation of the AWAKE experiment Vieira has been tackling a troublesome phenomenon known as hosing instability (HI). Unlike most plasma acceleration experiments, the large amplitude plasma waves generated in the AWAKE experiment will occur through another phenomenon called self-modulation instability (SMI), but HI, also known as ‘beam break-up instability’, can compete with SMI. “If you imagine a fireman’s hose that really violently wriggles around,” explains Vieira, “then this gives a physical picture of what happens to a beam under the influence of HI.” These oscillations and large amplitude wriggling keep growing in time and eventually lead to the break up of the beam.

“Any application, from medicine to material science, related to the imaging of small micrometric structures could potentially benefit from the X-rays emitted in plasma accelerators”

In a simplified model of HI mimicking the AWAKE experiment, Vieira gathered predictions of possible conditions that would suppress this instability, which could then be tested using 3D simulations. Homing in on a new mechanism for HI suppression, Vieira has found a way to make sure that SMI can grow, saturate and lead to the excitation of large amplitude plasma waves, thereby establishing the conditions for future experiments at CERN.

Though they may not be able to accelerate electrons to the same level as in the CERN experiment, the Stanford Linear Accelerator Centre (SLAC) provides conditions where Vieira can test some of the key physics concerning AWAKE, acting as a kind of surrogate for the future experiments. “The problems that we are dealing with are very complex from a conceptual and theoretical point of view,” states Vieira, “and the physics is very challenging. These experiments are also pushing the limits of these simulations and theories because we are working in very challenging regimes of plasmas.” It is in pushing these boundaries, however, that we are closer than ever to overcoming the limitations of conventional accelerator technology.

This project was part of a European Research Council Advanced Grant Accelerates (ERC-2010-AdG grant 26784 [11]), awarded to Luis O. Silva in 2010

Project title: Ultra-Relativistic Beam Plasma Interactions: From Miniaturized Plasma Based Accelerators to Extreme Astrophysical Conditions
Project leader: Dr. Jorge Viera, Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Portugal
Project details: This project was awarded 45 million core hours on SuperMUC @ GCS@LRZ, Germany
Keeping the flame alive

A long and continued endeavour of the combustion community has been to understand and predict the ignition phenomena. The EM2C laboratory and CERFACS have collaborated to model the “light-round” ignition process of annular combustors commonly used in aeronautics, the results of which could be used in the design of more efficient engines with reduced emissions and enhanced reliability.

In the aeronautical industry where gas turbines are used for propulsion, there is a strong need to master the ignition process. It is important to ensure that flames are not accidentally extinguished during ignition and to make sure that all injectors are fully initiated. The capacity to reignite the combustor at high altitudes is considered in engine certification, and this can impose design constraints that conflict with the search for cleaner combustion.

Indeed, lean combustion has received considerable interest in recent years as a way of lowering NOx emissions without reducing engine efficiency. The problem is that leaner combustion raises concerns about flame stability and leads to less favourable conditions for ignition. This is even more critical when combined with the decrease in the number of injection systems, intended to reduce the cost and weight of the system but leading to less favourable conditions for flame transmission from unit to unit. Consequently, predicting ignition or re-ignition capability is crucial for the design of the next generation of cleaner aeronautical combustors.

In aero-engines, ignition is usually achieved with two spark plugs or torches located at opposite ends of the ring-shaped (annular) chamber, starting a “light-round” process which can be broken down into three phases: energy deposition, in which a spark produces an initial flame kernel; kernel expansion, where the kernel spreads and creates a flame that stabilises near to the fuel injector next to the initial spark; and flame propagation, in which the flame front traverses the whole annular space and progressively ignites the rest of the injectors.

“At the EM2C laboratory, we are now preparing a new generation of MICCA combustor that will be equipped with liquid injectors”

The physics of ignition during the energy deposition phase is quite complex and cannot be predicted accurately with current models. However, kernel expansion and flame propagation can now be investigated with methods developed more recently such as Large Eddy Simulations (LES) of reacting flows and these methods can be validated in well controlled laboratory scale models reproducing the main features of real combustors but allowing full visualization of the flame.

During his PhD thesis at CERFACS, Dr Matthieu Boileau simulated the ignition of an annular combustor similar to that found in a helicopter engine, but no comparison with experimental data on the flame dynamics was possible. Now at the EM2C Laboratory at the French National Centre for Scientific Research (CNRS), Boileau has been part of a project involving a team at this lab (comprising doctoral student, Maxime Philip and senior staff members including Ronan Vicquelin, Thomas Schmitt, Daniel Durox and Sébastien Candel) and a team at CERFACS (involving the senior researchers Eleonore Riber, Florent Duchaine and Bénédicte Cuenot). The project was intended to allow validation of the simulation methodology relying on the AVBP flow solver (co-developed by IFPEN and CERFACS) in combination
with the EM2C tabulated chemistry model using a novel combustor (designated as MICCA) designed by EM2C and to perform a cross comparison with the methods developed at CERFACS.

The project’s first task was to perform LES of the ignition process of the annular combustor MICCA. This device reproduces many of the features of a typical aero-nautical combustor allowing detailed imaging of the flame during the light-round. It was this objective that required extensive computing resources and the reason that the team initially sought to access the PRACE programme. While typical Tier-1 resources are generally sufficient to calculate a single-injector configuration, Tier-0 resources (15 million CPU hours on TGCC Curie running 6144-core jobs as part of the PRACE 5th Call for Proposals for Project Access) were necessary to handle the 16 injectors of the MICCA configuration.

“In parallel, we will develop new calculations of the ignition sequence including the spray modelling”

Two combustion models were tested and compared. One was the TFLES model, which was based on an artificial thickening of the flame front and had been extensively used by CERFACS in previous ignition calculations, while the other was the FTACLES model developed at EM2C, which was based on tabulated chemistry and spatial filtering of the flame front. By using the two models, the researchers were able to evaluate the importance of the description of chemical kinetics for the simulation of light-round ignition.

“Our results have been quite promising,” says Boileau. “We have simulated an ignition sequence, doing several runs at various operating conditions and using different combustion models. The computed flame and the direct visualisation of the experiment showed excellent quantitative agreement with experimental data. “This indicates that the LES can reliably reproduce the large-scale structures and dynamics of light-round ignition.”

The different stages of the light-round process were explicitly predicted by the LES. The expansion of the initial kernel rapidly produced an arch-shaped flame that split in two large fronts, which then propagated in opposite directions and finally merged. In each stage, the shape of the experimental flame was reproduced by the LES. In addition, the merging time predicted in the LES was quite close to the value observed for various experimental shots in the same conditions.

Using these results, Boileau and his colleagues are working on the development of a reduced-order model of the light-round process. “If we can take into account the key parameters that control the process, we hope to create a model that can provide engineers with quick answers in the design process of better combustors, but which does not require the large CPU resources and long restitution times that the LES approach requires.”

The current work is the first step in a long-term research programme that aims to investigate the ignition of multi-injector combustors using a combination of experimental and numerical approaches. A natural continuation will be to study the effects of heat transfer between the flow and the combustor walls. The current experimental campaign has showed that the thermal conditions of the combustor walls strongly influence ignition time, suggesting that an accurate modelling of heat transfer in the simulation is required.

