



no.2 2015

PDC Center for High Performance Computing

PDC Newsletter

BioExcel: New Centre of Excellence for Computational Biomolecular Research

- Erwin Laure & Rossen Apostolov, PDC, page 4

PRACE Fourth Implementation Phase Now Up and Running - Lilit Axner, PDC, page 8

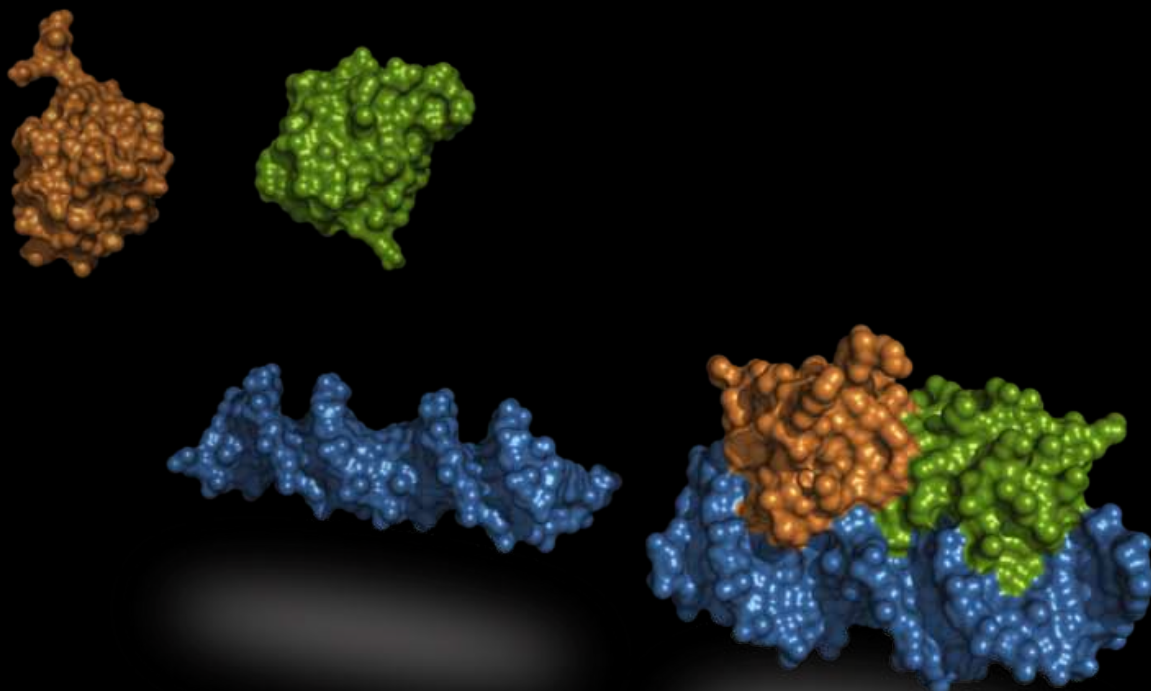
KTH Alumni First to Use New PDC Guide System - Gert Svensson, PDC, page 9

A Focus on Exascale - Erwin Laure, PDC, page 10

PDC's Application Expert Team Enlarged - Jonathan Vincent, PDC, page 12

PDC Summer School 2015 - Stefano Markidis, HPCViz, page 14

Milner Update - Mikael Djurfeldt, PDC, page 16





Erwin Laure
Director PDC and HPCViz

The PDC Newsletter is published by PDC at CSC, KTH.

PDC operates leading-edge, high performance computers as easily-accessible national resources. These resources are primarily available for Swedish academic research and education. PDC, which is hosted by CSC, KTH, is one of the six centres in the Swedish National Infrastructure for Computing (SNIC).

Editor: Erwin Laure
Editorial Staff: Genet Edmondson
Layout: Genet Edmondson
Graphic Design: Maria Malmqvist
E-mail: support@pdc.kth.se

ISSN 1401-9671

Cover

Docking and recognition of macromolecular assemblies - computational biomolecular research at the heart of the BioExcel Centre of Excellence

How to Contact PDC

Visiting address:
Teknikringen 14, "Plan 4",
KTH, Stockholm
Mail: PDC, KTH,
SE-10044 Stockholm, Sweden
E-mail: support@pdc.kth.se
www: <http://www.pdc.kth.se>
Phone: +46 8 790 7800
Fax: +46 8 247 784

Editorial

With our flagship system Beskow in full operation for almost a year, and our pre- and post-processing system, Tegner, also being in production for half a year, we are now focusing more on the application side of high performance computing (HPC) to improve the efficiency and productivity of our systems. We are expanding our team of application experts and have also started a number of high-profile research projects with application groups. The flagship project is our HPC Centre of Excellence for Computational Biomolecular Research – BioExcel, which is featured in our cover article. But we are also engaging in a number of other projects exploring different aspects of exascale computing: algorithms, particularly for Computational Fluid Dynamics (CFD), programming models, and input/output (I/O). These efforts are being complemented with a recent Swedish Foundation for Strategic Research (SSF) Research Infrastructure Fellowship Grant and our work on the Swedish e-Science Research Centre, SeRC, all of which aim to create a vibrant application scaling and optimization community around PDC.

With our links to the visualization activities at KTH and the VIC visualization studio we are starting to have a unique environment encompassing HPC hardware and expertise, visualization, and applications pushing the boundaries for Swedish research. This environment, modelled after international examples, will allow for much tighter interdisciplinary interactions expanding from pilot groups in CFD and Molecular Dynamics to further groups in Sweden. But before we see this in full operation, it's time to break and we wish all our users "Happy Holidays" and look forward to great new scientific discoveries on Beskow and with the other PDC services in 2016.