The current MICCA experiment is strongly simplified in that it uses an injection of a premixed gaseous mixture, whereas real aero-engines feature droplet spray injection systems. The use of liquid injection will introduce new physics that require dedicated modelling methods and involve a number of new controlling parameters. “At the EM2C, CNRS laboratory, we are now preparing a new combustor MICCA-Spray that will be equipped with liquid injectors,” states Boileau. “In parallel, we will develop new calculations of the ignition sequence including the spray modelling.” As the accuracy of the models of ignition improve, so too will their ability to contribute to a reduction in emissions from aeronautical vehicles.

**Project title:** SIMAC - Simulation of ignition mechanisms in annular multi-injector combustors and comparison with experiments  
**Project leader:** Dr. Matthieu Boileau, EM2C Laboratory – CNRS UPR288, Ecole Centrale, Paris, France  
**Project details:** Awarded 15 million core hours on CURIE Thin Nodes (TN) @ GENCI @ CEA, France
Golden nanostructures

Only recently has it become possible to fully explore the properties of a class of highly promising materials: ligand-stabilised gold nanoparticles. Now, for the first time, these systems are revealing important lessons on the birth of plasmon behaviour.

Ligand-stabilised gold nanoclusters are a highly interesting class of novel nanomaterial. For a while now, the use of thiolate ligand molecules to stabilise gold nanoparticles has been recognised as a handy way to synthetically achieve electrochemically, thermally and air-stable cluster compounds with tuneable sizes and properties at the nanoscale. Using light to excite the electrons in the metal, one can induce collective plasma oscillations. By enhancing their ability to absorb light, these materials are in theory able to carry much more information than conventional electronics can.

With characteristics as promising as this it is little wonder that their potential for application spans such a wide range of areas: virus labelling, drug delivery, sensor devices and nanoparticle catalysis are just a few. Hannu Häkkinen, a professor of computational nanoscience at the University of Jyväskylä (JYU) in Finland, heads a group specialising in these ligand-stabilized metal nanoparticles, exploring their electronic, optical, magnetic, chemical and catalytic properties. To achieve a microscopic understanding of the emergence of collective excitations in these nanostructures, Häkkinen has been running complex calculations that employ large-scale density functional theory (DFT) and linear-response time-dependent DFT using Hermit, the supercomputer housed at the High Performance Computing Centre Stuttgart (HLRS) in Germany. Allocated through PRACE, supercomputing facilities such as these are essential for carrying out calculations this demanding. “Nobody has tried to do this before because there are thousands of electrons to keep track of,” states Häkkinen, “and that requires very large parallel computer resources to do.”

Although known about for some time, it is only in the last decade that the chemistry to synthesise these metal nanoclusters at a detailed molecular level has been mastered. Without this, it would be impossible to achieve a precise understanding of
Plasmonics is a rapidly developing sub-field of nanoscience which aims at manipulation of light by using metal nanostructures such as nanoparticles, nano-bridges and “nano-antennas”. Possible applications include chemical sensors, non-intrusive detection and manipulation of biological reactions, and imaging and manipulation of biological systems.

While helping to establish the lower size limits of the plasmonic behaviour of thiol-stabilised gold, gold-silver and gold-copper nanoclusters, a side project provided an unexpected breakthrough. This kind of work usually focuses on gold, but an inorganic chemistry group in China discovered a series of very similar particles, this time made of pure silver. Being unknown at the time whether the same kind of ligand chemistry worked for silver, Häkkinen immediately began working with the group. “Using some of the core hours allocated by PRACE we were able to characterise the basic electronic structure and the absorption properties of these new particles,” Häkkinen explains. “It came as a surprise, but a very nice surprise.”

Among their wide array of potential applications, Häkkinen has begun to explore how the chemistry of these materials works with real bio-nanoparticles. Inspired by experimental collaborators at JYU using gold nanoparticles in electron microscopy, a new project aims to find out how the gold surfaces of these materials can be bound to virus proteins with precision and sensitivity. “The hope there,” says Häkkinen, “is that once we learn more about how to label viruses with these gold nanoparticles, then interesting possibilities might open up: can you somehow treat or kill the virus by exerting a lot of radiation through these metallic nanoparticles?”

As well as producing some unexpected breakthroughs, this research is an invaluable asset in setting the ground for further studies of ligand effects on plasmonic behaviour. Given the importance of plasmonics as a fast evolving field in nanoscience, these contributions to our understanding of the emergence of collective excitations in these materials will have a profound impact on the future of plasmonic applications.

**Project title**: Plasmonic ligand-stabilized gold nanoclusters  
**Project leader**: Prof. Hannu Häkkinen, University of Jyväskylä, Finland  
**Project details**: This project was awarded 18,358,272 core hours on Hermit @ GCS @HLRS, Germany
It’s only a phase: describing the quark-gluon plasma

The University of Wuppertal’s Dr Szabolcs Borsányi is delving into the furthest reaches of the universe’s history to describe a strange, short phase in its evolution that could help elucidate the mysteries of quantum chromodynamics.

For an infinitesimally short moment after the big bang there came into existence a hot, dense matter comprised of quarks and gluons which has come to be known as the quark-gluon plasma (QGP). Studying the few millionths of a second in which the plasma lasted, quantum chromodynamics (QCD) theory aims to expand our knowledge of this period in the universe’s evolution when quarks and gluons were briefly able to move freely.

Quarks and gluons are elementary particles which most of the time work together to form subatomic particles like protons and neutrons. Not long after QGP was brought to life in a blaze of heat, it rapidly began to cool and by the time it froze, the gluons had bound the quarks together into subatomic particles.

Thanks to particle accelerators, the conditions in which QGP is formed are reproducible but fundamental questions about this new form of matter remain unanswered. At what point, for instance, does the plasma break up, and down to what temperature does it survive? With funding from the German Research Foundation (DFG) and access to the Jülich Supercomputing Centre (JSC) awarded by PRACE, Dr Szabolcs Borsányi has been heading up an exciting investigation into the ephemeral plasma to find out.

There are, of course, challenges in measuring the properties of such short lived matter, not least because it is only detectable from the footprint it leaves after freezing. “It’s very mysterious because no one can actually see it,” explains Borsányi, “it has come from a theory and it used to be elusive, so I’m very happy that the existence of this strange thing has been confirmed.” But with only a few features of QGP known, it is impossible to properly define. In attempting to understand the plasma better, Borsányi and his colleagues have endeavoured to go beyond simple approximations and define this new form of matter with large-scale lattice simulations.

Lattice simulations are one of the best methods around for studying QCD and the only way that doesn’t resort to approximations. By putting space-time on a four dimensional lattice they can be used to recreate specific instants in the evolution of the plasma. Borsányi’s initial outings with JSC’s Blue Gene Q system were dedicated to pinpointing the transition temperature to determine from what moment onwards one can actually talk about a plasma. This

“We are not the only group working on this problem and to be on the edge of such competition, the PRACE access was absolutely essential to our success.”

 Success Stories

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is not the first attempt to extract such information but earlier efforts used experimental approaches requiring large amounts of modelling to interpret their data. Ideally, less is better since any modelling can break down at a certain point and the hadron resonance gas model employed in these experiments may be too simple and lacking in precision.

Sceptical of its simplicity, Borsányi replaced the model dependent part of the estimate using data gleaned from routine experimentation to tune the lattice simulations to a certain temperature. A considerable amount of parameters have to be added to ensure that a simulation is meaningful but this is no straightforward task. Nature realises a certain proton mass, for example, and this has to be reproduced in a lattice simulation. If the parameters are not right, then the simulation will not be reproducing nature. “One shouldn’t underestimate the effort that goes into this,” states Borsányi, “if we make a mistake and simulate a different nature then all the results will have a systematic error.”

After setting the parameters and mapping different temperatures, for example, lattice simulations allow you to measure the pressure, the energy density or, as in this project, the grand canonical fluctuations of the various cause of charges. Using a separate simulation for each temperature of interest, one can compare the single instant observed in an experiment against the lattice simulations to find a match. This match gives the most likely temperature. A great deal is going on in the lifetime of QGP, however, meaning yet more simulations may be needed to account for new observables, as Borsányi explains: “When we do lattice simulations it means that we always do lots of lattice simulations with lots of parameters.” In this way, Borsányi’s team could identify certain temperature points for certain phenomena up to the point when the whole plasma broke up.

During the 90 million allocated core hours CPU time, this intensive process does not appear to have descended into rigmarole for the team: “I really enjoyed working on the Blue Gene Q system,” Borsányi enthuses. “We are not the only group working on this problem and to be on the edge of such competition, the PRACE access was absolutely essential to our success.” By comparing several possible temperatures and finding a match, the team is able to put non-trivial constraints on what the actual temperature is at the moment of last inelastic scattering. In doing so, Borsányi can show that this temperature is almost 157 mega-electron volts (MeV), meaning the plasma’s freeze out likely coincides with QCD transition. These results provide nothing less than the theoretical background necessary for heavy ion experiments currently underway at the Large Hadron Collider (LHC) and the Relativistic Heavy Ion Collider (RHIC).

Already, Borsányi has extended the project in hot pursuit of the next goal: finding the plasma’s chemical potentials. With access again afforded by PRACE to Tier-0 supercomputing facilities (88 million core hours at Forschungszentrum Juelich and 73.2 million core hours at CINECA), the team is running experiments with various different collision energies so that the density of the plasma at the point of break up will be strongly dependent on them. It is hoped that such an approach will enable the team to further describe the plasma by chemical potential just before the point of break up. “I hope there will be results in the not very distant future,” says Borsányi, “but it’s not the only direction in which we can go and there will be more experiments yet.”

The QCD phase diagram requires a lot of investigation both theoretically and experimentally, but Borsányi is confident that these projects will continue to push the envelope and help solve QCD theory.

**Project title:** Heavy ion phenomenology form lattice simulations  
**Project leader:** Dr. Szabolcs Borsányi, Bergische Universität Wuppertal, Germany  
**Project details:** This project was awarded 91,791,360 core hours on JUQUEEN @GCS@Južlich, Germany. Resources on Fermi was awarded 73.2 million core hours at CINECA
Making it rain

ARIA Technologies, a French SME, is providing insurance companies with an improved ability to calculate risk of flooding by simulating extreme rainfall events at high resolution. This approach is particularly useful for situations in which the data available on real extreme events is scarce, or to account for climate change effects on natural hazards.

Reinsurance has long played an important role in the management of extreme events such as natural disasters. It infers risk calculation by using statistics to calculate the risk of such events occurring, collecting data from local regions based on real past events to build databases on which these calculations can be made. However, in many cases there is a lack of large amounts of data for such catastrophes, making it difficult to accurately predict future events. Past events also do not reflect the current state of climate change, which evolves rapidly nowadays. Recent research efforts have tried to counter this by expanding existing databases using “synthetic realistic event generators”. Using models of large-scale meteorological conditions that can satisfactorily mimic real past events, researchers have been able to simulate new events with physically realistic footprints and intensities.

Bruno Guillaume of ARIA Technologies (one of the partners of the Climate-KIC, the EU’s main climate innovation initiative) has been looking to use this approach to improve the risk assessment of extreme rainfall events in the Netherlands. The flat, low-lying topography of the country makes it largely vulnerable to pluvial flooding from ocean entries, and so the ability to accurately evaluate the risk of high impact regions with large amounts of houses is important. “Ideally, you want to look deep into the past and have as large a dataset as possible on the region you are studying,” explains Guillaume. “However, with extreme flooding events being few and far between, happening around every 50 to 100 years, it is not possible to have large databases of real events. In the last 20 years we have had computers capable of dealing with big data, and as such we have good data from this period, but at the beginning of the century it was not so easy.”

Classically, insurance companies have simply extrapolated from the available data, but the statistical methods used to do this suffer from the sparseness of this data and the results are quite biased. Adding simulated events to the pool of real events is thus a necessity, but although the idea is not a new one, this technique has not been used at such high cost levels before.
The simulation tools used to generate these synthetic events are developed in meteorological offices such as the NCAR/NOAA US meteorological services, the MET Office in the UK and Météo-France. One of these models, called WRF and developed by NCAR/NOAA has been used extensively by ARIA Technologies to make independent meteorological forecasts. “Our idea was to use this tool to cover the entire Netherlands with a resolution of 3km, meaning that for every 3km in latitude and longitude, the numerical model will generate information on the possible impact of rainfall events,” says Guillaume.

This precise model for rain was then combined with coarse resolution data for fields of atmospheric pressure from the NOAA20CR database, which has used a state-of-the-art data assimilation system and surface pressure observations to generate a six-hourly, four-dimensional global atmospheric dataset in current climate conditions (1990-2010)

For this project, use was made of the NOAA20CR database, produced by the American NCAR who “perturbed” the global atmospheric conditions of the 1990-2010 period slightly, producing 56 slightly different variations of what might have happened during this period in terms of atmospheric pressure. “This gives us a range of uncertainty – 56 differing representations of reality,” explains Guillaume. “We have used the data from this pre-developed database, which describes the positions of cyclones and anticyclones at a coarse resolution of 200km x 200km, and paired it with our fine resolution rainfall model.”

Using these 56 variations of atmospheric pressure over the last 20 years as input into the rainfall model, Guillaume and his team were able to simulate realistic rainfall events in the Netherlands, using a total of 6 million core hours on the CURIE supercomputer hosted by GENCI in France. However, the amount of core hours it would take to fully simulate 56 versions of 20 years of rainfall would be impossibly large. Instead, the researchers used a screening method that allowed them to search for favourable rainy events, at which point the full algorithm could be run. The researchers have thus produced a large database (around 69,000 separate events) providing a detailed view, event-by-event with footprint, of the physically possible extreme rainfall events over the Netherlands for the current climate time slice. This database is currently being plugged as an expert hazard module on pluvial flooding risk in the OASIS platform for reinsurers.

ARIA Technologies are now in the process of simplifying the algorithm. “What we have achieved with the CURIE supercomputer is a demonstration of what can be done, but using that amount of processing power and such a high-cost algorithm is obviously not practical most of the time,” Guillaume states. “We have been looking at ways of making it more efficient. We want to be able to retain 80 percent of the quality while only using 20 percent of the data.”

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“"We have been looking at ways of making it more efficient. We want to be able to retain 80 percent of the quality while only using 20 percent of the data"
You were there at the start of PRACE. Do you think PRACE 1.0 has fulfilled its objectives?

Sanzio Bassini: In 2010, there was a common understanding amongst many of the member states of the EU that there was a need to pool high-performance computing resources at a European level. Consequently, the Partnership for Advanced Computing in Europe (PRACE) AISBL association headquarters were set up in Brussels, as an association of the member states represented by their appointed delegates. Four of the member states (France, Germany, Italy and Spain) committed the equivalent of €100m over the next five years through access to their supercomputing resources, most of which were rated very highly worldwide at the time.