Erwin Laure, Director PDC and HPCViz



Above: Coffee break at PDC Summer School 2015

EASC2016

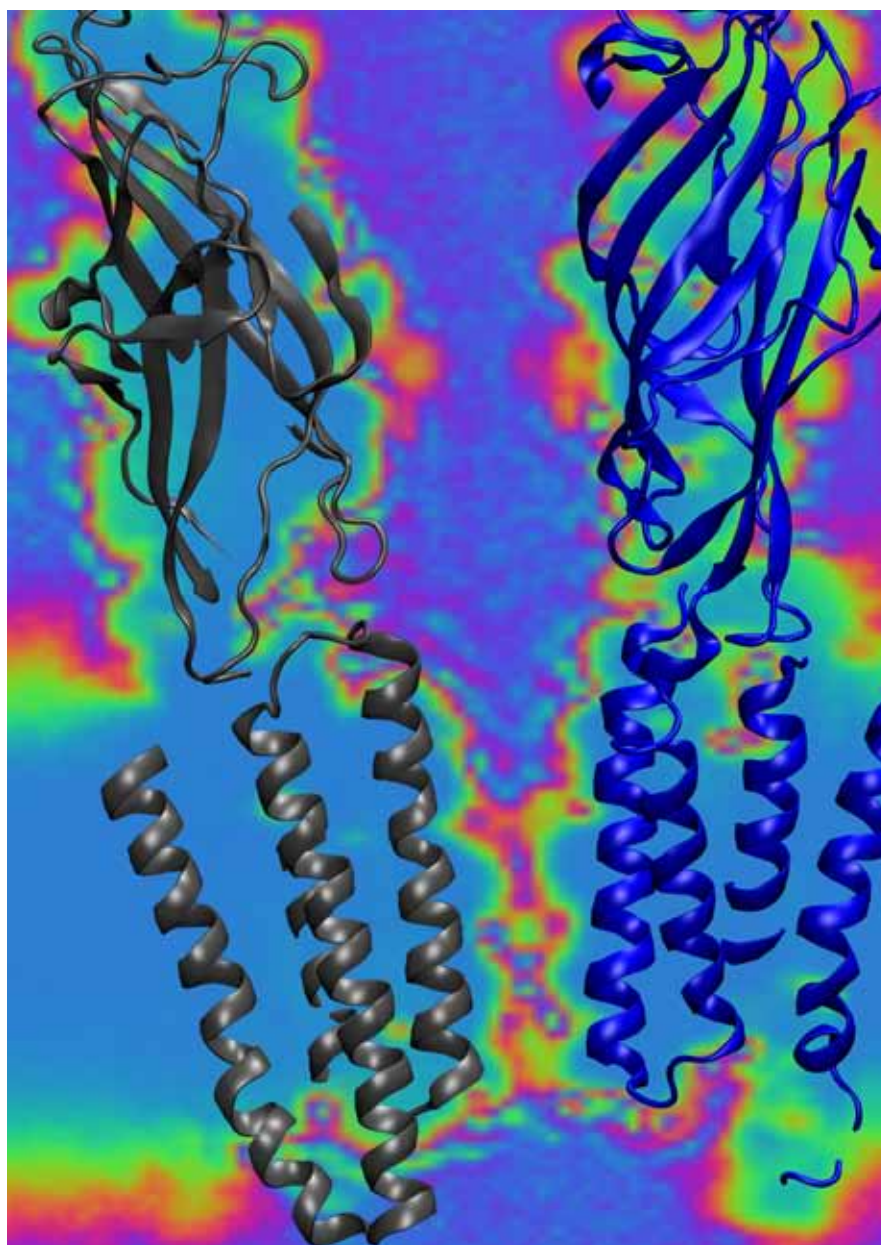
Exascale Applications and Software Conference

26-29 April 2016
Stockholm, Sweden

The EASC2016 Conference on Solving Software Challenges for Exascale is being organized by KTH in association with the Swedish e-Science Research Centre (SeRC).

The Call for Papers is currently open. For further information and registration details, see

<https://www.pdc.kth.se/easc2016>



In This Issue

Editorial

Erwin Laure 2

Staff Focus

Polina Vasiljeva 10

Magnús Benediktsson 11

Cristian Cira 12

BioExcel: New Centre of Excellence for Computational Biomolecular Research

Erwin Laure & Rossen Apostolov....4

PRACE Fourth Implementation Phase Now Up and Running

Lilit Axner8

KTH Alumni First to Use New PDC Guide System

Gert Svensson 9

A Focus on Exascale

Erwin Laure 10

PDC's Application Expert Team Enlarged

Jonathan Vincent 12

PDC Summer School 2015

Stefano Markidis 14

Milner Update

Mikael Djurfeldt 16

PDC-Related Events 16

HPC Sources 16

Left: *Gloeobacter* Ligand-gated Ion Channel (GLIC) ion channel protein

This is typical of the types of visualization produced in the area of computational biomolecular research which underlies the recently launched BioExcel Centre of Excellence, led by PDC. The centre will work on improving the performance of key scientific codes that are used for such research, improving the usability of related tools, and offering training and consultancy services to academia and industry.

BioExcel: New Centre of Excellence for Computational Biomolecular Research

Erwin Laure and Rossen Apostolov, PDC

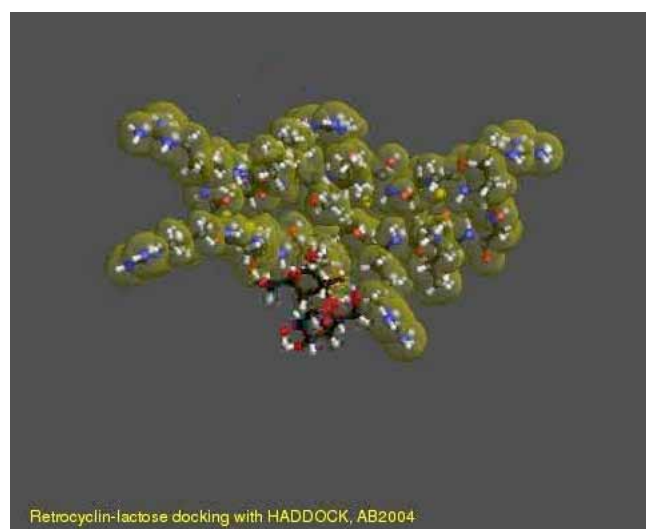
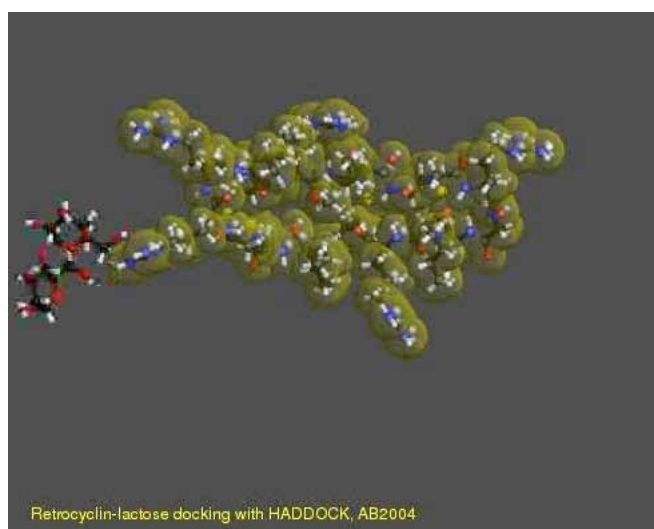
Introducing BioExcel

PDC, along with ten other European partners has recently been awarded funding to establish a Centre of Excellence for Computational Biomolecular Research through the EC Horizon 2020 program. The project, BioExcel, will be coordinated by PDC. Researchers from the KTH Department of Theoretical Physics will participate in the project along with academic and industrial research partners from Utrecht University (Netherlands), the Institute for Research in Biomedicine (Spain), the Jülich Research Centre (Germany), The University of Edinburgh (UK), The University of Manchester (UK), the European Molecular Biology Laboratory (Germany), the Max Planck Institutes (Germany),

Forward Technologies (Sweden), the Barcelona Supercomputing Center (Spain) and Ian Harrow Consulting/Pistoia Alliance (UK).

The Need for BioExcel

The general area of life science research, which includes the more specific discipline of biomolecular research, is having a greater and greater impact on our daily lives – particularly in relation to health (as it helps in the creation of new medical treatments and drugs) and new developments in agriculture and the food production industry. Biomolecular modelling techniques have produced computational tools and programs that are widely used in applied research and industrial development. Meanwhile new technologies in imaging and gene sequencing have drastically increased the amount of data that is produced and that must be analysed. For example, state-of-the-art techniques, such as cryo-electron microscopy, depend just as much on refining data via computers as on collecting initial data through experiments. As a result of such developments, life science research is becoming increasingly “digital” rather than focussing solely on practical laboratory studies, and hence the number of people within the life science research community who are working with high-end computing is increasing. This, in turn, is creating greater and greater demands for better computational performance and throughput from the available life science computational tools.

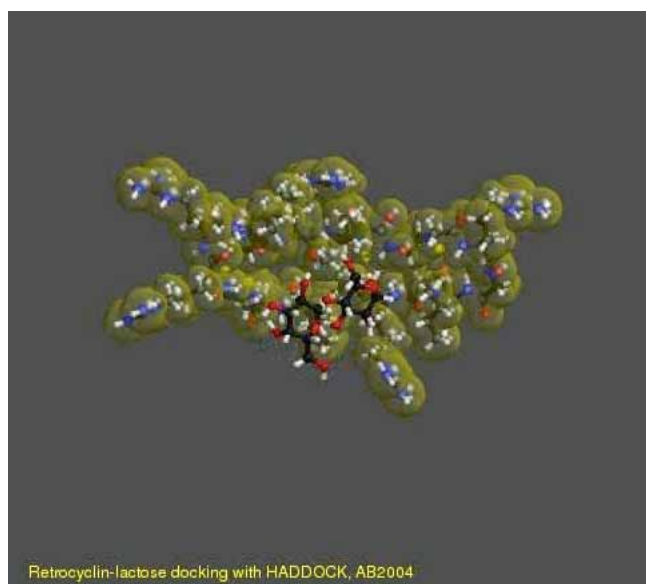
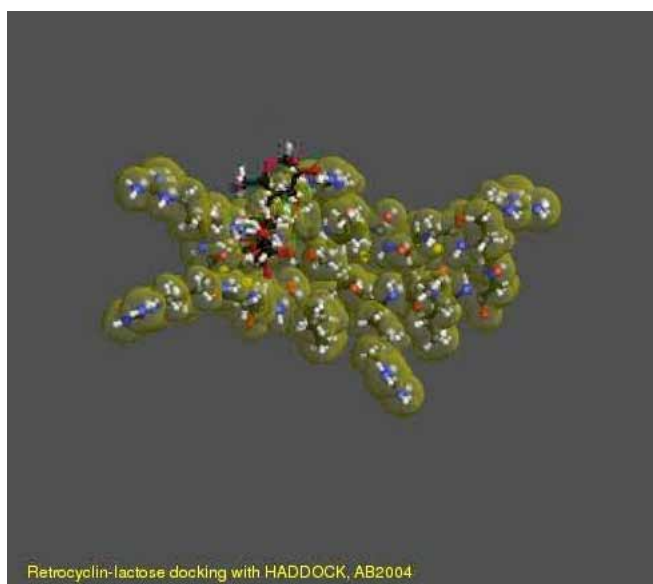


Above and on the next page: This sequence of images, which has been produced with HADDOCK, illustrates a typical docking process for “virtual drug screening”, that is, the process of searching for small molecules with a high affinity for binding to a protein enzyme receptor.