I believe PRACE has done an excellent job of pooling these systems and creating a single access point to high-end computing resources and services for European researchers. It has helped them maintain competitiveness with the rest of the world in terms of computational science, as well as providing a system of access based on the excellence of research and the
merit of the scientific work. Since mid-2010, there have been 10 PRACE Calls for Proposals from which over 10 billion core hours have been provided to researchers.

One of the major achievements of PRACE has been defining a method of deciding who has access to resources that are fairly limited. Typically, only one third of the demand for high-performance computing can be satisfied by the total amount of core hours available. Many projects are put forward and considered at a level of excellence and scientific merit in a blind and independent peer review process, and many are deemed eligible, but only some of them will gain access to the resources. This is decided by ranking the projects based on a transparent and fair process that has been developed by PRACE.

Another major achievement of the last five years has been the measurable improvement of scientific outcome in terms of scientific publications. The competitiveness of European systems has increased with respect to the rest of the world. Looking at statistics from Web of Science, one can see that both the number of publications and the impact factor of those publications have increased.

Where does PRACE go from here? What will PRACE 2.0 bring that is not merely a continuation of PRACE 1.0?

SB: We are now approaching the end of the first period of agreement in 2015. What we want to work towards now is the long-term vision for European HPC infrastructure that can include and provide opportunities for potential joint procurement and management of the infrastructures. This will truly allow the European HPC landscape to become competitive with the rest of the world.

It is now time to start addressing the next period of agreement — PRACE 2.0 — and the challenges that will come with that. The PRACE Council is finalising a model this year that will help to do this. Certainly many aspects of PRACE 1.0 are contained in PRACE 2.0, but as in software, the next version is always an improvement of the previous, including new features and improved functionality. And this is exactly what we will do. Already now we are developing new services or improving and expanding existing ones like our training offer via the PRACE Advanced Training Centres (PATCs).

One of the most pressing issues is the participation on all members of the association to the operational costs of the infrastructure, and the sustainability of the model moving forwards. There is a lot of debate going on at present in regards to what makes a fair basis for participation. Perhaps it should be based on the GDP of the different countries. We are not yet in a situation for potential joint procurement and so the investments remain the affairs of each of the member states, but we need to ensure that we have a method for ensuring fair distribution of all the contributions.

There are a couple of other significant issues in our agenda that we will have to face in the coming months and one is related to a substantial participation of the European Commission. Aside from the commitment and the fairness of contributions of different member states, it is also mandatory that the EC participates to the persistency of PRACE as a Pan-European Research Infrastructure. From this point of view we think that strong actions could involve different movements; firstly a bottom-up movement from the different scientific communities and member states, but also a top-down one in terms of strategy that the EC puts in place toward HPC in Europe.
Key Performance Indicators for PRACE

With so much calculating power in the PRACE portfolio, numbers about PRACE itself are becoming increasingly important to highlight its impact on HPC based research, on HPC know-how in Europe, as well as on European industry engagement in HPC.

In 2014, the PRACE Council approved a set of Key Performance Indicators (KPI) for PRACE that will allow a deeper analysis and evaluation of its achievements and successes.

PRACE impact on evolving research

Number of projects

A clear upward trend is observed in the number of project applications received via the PRACE Calls for Proposals for Project Access (Figure 1). A downward trend of rejected projects above the technical quality threshold is noted until the 5th Call, but a reversal is visible in more recent Calls. This evolution confirms the maturation process of proposal submissions, in which researchers put more effort into the quality of their proposals, but the competition has become increasingly fierce, also influenced by the amount of resources available. Moreover, the evolution reflects the good outcomes of PRACE Preparatory Access calls (including access type C) that enable prior technical support for application and scalability tests.

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

![Figure 1: Number of projects requested (blue), above technical threshold (red) and awarded (green).](image-url)
**Project resubmission**

PRACE also keeps track of the submission of project proposals by recurrent principal investigators (PIs) (Figure 2). The ratio of recurrence is relatively low: over 40 per cent of PIs who submitted the most recent proposals were recurrent applicants to a PRACE Call for Proposals for Project Access.

This highlights a good balance between a healthy renewal of demand, and recurrence of scientists whose research benefits from PRACE allocations.

**International cooperation**

A total of 60 per cent of the projects that are awarded with PRACE resources, and two-thirds (63 per cent) of those resources are awarded to “foreign projects” (i.e. projects with PIs from a different country (recorded as the primary institution of the PI) than the machine on which the research is executed). The evolution of the ratio of awarded foreign projects remains rather stable over time (Figure 2). This proves that the nationality of the PIs institution does not impact the chances of a project being awarded and underlines that the PRACE peer review process works with scientific excellence as its main criterion. This also demonstrates PRACE’s impact in the enhancement of European and International collaboration.

Co-funding for PRACE-awarded projects shows a downward trend (Figure 3), despite the clear increase between the 8th and 9th Calls. A particular increase of national co-funding is observed between the 8th and 9th Calls.

The slight increase of EC support for the projects awarded by PRACE illustrates the outcomes of EC funding policies, aligned with the support to HPC as a key enabler technology.
PRACE's impact on scientific production

Considering that it is only possible to measure the impact of PRACE Access calls on scientific production one year after the project end, Figure 4 only presents the evolution of scientific production supported by PRACE until the 5th PRACE Call for Proposals for Project Access (end of 2013).

Until the 5th PRACE Call for Proposals for Project Access, PRACE has supported 158 PhD theses, 507 publications and 719 scientific talks. On top of that, two patents resulting from projects supported by PRACE have been filed. This data reflects an increasing trend in all types of scientific production supported by PRACE.

The increase in scientific production (Figure 4) is partly related to the increase in PRACE HPC resources made available and therefore the possibility of awarding a larger number of project applications. Of course, a higher number of publications raises the chances of a higher impact in science, but a future analysis of the impact-factor of published papers will reveal quantitatively whether the quality of scientific production also improves over time.

![Figure 4: Scientific production supported by PRACE.](image)

PRACE's impact on growing know-how in Europe

Since 2008 PRACE is engaged to provide top-class education and training for computational scientists in Europe through the PRACE Advanced Training Centres (PATC), the International HPC Summer School, and PRACE seasonal schools, with a clear increase of participants registered (Figure 5). PATC courses, seasonal schools and the International HPC Summer School are offered free of charge to eligible participants.

![Figure 5: Number of person-days registered at PRACE Training days between 2008 and 2014](image)

Between August 2008 and December 2014, PRACE has provided 19,686 person-days of training through attendance-based courses, with an upward attendance trend. 5,249 unique individuals attended PRACE courses. This shows the effectiveness of PRACE in attracting, training and retaining competences.

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

The average rate of recurring participation in training is 30%. This excellent ratio proves that PRACE training is not a closed circuit where the majority of attendees are the same people.
PRACE impact attracting the industrial sector

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

The interest of industry in PRACE at high-level international events has increased steadily over the past years (Figure 7). The total number of industrial participants showing interest in PRACE during the two main HPC events (Supercomputing (SC) in the USA, and the International Supercomputing Conference (ISC) in Germany) between 2008 and 2013 was 695 unique individuals.

![Figure 6: Number of person-days registered at PRACE training days in 2014.](image)

In 2014 the number of participants registered in PATC courses was 2,545 (2,175 from academia and 274 from non-academia affiliation). More than 90% of participants attending PATC training days have academic affiliation (2,175), illustrating the impact of such events on research and scientific communities, in particular for early stage researchers and PhD students.

![Figure 7: Number of industrial attendees that made contact with the PRACE booth at ISC and SC.](image)

However, as observed in Figure 6, the total number of attendances registered is not dependent on the number of training days and courses. Despite the number of PRACE training days being the lowest in the third quarter, the number of attendances registered is the highest observed for 2014.

The ratio of companies that repeat their contact with PRACE during the main HPC events has stabilised at around 50 per cent for SC and 64 per cent for ISC event. This extremely high level of recurrence is an indicator that industrial interest in PRACE is genuine and not mere curiosity.
Industrial participants in PATCs

The average participation of industry in PATC training is 14 per cent. The increasing interest from industry to participate in HPC training is visible in Figure 8. A total of 250 industrial participants were trained by PRACE. Eligible industrial participants enjoy the same service as academic trainees and can attend PATC courses free of charge.

![Graph showing the percentage of industrial attendees contact with the PRACE booth at ISC and SC.](image)

**Figure 8:** Number of industrial attendees that made contact with the PRACE booth at ISC and SC.

Industrial use of PRACE HPC resources

PRACE opened its Calls for Proposals to industrial applicants in mid-2012. Industrial participation can take the form of a project led by a principal investigator coming from an industrial enterprise, or of a researcher from industry collaborating in an academia-led project. The reduction and stabilisation of projects awarded after the 7th Call has a strong impact on the number of projects awarded with industrial participants (Figure 9), but also in the amount of CPU hours allocated to industry.

![Graph showing industry participation in PRACE allocations.](image)

**Figure 9:** Industry participation in PRACE allocations.

Regarding the SHAPE pilot, PRACE can report 10 success stories of SMEs from 6 different countries benefitting not only from PRACE HPC resources, but more importantly from the know-how in the PRACE centres.
Q&A: Driving Europe to graphene success

The Graphene Flagship is a €1 billion European Commission funded project that is aiming to give Europe a head start in graphene research and development over the next ten years. Professor Jari Kinaret, director of the Graphene Flagship, explains the goals of the project and the role that HPC resources will play in achieving them.

- **What is the overall goal of the Graphene Flagship?**
  Jari Kinaret. We want to take graphene and related materials from academic laboratories into society as new products as a means to contribute to economic growth. Graphene technology is only at its very early stages, and it will still be a while before we see it widely integrated in real life applications. At present, the consortium is mainly made up of research institutions, but I expect the balance will move towards more companies as time progresses and we look to start creating real products.

- **How will you achieve your goals?**
  JK. Our basic mode of operation is to bring together world leading expertise from academia, research institutes and industry. With these people gathered, the next pertinent question is: what do we do? We have done a very careful job of analysing the field and have recently published a roadmap article outlining current global knowledge of graphene, where research is moving, and where opportunities lie.

  On the one hand we are looking from the technological “push side”, i.e. what is it possible to achieve with graphene? On the other hand we are looking from the “pull” side, i.e. what technological developments are needed, and what can we make of value? The challenge is to strike a balance between the push and the pull.

- **PRACE have allocated HPC core hours to a number of the Graphene Flagship’s researchers. How will these be used?**
  JK. Some of our researchers are doing very computer heavy work, and this is where the PRACE allocations are vital. For example, Professor Stephan Roche of the Catalan Institute of Technology has made extensive use of HPC resources as head of the spintronics work package, with the goal of establishing the ultimate potential of graphene for spintronics, targeting efficient room temperature spin injection and detection but also spin gating and spin manipulation in graphene spintronic devices.

  In general there is less computationally heavy work in areas such as component modelling and systems modelling in which variability of components is high, making it difficult for numerical modellers.

- **How do you bring all of the research and knowledge together effectively?**
  JK. It is certainly a difficult job; we already have 142 partners from 23 countries involved, with each partner having anything from one to ten researchers. To organise the project effectively it is divided into sixteen work packages, each of which is divided up into tasks. For instance, the work package for energy applications has a task on battery technology, a task on supercapacitors, and more. These tasks are encouraged to collaborate closely, as are work packages that are likely to have crossover in terms of the research they are carrying out.

  Find out more about the Graphene Flagship at graphene-flagship.eu
Professor Stephan Roche was awarded for a total of 22 million core hours from PRACE (see more here: www.prace-ri.eu/roche-2014):

- The project entitled “Linear Scaling Methods for Quantum Hall Transport Simulations” was allocated 200,000 core hours on CURIE @ GENCI@CEA, France, and 50,000 core hours on HERMIT @ GCS@HLRS, Germany, under the 9th cut-off for PRACE Preparatory Access (Type C).

- The project entitled “Longitudinal and Transverse Electronic Transport in Atomically Doped Graphene from First Principles” was allocated 14.3 million core hours on CURIE @ GENCI@CEA, France under the 6th Call for Proposals for PRACE Project Access.

- The project entitled “Longitudinal and Transverse Electronic Transport in Atomically Doped Graphene from First Principles” was allocated 22.1 million core hours on CURIE @ GENCI@CEA, France under the 8th Call for Proposals for PRACE Project Access.

PRACE has also supported four other projects linked to the FET Flagship Graphene with a total of over 90 million core hours

- “Effects of irradiation on nanostructures from first principles simulations” by Arkady Krasheninnikov (Call 3) was awarded 10 million core hours on CURIE TN @ GENCI@CEA, France.

- “EPIGRAPH – Electronic and optical properties of graphene nanoribbons on metal surfaces” by Andrea Ferretti (Call 6) was awarded 17 million core hours on FERMI @ CINECA, Italy

- “Controlling Hydrogen Binding to Corrugated Graphene” by Valentina Tozzini (Call 7) was awarded 38 million core hours on FERMI @ CINECA, Italy

- Under the 9th Call, the project entitled “AESFTI” led by Matteo Calandra of CNRS, France, is a partner in the Graphene Flagship Initiative. The project received 9 million core hours on CURIE @ GENCI@CEA, France.
Since 2014 the six PRACE Advanced Training Centres, located in Finland, France, Germany, Italy, Spain and UK, offered 84 courses in the framework of their mission to serve as European hubs of advanced, high-quality training for researchers working in the computational sciences.

The PATCs followed a jointly developed curriculum, designed and coordinated by PRACE with input from user communities and thus promoting a common PRACE brand, representing the whole PRACE community rather than only the hosting sites.

The following table (below) shows the key output from the six PATCs for the academic years since 2012.

**Key 2014 PATC highlights include:**
- The mobile nature of PATCs – a number of PATC courses were delivered in non-PATC hosting countries.
- A greater percentage of PATC participants from non-academic institutions.
- PATC events with a specific industrial focus.

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### Seasonal Schools

During 2014 three PRACE seasonal schools took place in various (and geographically spread out) non-PATC PRACE partner countries:

**PRACE Winter School 2014**

The PRACE Winter School 2014 was held from 10 to 13 February 2014 at Tel Aviv University, Israel.

Organised by IUCC in collaboration with the LinkSCEEM-2 project under the title “The Future of HPC: Israeli Innovation and PRACE Introductory Workshop”, the event attracted 43 participants and targeted two separate user groups.