At the same time that the life sciences are becoming critically important for the industrial sector in Europe, the use of e-infrastructures to help meet these demands is still relatively new compared to the situation in some other disciplines. (E-infrastructures are essentially networks of computational hardware and software, along with data management services and appropriate connections and communications between the various parts of the network, which are used to support collaborative research.) At present, many advanced life science computational techniques are not being applied commercially due to limited experience. Thus we have a situation where there are a lot of life science researchers who are not computing experts but who need to use complicated computationally intensive biomolecular modelling tools.

We need some way of providing these researchers with the necessary level of support so they can use the available e-infrastructures efficiently, for example, by providing suitable computational workflows to help the researchers handle the vast amounts of data that are needed for the types of calculations used in biomolecular modelling. In addition we need to improve the performance and applicability of various key life science programs and applications to handle the increasing quantities of data and enable them to run efficiently on the progressively more powerful systems that are becoming available.

Having said all of that, it is important to remember that the life sciences cover a vast field that ranges from nanoscale quantum mechanical descriptions of atomic systems (which can, for example, be used to investigate interactions between molecules) to working with whole complex organisms (such as human beings). The huge range of scales that is covered means that the equations needed for modelling the relevant biological systems (for example, molecules, cells, brains or whole bodies) differ enormously, and hence a single Centre of Excellence cannot realistically provide adequate support for all aspects of the life sciences. This is why, given the key role of molecular-level investigations for many aspects of life sciences (including medicine, genetics, pharmacology, and the food industry), the BioExcel centre will focus on providing expertise and support for research on the main building blocks of living organisms. BioExcel will cover structural and functional studies of the building blocks of living organisms: proteins, DNA, saccharides, membranes, solvents and small molecules (like drug compounds), which are all areas that are being studied extensively in European academia and industry. Thus we will mainly work on biomolecular models up to the level of a single cell, although our expertise also covers techniques to model interactions between molecules and to handle coarser-level models for investigating the interactions between even higher levels of biological structures.



Below: BioExcel's basis – three pillars of excellence



The question then is how will we help life sciences researchers make good use of the great e-infrastructures that are available to support biological research. The BioExcel project will be based on three pillars, namely providing:

- excellence in biomolecular science,
- excellence in application usability, and
- excellence in consultancy and training.

Excellence in Biomolecular Science

In terms of “Excellence in Biomolecular Science”, BioExcel personnel will improve the performance, efficiency and scalability of three of the major software codes used in biomolecular science: GROMACS, HADDOCK and CPMD, with a particular view to their use on next-generation high performance computing (HPC) systems.

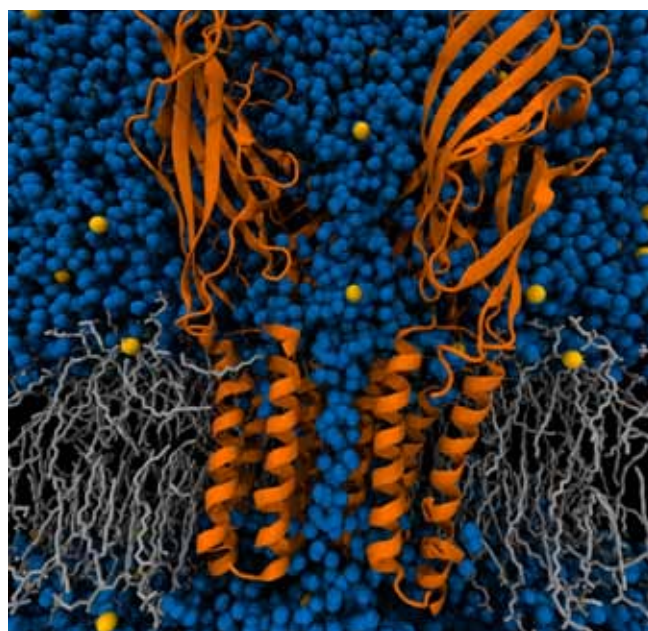
GROMACS is an extremely widely used program for molecular dynamics simulations. It was primarily designed for running simulations of the interactions between proteins, lipids and nucleic acids – it is used both in industry, for example, for the development of novel drugs and also extensively in academic research. The illustration on the right shows a model of an ion channel protein embedded in a lipid membrane. During simulations, scientists can observe the dynamical changes in the system, and based on the collected trajectory data understand the basis for many of the underlying phenomena.

HADDOCK is used for modelling the way that large molecules (macromolecules) can interact to form even larger structures or assemblies. These processes, which can change the internal structure of the initial macromolecules, are known as docking processes. The sequence of images on the previous pages is typical of the type of research performed with HADDOCK.

CPMD is used to model processes using hybrid quantum mechanics/molecular mechanics methods. In the life sciences domain it is typically used for studying processes (for example, relating to enzymatic reactions, photochemistry and electron transfer) in which chemical bond formation and breakage are modelled and studied. The figure on the next page shows an example model system where parts of the model (several water molecules) are treated quantum mechanically while the rest is subject to classical molecular mechanics modelling.