A half day mini-workshop titled “The Future of HPC: Israeli Innovation”, showcased Israeli companies and researchers who are developing the future HPC technologies for the next 5 years.

**PRACE Spring School 2014**

The PRACE Spring School 2014 was held from 15 to 17 April 2014 at Research Institute for Symbolic Computation (RISC), Castle of Hagenberg, Austria.

Organised by the Johannes Kepler University Linz (JKU) and the University of Ostrava and IT4Innovations Centre of Excellence (VŠB-TUO) under the main training event programme was designed to accommodate trainees with varying expertise level and professional backgrounds and to give a very thorough overview and training in fundamental HPC topics and to introduce topics of importance and interest to the computational science community. It included topics covering parallel programming techniques, MPI (lecture and hands-on), OpenMP (lecture and hands-on) as well as sessions on core skills, CUDA programming, HPC system architectures and supercomputer design, visualisation techniques and more.

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the title of “Software Engineering for Supercomputers in Research and Industry” the event attracted 42 participants and this three day event included:

- A one-day HPC usage for industry track bringing together researchers and attendees from industry and academia to discuss the variety of applications of HPC in Europe.
- A two two-day track on software engineering for parallel and emerging computing architectures which included a deep insight into solving multiphysical problems with Elmer on large-scale HPC resources with lectures delivered by industrial and PRACE members.

**PRACE Autumn School 2014**
The PRACE Autumn School 2014 was held from 25 to 28 November 2014 at the training Centre of the Hellenic Telecommunications Organisation (OTE Academy) in Athens, Greece.

Organised by the Greek Research and Technology Network (GRNET) under the title of “HPC Programming Techniques”, the event attracted 54 participants and addressed existing and potential users of high performance computing systems in Europe. Researchers and students from Europe received advanced training in programming models and optimisation techniques, MPI/OpenMP and hybrid programming, profiling and benchmarking. The event focused on in-depth presentations for thorough understanding of these HPC topics, followed by hands-on training.

**International HPC Summer School 2014**
The International HPC Summer School 2014 was held from 1 to 6 June 2014 in Budapest, Hungary.

The school was a collaboration between PRACE, the USA’s National Science Foundation’s eXtreme Science and Engineering Discovery Environment (XSEDE) project, Canada’s Compute Canada and Japan’s RIKEN Advanced Institute for Computational Sciences (RIKEN) under the title “HPC Challenges in Computational Sciences”.

The school attracted 79 participants, 10 of whom came from Japan, 10 from Canada, 29 from the USA and the remaining 30 participants from sixteen European countries.
A wide variety of topics were covered in the school including:
- Access to EU, US, Japanese and Canadian HPC-infrastructures
- HPC challenges by discipline (e.g. bioinformatics, computer science, chemistry, and physics)
- HPC programming proficiencies
- Performance analysis and profiling
- Algorithmic approaches and numerical libraries
- Data-intensive computing
- Scientific visualisation

“It is clear that the PRACE Training Portal continues to reach a global audience”

Training Portal
The PRACE Training Portal continues to serve as a single source of training material, tutorials, and information on upcoming training opportunities and throughout 2014 has attracted many visitors from around the globe.

The PRACE Training Portal now hosts 27 PRACE video tutorials, the training material from 89 PRACE training events which represents over 380 different items of training material (with each item grouped together with other material related to similar topics). Close to 120 of these include a video of the lecture where both the presenter and the slides can be viewed simultaneously. Training material includes the slides of the presented lectures in Portable Document Format (PDF) format and whenever a hands-on session was held, the exercises and solutions (software code etc.) are also included where possible. In total, the number of documents hosted by the training portal exceeds 900 documents.

In 2014 a link between the PRACE Training Portal and the XSEDE Training Portal (and vice versa) was established. This is the first step towards a possible future collaboration between PRACE and XSEDE with regards to the distribution of training material. Similarly, links to some PRACE partner local training portals were added to the landing page of the training portal.

The visitor statistics for the training portal covering the full year of 2014 are summarised in the figure below.

It is clear that the PRACE Training Portal continues to reach a global audience. It is interesting to note the increased amount of traffic emanating from the USA – which is of similar (and sometimes higher) level to PRACE member countries. One should also take note the relatively high amounts of traffic from India. The PRACE Training Portal has built up an extensive user base making it a significant training resource for the global HPC community.

Visit the training portal at: http://www.training.prace-ri.eu
The PRACE User Forum

In 2014 the PRACE User Forum (UF) held its second general assembly in Barcelona during the PRACE Scientific and Industrial Conference (PRACEdays14), which was held from 20 to 22 May 2014 (see page 45 of this Annual Report).

The members of the PRACE User Forum Programme Committee that attended that conference (Derek Groen, Troels Haugbølle, Koen Hillewaert and Gustavo Yepes) organised the session.

The format of the general assembly worked very well. It was largely unchanged with respect to the first one organised in 2013 during the CSC2013 conference in Cyprus (see our contribution to the PRACE Annual Review 2013 for more information).

However we noted a significant less number of people attending the User Forum session in Barcelona, probably because the session was placed before the official opening of the conference. In future PRACE conferences, we will plan to allocate the UF session in a better time slot and to spread out more information among the participants of the conference. In order to reach more users, other activities are being planned (cfr. infra).

Nevertheless, the interaction with the audience was very positive and there were several interesting discussions raised during the UF session on the following topics:

• Users would like to rationalise access modalities and PRACE accounts for projects which run on multiple machines or even between different projects;
• Over-subscription of queues, conflicting with the planned timing of CPU consumption. Overall interaction with HPC centres very positive regarding re-planning of activities;
• Storage facilities and data retention beyond the project duration;
• Facilitate follow up PRACE projects on Tier 1 systems for e.g. post-processing the data or small additional computations;
• Special project category for post-processing;
• Some computations require complex work flows / co-processing, in that sense, the UF will elaborate a report on use cases and suggestions from user feedback;
• Rigid duration and synchronous end dates of PRACE projects.

The conclusions of the general assembly were summarised by the User Forum Programme Committee, and sent to the PRACE Board of Directors (BoD) for further consideration.

Social media
To keep communications with the PRACE User Community transparent and efficient, the PRACE User Forum has started and maintains a social media presence on LinkedIn and Twitter, where the discussions of the above topics, or other ones raised by users, can then be followed by a larger audience.

We remind you that the PRACE User Forum can be found at www.linkedin.com/groups/PRACE-user-Forum-4793989 on LinkedIn and at @PRACEuserForum on Twitter. The LinkedIn group contains details of the discussions at the User Forum general assemblies held at CSC2013 and in PRACEdays14 conferences. But it is also open to contributions from any PRACE Users, or prospective users.

Renewal
The programme committee of the User Forum is also looking for new members of the major scientific and industrial disciplines that are currently using PRACE HPC infrastructures. The chair and vice-chair of the programme committee is renewed annually, but keeping some line of continuation. The current vice-chair (Koen Hillewaert) will take the chair position in 2015, while Troels Haugbølle will take the position of vice-chair. The current chair, Gustavo Yepes, will be appointed as out-going chair.

PRACEdays15. The PRACE User Forum is taking part in the organization of PRACEdays15 conference that will be held from 26 to 28 May in Dublin (Ireland). The 3rd General Assembly of the User Forum will be hosted by this conference. We encourage all the PRACE users that will attend PRACEdays15 to participate in the User Forum session.