Excellence in Usability

When it comes to “Excellence in Usability”, BioExcel’s main focus will be on making it easier for academic and industrial biomolecular researchers to use the available information and communications technologies (ICT), particularly by devising efficient workflow environments



Above: An example of the type of simulation work that GROMACS is used for: modelling an ion channel protein which is embedded in a lipid membrane

with associated data integration. Workflow environments or management systems allow people to easily set up, run and monitor a series of computational or data management tasks, without having to be programming experts. Consequently these types of easy-to-use tools are of great benefit to researchers whose expertise is in biomolecular areas, rather than in computing or data management.

Excellence in Consultancy

The purpose of BioExcel's "Excellence in Consultancy" is to build competence amongst biomolecular researchers by training them to follow recommended "best practices" and make the best use of both the software and computational infrastructures that are available to them. BioExcel will offer help to academic/non-profit and industrial researchers who are using biomolecular software, as well as aiding academic developers of biomolecular-related software and also independent software vendors (ISVs) producing biomolecular products. The project will also be available to assist both academic HPC centres and commercial biomolecular resource providers.

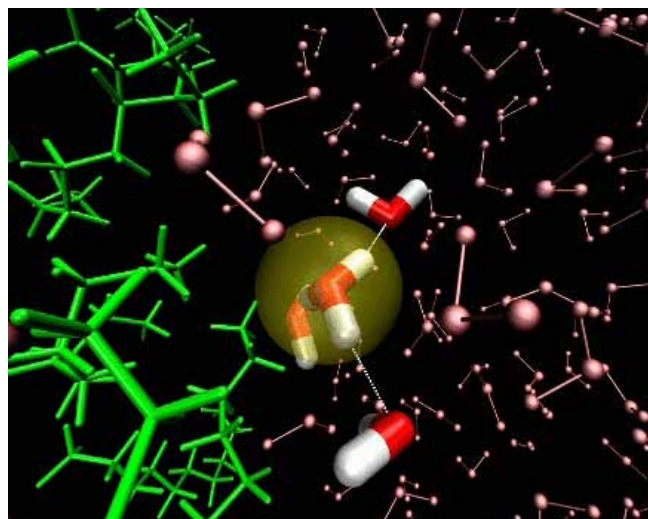
Sustainability

In addition to building its three pillars of excellence, BioExcel has a fourth objective – to achieve sustainability. To this end, the project will work on developing appropriate governance structures and a sustainable business plan to enable the work of the project to continue after the initial project phase.

BioExcel in a Nutshell

In summary, BioExcel will focus on improving the usability of technologies for biomolecular researchers and also the efficiency and scalability of important software packages for biomolecular research. In addition, the project will provide training to help life sciences researchers make good use of the available software and e-infrastructures, and help them to be aware of the "best practices" for the relevant combinations of software and hardware. This will definitely

Below: An example of CPMD modelling



strengthen current world leading European work in biomolecular research. It will also establish a European node in the international network of biomolecular research centres as we will be collaborating with other European projects and initiatives, such as the **ELIXIR** and **INSTRUCT ESFRI** initiatives, e-infrastructure projects such as PRACE, EGI and EUDAT, and also global and national resource providers such as Amazon. In addition, BioExcel will collaborate with some of the research centres in the USA (Oak Ridge National Laboratory) and Asia (RIKEN, Japan). Important partnerships with the industrial alliances Pistoia (pharmaceuticals), CEFIC (chemicals) and FoodDrinkEurope (food industry) are also planned.

The BioExcel project officially started on the 1st of November 2015 and there was a kick-off meeting at the KTH Royal Institute of Technology in Stockholm on the 3rd of November. The project has funding for three years, however it is important to remember that one of the goals of the project is to develop sustainable resources, so the benefits of the project should continue to be available to researchers even after the initial three year period is over.

For further information about BioExcel, please see the project website <http://www.bioexcel.eu> (which was under development at the time of writing) or contact Rossen Apostolov (rossen@kth.se).



PRACE Fourth Implementation Phase Now Up and Running

Lilit Axner, PDC

On the 28th of April PRACE started its fourth implementation phase (known as PRACE-4IP) with a kick-off meeting in Ostrava-Poruba, Czech Republic. Just as with the previous PRACE implementation phases, the ambitious goal of PRACE-4IP is to provide a pan-European world-class high performance computing (HPC) infrastructure to support the advanced modelling and simulation needs of European researchers across the scientific and industrial domains. The objectives of PRACE-4IP are to:

1. achieve long-term sustainability of the PRACE infrastructure,
2. promote Europe's leadership position in HPC applications,
3. build up European human resources skilled in using HPC and HPC applications,
4. provide a balanced ecosystem of HPC resources for Europe's researchers,
5. evaluate new technologies and define Europe's path for using exaflop resources, and
6. disseminate the PRACE results effectively.

In terms of Sweden's participation in PRACE-4IP, the Swedish National Infrastructure for Computing (SNIC) is continuing its active role in PRACE as one of the early partners while PDC continues to be the coordinating HPC centre for SNIC within PRACE.

During the initial three implementation phases of PRACE from 2010 to 2014, researchers from Sweden were very successful in using the PRACE HPC facilities and services. The recently published [SNIC-PRACE Digest No.1](#) sum-

marizes these achievements for the PRACE first to third implementation phases. SNIC's participation in PRACE is of major importance when it comes to maintaining the competitiveness of research in Sweden by enabling researchers to use these world-class HPC infrastructures.

The transition period from the third implementation phase to the fourth has not been trivial for PRACE. In particular, it was important to ensure that researchers had continuous access to the PRACE HPC facilities during the gap of several months between the end and start dates of those two phases, so PRACE continued its activities as usual even during the interim period.

The PRACE 11th Call for Proposals was launched in February 2015. This time the call had something more to offer, namely a pilot call for joint data storage services and resources. This pilot call was proposed jointly with PRACE associated members and partners willing to provide storage and associated data services under the PRACE umbrella including [EUDAT](#), [EU-To](#), [BSC](#), [CaSToR](#), [EPCC/EP SRC](#) and [SURFsara](#). These data services and facilities were intended for researchers who needed to share their project data over a large network of users or to store it for a longer period. There have been two successful Swedish applications that were awarded time allocations from this PRACE 11th Call – the projects were allocated 15 million core hours on the [MareNostrum system](#), which is based at [BSC](#) in Spain, and 35 million core hours on [FERMI](#), which is run by [CINECA](#) in Italy.

When it comes to the Call for Proposals for [PRACE Preparatory Access](#), this is a call that is continuously open but which has regular quarterly cut-off dates for assessing applications. The results from the 21st cut-off date are [now available](#) and the process

continues with the most recent cut-off date being on the 1st of December 2015.

PRACE also runs a program to help European small to medium-sized enterprises (SMEs) take advantage of the innovation possibilities opened up by HPC techniques and technology. This SME HPC Adoption Programme in Europe is known as SHAPE. The second SHAPE Call for Proposals was held earlier this year and supported **eleven projects** from European SMEs. These companies are receiving support from PRACE and its partners to assess how the use of HPC can increase their competitiveness. The third SHAPE call for SMEs is currently open for applications and will close on the 14th of January 2016.

There was a minor delay with the launch of the latest PRACE Distributed European Computing Initiative (DECI) calls. This delay was a result of internal restructuring of the PRACE infrastructure. As a consequence of these changes, DECI will no longer be part of the PRACE implementation phases but will instead be directly under the coordination of the PRACE infrastructure as an optional program. For applicants, this change does not have major implications except that the possibility of the support of PRACE application experts for DECI projects for up to six months will be decreased to a minimum required amount.

The DECI13 call under the PRACE optional program opened on the 14th of August and closed on the 21st of September. One hundred and fifteen DECI applications from twenty-eight countries were submitted of which five were from Sweden. All five Swedish application were accepted and will have access to the DECI systems starting from the 18th of January 2016. The 12th PRACE call for Project Access was opened on the 30th of September and closed on the 12th of November 2015. The results of the 12th call will be known in March 2016.



KTH Alumni First to Use New PDC Guide System

Gert Svensson, PDC

If you have ever been on one of the tours of the PDC computer hall, you will know that it is a noisy environment; people who work in there need to wear some kind of ear protection to protect their hearing. This makes it very hard for people to discuss what is going on when a tour group enters the computer hall. To overcome this, PDC recently purchased a wireless guide system. The guide who is leading the tour of the computer hall can speak into a microphone and there are ten sets of earphones that the visitors can wear so they can listen to the guide. The earphones also reduce the noise from the computers. The images show the first PDC visitors to use the new guide system – on the 2nd of September, 20 former KTH students (who had started studying Engineering Physics at KTH in 1965) toured the PDC computer hall, and were split into groups of ten to use the guide system.



Above: KTH alumni visiting the PDC computer hall during their 50 year reunion were the first to use the new wireless guide system, 2 September 2015

Staff Focus



Polina Vasiljeva

Polina Vasiljeva joined PDC in June 2015 to work in the Support group. Polina has a Bachelors degree in chemical engineering from KTH and is currently enrolled in a Masters program in mathematical statistics at KTH. Before starting her studies at KTH, Polina studied French language and linguistics, both in Stockholm and in Paris.

Polina enjoys spending time with her friends, trying out new restaurants, travelling and Fridays. She practices yoga, and her dream place on Earth is California, where she was lucky to spend the summer of 2014 as a research intern at Stanford University.

Free AVL FIRE License

If you are interested in running AVL FIRE at PDC, please contact support@pdc.kth.se to request a free license.

In your email please include your name and contact information, along with details of the research project(s) or course(s) where you would like to use AVL FIRE.

For details about AVL FIRE, see <https://www.avl.com/web/ast/fire>.

A Focus on Exascale

Erwin Laure, PDC

Reaching exascale (10^{18} floating point operations per second) is the next major goal the high performance computing (HPC) community has set itself. Although exascale systems are unlikely to appear during the next ten years, there is intense research and development being undertaken on both the hardware and software aspects of such systems. In particular, the hardware developments (like many-core processors, accelerators, and non-volatile memory) are gradually being introduced and thus it is important to study how applications and underlying system software are coping with those developments.

PDC has been active in exascale research for many years, including working on prototype developments within PRACE, the CRESTA flagship project, and more recently in the EPiGRAM project which is just preparing for its last year of operation. While our focus in CRESTA has primarily been on software applications that are important for Swedish research (especially GROMACS and Nek5000) as well as supporting runtime technologies, within EPiGRAM we concentrate on exploring possible evolutions of programming models towards exascale, particularly with respect to MPI and the Global Address Space Programming Interface (GASPI).

The start of the new EC framework program, Horizon 2020, has brought an increased focus on HPC and exascale research, and PDC/HPCViz has been very successful, with funding being granted for four projects. These projects, which started in October 2015, cover a wide spectrum of exascale research from algorithmic developments and programming models to hardware advances.

The ExaFLOW project, which is being coordinated by PDC, is addressing algorithmic challenges to make it possible to use accurate Computational Fluid Dynamics (CFD) simulation models in exascale environments. Driven by problems of practical engineering interest, it focuses on important simulation aspects including:

- error control and adaptive mesh refinement in complex computational domains,
- resilience and fault tolerance in complex simulations,
- heterogeneous modelling,
- evaluation of energy efficiency in solver design, and
- parallel input/output and in-situ compression for extreme data.