Outreach
Apart from PRACEdays, the programme committee has considered that the User Forum should also have visibility in other more user-oriented HPC conferences in Europe in order to reach more potential users. Currently, the User Forum has organised mini symposia / sessions in the ECCOMAS conference in 2016 (http://www.eccomas2016.org) and in the ICCS 15 conference in Reykjavik (Iceland) (http://www.iccs-assembly.org/iccs2015/registered-workshops/#ws27)
After the successful closure of the 1st Implementation Project (PRACE-1IP) at the end of December 2013, the 2nd and the 3rd Implementation Projects (PRACE-2IP and PRACE-3IP) were running in parallel during 2014 supporting the implementation of the PRACE Research Infrastructure. Some highlights of the work of the PRACE projects are reported in detail in other parts of this annual report. This is the case especially of SHAPE, the SME HPC Adoption Programme in Europe, the extensive training activities of the PRACE Advanced Training Centres or the dissemination actions like the presence of PRACE at numerous HPC exhibitions and events.

After 36 months of intensive and effective project work the PRACE-2IP project had its final review in October 2014 and received an overall rating of ‘good’. The project has made very good progress, especially in the areas of training, porting/tuning applications and engagement with the industry. A highlight of the project is the PATC training, where the curriculum developed is best practice for a top class university and has been well received and evaluated by the users. On the operational side, support of the project is excellent, as is the support for research into new algorithms.

In order to assure a smooth continuation of the work (e.g. user support, training, dissemination) for the PRACE Research Infrastructure until the new PRACE project starts, PRACE-3IP was extended by 7 months and ended its activity on 31 January 2015. Only the Pre-Commercial Procurement (PCP) related tasks will continue till 2016. In October 2014 a periodic project review took place and PRACE-3IP received the highest possible rating of ‘excellent’, except for Work Package 8 (PCP). During its 31 months the project submitted 45 deliverables on schedule and produced excellent enabling work that lead to excellent white papers.

Highlights of the project are the dissemination and outreach activities, the excellent training offers, and the valuable collaborations such as with XSEDE and with industries through the SHAPE pilot.

In 2014 the proposal for the PRACE-4IP project was created and submitted on 2 September 2014. The proposal was accepted and the consortium was invited to prepare the grant agreement. The PRACE-4IP project start was confirmed as 1 February 2015.

In the following pages are some highlights of the project work in 2014:

**Summer of HPC 2014**

Summer of HPC (SoHPC) continued in 2014, following on from a very successful programme in 2013. SoHPC is an outreach programme targeting undergraduate and postgraduate students, offering them a chance to complete a project during the summer at a HPC centre in Europe. In 2014 five European HPC centres hosted two students each for two months during summer. The application and selection process was rigorous and the top ten students were selected to participate.

Each centre included the students in one of their projects and a dedicated project mentor supervised their scientific development. The students wrote articles about their personal and professional experiences. These articles and information on SoHPC 2013, 2014 and 2015 can be found on the programme’s website (http://www.summerofhpc.prace-ri.eu).

All students successfully completed their projects and at the end of the programme all mentors were asked to evaluate the work of each student. The student adjudged to have been the most successful was awarded the ‘Best SoHPC Student’ of 2014 prize. Each project mentor was very satisfied with the attitude and the knowledge of their mentees, so it was not easy for them to choose only one, but finally they came to the decision that Nicola Luminari from Italy, who was hosted at VSB – Ostrava, Czech Republic was the winner.

We are pleased to say that based on the feedback from the project mentors and mentees the programme was a success. The experience for the students was so influential that some of them decided to continue their studies in areas closely related to the scientific project they were working on during the summer. SoHPC 2014 has come to a successful close but SoHPC 2015 is just beginning.

Nicola Luminari - Winner of PRACE Best SoHPC Student 2014
IP PROJECTS

Operations
PRACE sites have implemented a set of common services which enable interoperation among PRACE systems, such as for data transfers, job submission and login, and using the same credentials for authentication and authorisation for all these services. Also a dedicated network is operational which interconnects most of the sites. Because of the inter-dependencies of these integrated services between sites, a tight collaboration between those sites is required. PRACE implemented an operations team which coordinates the daily operation of the common production services.

A change management procedure has been implemented to guarantee reliable and available services. The procedure has been loosely based on IT Infrastructure Library (ITIL) principles. A proposed change must address the following topics: description of the change, security impact, installation instructions, monitoring facilities, user documentation, pre-production tests and their results, service certification tests, and a planning of the change. The latter also includes roll back measures for large changes. The acceptance procedure of a change depends on the impact, e.g. the introduction of a new service has more requirements before it will be accepted for implementation than for just a configuration change at one of the partners. Also important is that each service, sustainable support is guaranteed by the experts of the PRACE partners. Each week a PRACE partner is responsible for overseeing the status of the services, using the available monitoring information and the status of problem reports. Escalation procedures for problem management are implemented too.

The security of the infrastructure is important; PRACE sites must trust each other that good security practices are implemented. A security forum, with membership of security representatives from all sites, is responsible for the policies and the procedures used by the PRACE partners for the operation of common services. This forum also is responsible for the management of security incidents which may have an impact on the infrastructure.

For monitoring the results of the operational activities a set of Key Performance Indicators has been defined and measurements have been implemented. The results can be used to further enhance the quality of the provided services and to describe service levels.

Figure 1 shows the different processes that have been described above and which together have implemented the operation of sustainable services for the PRACE infrastructure.

Code enabling and white papers
While the focus of the applications enabling activity remains supporting European researchers to efficiently exploit PRACE supercomputers, recent activity also includes work on enabling applications to address key socio-economic challenges from the “PRACE Scientific Case for HPC in Europe”. It is a key priority to disseminate the results to the European HPC community through white papers and best practice guides.

The efficient use of the largest HPC systems places high demands on the software and often requires advanced optimisation work. This requires a high level of experience and advanced knowledge of different concepts, programming techniques and parallelisation strategies. PRACE provides access to supercomputing experts who have the skills and knowledge required to collaborate with users so that they can undertake their computational research. Through preparatory access and DECI (Distributed European Computing Initiative), we are able to support researchers from throughout Europe in using systems in different countries to produce high quality research outputs.

“The security of the infrastructure is important; PRACE sites must trust each other that good security practices are implemented”

For the applications selected on the basis of their socio-economic importance, we described key best practices, such as multi-discipline modelling. White papers were produced describing the results from these projects, including modelling the human heart, scalable simulations of aircraft designs, and environment safety simulations.

Having previously surveyed a number of tools and techniques of interest for future petascale systems, we exploited the most promising of these on well-known community applications codes through a variety of different enabling projects. Each of these produced a white paper, now available on the PRACE website for interested readers, and the results were also summarised in a public deliverable.
As well as a wide variety of enabled applications and public deliverables, we have produced around 40 new white papers this year (http://www.prace-ri.eu/white-papers/) and five best practice guides (http://www.prace-ri.eu/best-practice-guides/). These are available as part of the valuable documentation resource on the PRACE website that ensures that the expertise of the PRACE partners benefits the HPC community throughout Europe.

**CASE STUDY - Social challenge**
Computational model of the human heart created with the ALYA_RED code, with coupled fluid-electro-mechanical interactions

**CASE STUDY – Preparatory Access**
The subject of one of the recent Preparatory Access projects was the optimisation of the quantum-mechanics software package Wannier90 [1]. For the discovery and design of new, improved materials e.g. for transparent electrodes of solar cells or for non-volatile magnetoresistive random access memories (MRAM), simulation codes like Wannier90, capable of predicting desired and undesired material properties, are an inevitable complement to practical experimentation.

“The efficient use of the largest HPC systems places high demands on the software and often requires advanced optimisation work”

Most runtime-critical computations of Wannier90 are dominated by dense matrix operations (double precision complex), in particular by matrix-matrix multiplication and diagonalisation. In the course of this six month-project in a close collaboration between PRACE experts and the scientists from Johannes Kepler University (Austria) and the Institute of Physics of Polish Academy of Science (Poland), these computations have been speeded up by a factor of five and higher by using BLAS for matrix products and by algebraically rearranging matrix multiplications (exploiting associativity) and reusing intermediate results. Also the scalability of Wannier90 has been improved significantly by parallelising several previously serial computations.

As can be seen in Figure 2 and Figure 3, the new code version of Wannier90 exhibits near-to-perfect strong scalability up to 2048 processes for sufficiently large problem settings. In addition, for the main computation module (berry_main), optimal weak scalability has been demonstrated up to 16-thousand processes making it perfectly suitable for future scientific production using PRACE regular calls.

![Figure 2: Strong scalability comparison for the original (dashed lines) and the new (solid lines) code version of Wannier90 for computations with 8 up to 128 atoms. Performance has been increased significantly; scalability is now optimal up to 2048 processes.](image)
Pre-Commercial Procurement

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

In 2014 the PRACE-3IP project achieved during the second year of the PCP the finalisation of the tendering material, the launch of the PCP call for tender from November 2013 to February 2014, the assessment of the offers from March 2014 to June 2014, and the signing of the framework contract and Phase I contract with four selected bidders from June 2014 to September 2014. The launch of the 1st Execution Phase has been formalised on 9 September 2014, with the following bidders:

- BULL SAS, France;
- E4 Computer Engineering SpA, Italy;
- MEGWARE Computer Vertrieb und Services GmbH, Germany;
- Maxeler Technologies Limited, United-Kingdom.

During this period a Benchmark Code Owners (BCO) group has been put in place in order to prepare benchmarks that will be used for the evaluation of improvements in energy efficiency through the use of real production applications codes in use by PRACE today.

The selected codes are part of the European Unified Application Benchmark Suite:

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

The 1st Execution Phase of the PCP will be closed on 9 March 2015 and a new call for tender will be issued for the 2nd Execution Phase of the PCP, restricted to the four vendors who signed the Framework contract and Phase I contract.

Events

PRACE on the road

Each year PRACE is present at the largest international HPC events: ISC in Germany and SC in the United States. In 2014 PRACE combined its annual Industrial Seminar and its annual Scientific Conference into a new event called “PRACEdays”.>
PRACEdays14 concludes with three awards

In 2014, PRACE organised its first Scientific and Industrial Conference – the first edition of “PRACEdays” – under the motto “HPC for Innovation – when Science meets Industry” from 20 to 22 May 2014 in Barcelona, Spain. Hosted by PRACE and supported by the Barcelona Supercomputing Centre, the conference attracted over 200 participants from academia and industry.

The conference counted two satellite events: an open session of the PRACE User Forum, and a workshop on exascale and PRACE prototypes.

Highlights of the conference were keynote speeches by well-known academic scientists and industrial researchers from the US and Europe, as well as by high-level representatives from the European Commission and from industry. A full parallel stream was dedicated to presentations from SMEs who have already benefited from the PRACE SHAPE pilot programme (http://www.prace-ri.eu/shape - see page 5 of this annual report). The final panel on 22 May brought together the keynote speakers for a discussion on economic and scientific impact of collaboration between science and industry.

The PRACEdays14 Award for Best Scientific Presentation went to Teodoro Laino of IBM Research – Zurich, Rüschlikon, Switzerland for his presentation entitled “Shedding Light On Lithium/Air Batteries Using Millions of Threads On the BG/Q Supercomputer.”

The PRACEdays14 Award for Best Industrial Presentation went to Mathis Bode of RWTH Aachen University, Germany for his presentation entitled “High fidelity multiphase simulations studying primary breakup.”

Last but not least, the PRACEdays14 Award for Best Poster was given to Kannan Masilamani of University Siegen, Germany for his poster entitled “Simulating and Electrodialysis Desalination Process with HPC.”

PRACEdays15 packed with excellence

PRACEdays15 will be held at the AVIVA Stadium in Dublin from 26 to 28 May 2015.

One of the main highlights of the conference will be a keynote speech by Masahiro Seki, president of the Research Organisation for Information Science and Technology (RIST), Japan.

Six talks by renowned researchers from science and industry will underline the theme of the conference: “enable science, foster industry”. This theme will be further explored in 12 parallel talks during the second day of the conference. A panel session entitled “Science and Industry: Partners for Innovation” and moderated by Tom Wilkie of Scientific Computing World, will conclude the conference.

Participants to PRACEdays15 will have the opportunity to attend two satellite events – one on exascale and one on women in HPC – as well as the EESI2 Final Conference, free of charge.

PRACEdays16 – there is always more to come

PRACEdays16 will be held from 10 to 12 May 2016 in Prague, Czech Republic. Keep an eye on the PRACE website for more!
PRACE at ISC’14 Conference
At the Opening Session of ISC’14, on Monday 23 June 2014, the PRACE-ISC Award was announced for the paper entitled “Sustained Petascale Performance of Seismic Simulations with SeisSol on SuperMUC”.

On Tuesday 24 June, International Data Corporation (IDC) announced the seventh round of recipients of the HPC Innovation Excellence Award. One of the winners was PRACE Member CINECA, Italy. Engineers from THESAN srl, an Italian SME active in the renewable energy sector, teamed up with the Italian supercomputing centre CINECA to develop simulation driven engineering of hydroelectric turbines. The research was conducted in the framework of the PRACE SHAPE (SME HPC Adoption Programme in Europe) programme.

Wednesday evening was cause for celebration for PRACE Member EPCC, with their team from the University of Edinburgh breaking the Linpack record during the ISC’14 Student Cluster Competition.

PRACE at ISC’14 Exhibition
The PRACE booth attracted more than 230 visitors with various activities. International press visited PRACE on Monday evening, just before the official opening of the ISC’14 Exhibition during which PRACE invited visitors to a cocktail and informal networking session.
PRACE at SC’14
PRACE’s presence at SC’14 in New Orleans, Louisiana in November was a focal point and attracted a great deal of international attention.

For the first time, three PRACE and PRACE Partners won 3 HPCwire Reader’s Choice Awards:
- Best use of HPC in automotive - Biggest car optimisation study by Renault SAS on PRACE resources.
- Best HPC Collaboration Between Government & Industry - PRACE SHAPE helps European SMEs overcome barriers to using HPC
- Top Supercomputing Achievement - Max Planck Institute for Astrophysics for using CURIE to simulate the entire known Universe from its birth to present day

A SHAPE project participant, Nexio Simulation, was a recipient of the IDC HPC Innovation Excellence Award. Nexio Simulation is a French SME located in Toulouse who partnered with Bpifrance (the French public bank dedicated to SMEs), Inria, and GENCI for using HPC to scale out their electromagnetic studies to a full plane.