The algorithms developed by the project will be prototyped in major open-source simulation packages in a co-design fashion, exploiting software engineering techniques for exascale.

In the INTERTwiNE project, coordinated by EPCC (formerly the Edinburgh Parallel Computing Centre), we continue our work on programming models, started within EPiGRAM, with a particular focus on how different models can interoperate within an application. Due to the increasingly heterogeneous nature of HPC systems, the combination of different models becomes more important in order to exploit the most efficient combination given a certain hardware base. However, if you have ever tried to combine say MPI with PGAS approaches, you will have realized that this is far from easy and is often inefficient due to interoperability issues. The INTERTwiNE project is setting out to ease the combining of different models and will thus contribute to the ease of programming and the efficiency of software for exascale systems.

A different approach is being pursued by the AllScale project, coordinated by the University of Innsbruck. In this project, a higher level programming approach is being pursued, following a recursive task-based model combined with advanced compilation and adaptive runtime technologies. AllScale aims to decouple the specification of parallelism from the associated management activities during program execution.

Finally, with storage and input/output becoming more and more of a bottleneck when it comes to highly parallel computing, the development of intelligent data storage – uniting data processing and storage as two sides of the same rich computational model, as pursued by the SAGE project coordinated by Seagate – is another stepping stone towards exascale. This project will enable sophisticated, intention-aware data processing to be integrated within a storage systems infrastructure, combined with the potential for exabyte-scale deployment in future generations of extreme-scale HPC systems.

Our involvement in these projects will ensure that Swedish HPC stays abreast of the latest HPC developments and that Swedish researchers will be able to take advantage of the best breeds of hardware and software. Together with the HPC Centres of Excellence (of which we are coordinating the biomolecular one, BioExcel, as discussed in the cover article, and are also involved in a materials science one, MAX), these projects will ensure that Sweden and Europe are well equipped for the challenges to come and stay competitive with similar efforts in the US, China and Japan.

Staff Focus



Magnús Benediktsson

Magnús obtained a B.Sc. in physics from the University of Iceland. After that he did an M.Sc. in physics at Chalmers University of Technology. Now he is studying towards an M.Sc. in machine learning at KTH.

Magnús started working in the PDC support group in June this year. In his "leisure" time, Magnús likes to do stuff that involves sitting still, such as reading science fiction. In his earlier years Magnús has been involved in activities that require moving about, specifically taekwondo and Brazilian jiu-jitsu, but he last did those a year and a half ago.

Magnús is interested in science fiction and artificial intelligence which is partly the reason he chose his current Masters programme.



Above: PDC Summer School lectures, August 2015

Staff Focus



Cristian Cira

Cristian Cira fell in love with technology at the age of 12, in the spring of 1991, when his father brought home an IBM XT machine. The early 1990s were marked by events that were to forever change the life of millions: Romania switched from a totalitarian regime to a democracy, the World Wide Web was launched and the European Union was born. It was in this new information age that Cristian discovered a passion for mathematics and computers. After graduating from Computer Science studies at the West University of Timișoara, Cristian went on to pursue a Masters at RISC in Linz, Austria, only to return home for a doctorate. During his five year Ph.D., Cristian worked as a teacher in his hometown university. The end of his Ph.D. marked another important decision in Cristian's life. A scholarship allowed him to pursue a Masters in high performance computing in the USA that led to a job at the Oak Ridge National Laboratory. After five very valuable years there, that were influential for his career, Cristian decided to return to Europe with high ambitions to contribute to shaping a better, brighter future on the continent that he calls home.

...continued on page 13

PDC's Application Expert Team Enlarged

Jonathan Vincent PDC

PDC is in the process of enlarging the Application Expert team: Cristian Cira recently joined PDC where he will be working on code optimisation, and Thor Wikfeldt has just started at PDC as an application expert in the area of molecular dynamics. Thanks to a number of successful projects, including BioExcel and ExaFLOW, and the Swedish Foundation for Strategic Research (SSF) Research Infrastructure Fellowship, we will hire further researchers in the areas of molecular dynamics, computational fluid dynamics (CFD), and optimization for novel architectures (such as accelerators).

In other changes, Radovan Bast moved to Poland earlier this year and has been replaced by Jaime Axel Rosal. Additionally, from November onwards, Rossen Apostolov has been working full-time with the BioExcel project and similarly Mikael Djurfeldt will be based within the Human Brain Project. Jonathan Vincent, Jing Gong and Henric Zazzi all continue to be available at PDC to provide help with tuning your applications – so, if you have any queries for our Application Expert team, please contact support@pdc.kth.se.



Thor Wikfeldt

Computational Chemistry and
Chemical Physics
(Ph.D., Stockholm)

Previous research and work

- *computational research on*
 - liquid water and ice surface systems,
 - hydrogen-bonded ferroelectrics,
 - surface diffusion on metals,
 - low-temperature dynamics, and
 - quantum tunnelling
- *expertise in*
 - molecular dynamics (including *ab initio* and path-integral methods),
 - adaptive kinetic Monte Carlo,
 - density functional theory, and
 - classical and advanced polarizable force fields

Current work

- *research in computational chemistry and chemical physics*
- *setting up and optimising molecular dynamics codes*

Can help PDC users with

- *advanced support in molecular dynamics (MD) and other simulation methods*



Jaime Axel Rosal
Theoretical Chemistry
and Biology
(Ph.D., Stockholm)

Previous research and work

- *high performance and low-complexity algorithms for quantum chemistry*

Current work

- *parallelizing the QM/CMM (Quantum Mechanics/Capacitance-polarizability Molecular Mechanics) project in Dalton, and merging it with the CPP (Complex Polarization Propagator) code*
- *efficient implementation of the ADC (Algebraic-Diagrammatic Construction) propagator method for calculation of molecular spectroscopy*
- *installation and optimization of QM codes*

Can help PDC users with

- *(hybrid) parallelization*
- *code optimization for high performance architectures and quantum chemistry software*



Cristian Cira
High Performance
Computing
(Ph.D., Timișoara)

Previous research and work

- *non-volatile memory architecture*
- *profiling, tracing and analysing the communication characteristics of high performance computing scientific applications running on petascale systems – some examples of the applications that were analysed are CESM (Community Earth System Model), LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), NRDF (Non-Equilibrium Radiation Diffusion), QMCPACK (Quantum Monte Carlo simulation code) and WL-LSML (Wang Landau locally self-consistent multiple scattering method)*

Current work

- *VASP*
- *PRACE*

Can help PDC users with

- *VASP*
- *application profiling/tracing*
- *performance analysis*
- *general scientific computing problems*

...continued from page 12

In Cristian's free time, he strives to balance all the important aspects of life including enjoying cooking with fresh produce. Gathering people around this activity seems to be easier nowadays as more of us become conscious about the health issues associated with the food industry. Cristian also follows sports, world politics and lots of technical documentaries. He and his friends often strive to find ways to help reduce the imbalances that occur in various aspects of life in this world. Issues like global warming, conflicts, education, ethics and technology are frequently among the hot topics that he discusses with friends and family.

Juvenal's famous verse "Mens sana in corpore sano" always resonated with Cristian. Although he was never involved in professional sports, he enjoys snowboarding, climbing, and playing tennis or football. Swimming, hiking and skydiving are among the activities that he does occasionally but would like to do more often! The latter is especially dear to him since five of his very close friends are professional skydivers with remarkable international achievements. Spending time among world-class top athletes in such a "cool" discipline is very rewarding and inspiring. One can imagine their daily work involves being surrounded by lots of positive vibrations and thoughts. The community that is formed is such an example of multiculturalism, collaboration, resource management, respect and optimistic attitude that Cristian cannot help but wonder if we could all learn from such examples of human interaction and apply it in other aspects of our lives to build a better future.

PDC Summer School 2015

Stefano Markidis, HPCViz

Students at the PDC Summer School, “Introduction to High Performance Computing”, enjoyed soaking up the sun and getting to know each other during a picnic in the KTH courtyard on the first day of the course.



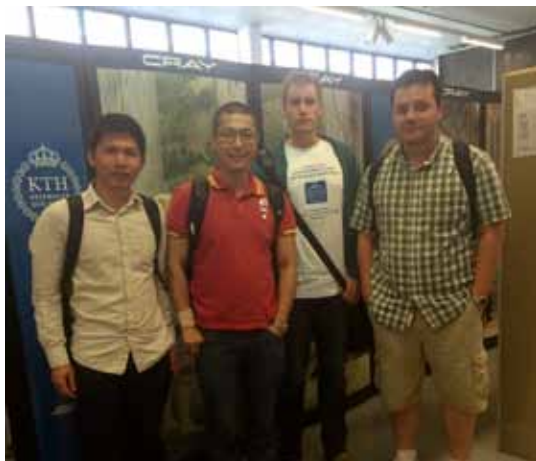
While many of the students are from Sweden (with Gothenburg, Linköping, Lund, Stockholm, Umeå and Uppsala all being represented), some attendees came from as far afield as Bosnia, France, Italy and Japan!



However life is not just a picnic - the summer school also includes lectures and lab work...



...but there are plenty of breaks for refreshment too!



The PDC Summer School not only gives a great introduction to high performance computing but also introduces participants to our main system, Beskow (which is currently the fastest academic supercomputer in the Nordic countries), and the infrastructure services necessary for running supercomputer systems like these (which are needed in case of power failure or fire, for example).

Here are some of the participants from this, the 20th year of the summer school, shown during the computer hall tours on the afternoon of the 18th of August 2015.



Milner Update

Mikael Djurfeldt, PDC

Our system Milner, intended for research in neuroinformatics, is a Cray XC30, based on 2.5 GHz Intel Ivy Bridge 10-core processors and Cray's Aries interconnect. The aggregate peak performance is 48 TF and the aggregate compute memory is 3.75 TB. The system also includes a Lustre file system with a usable capacity of more than 150 TB.

New developments

In the EU project **CENTER-TBI**, Cecilia Åkerlund is working on analysing data from patients with traumatic brain injuries. In intensive care units, the condition of each patient is monitored using many different monitoring systems which generate large amounts of data with varying time resolutions. Within the framework of the **CENTER-TBI** project, such data is collected, for example from the **Neurosurgical Intensive Care Unit** at the Karolinska University Hospital, and analysed. The data consists of hundreds of parameters, from details about a patient's socioeconomic background to X-ray images, continuous heart rate monitoring and EEG recordings. The goal of this study is to find ways to define the stages of disease progression after traumatic brain injury, and also to understand what the transitions between these stages look like. Cecilia will carry out her analysis on Milner.

Along with the 48-node SpiNNaker system, which is also part of the neuroinformatics research platform, Milner will be part of the Swedish participation in the Human Brain Project during its next phase, and is opened up for development work within that project.

PDC-Related Events

Introduction to PDC Systems

10 February 2016, PDC, KTH, Stockholm

<https://www.pdc.kth.se/events/event-repository/introduction-to-pdc-systems-february-2016>

Allinea Performance and Debugging Tools Workshop

26 January 2016, PDC, KTH, Stockholm

<https://www.pdc.kth.se/events/event-repository/allinea-performance-and-debugging-tools-workshop>

EASC2016

26-29 April 2016, Stockholm

<https://www.pdc.kth.se/easc2016>

PDC Summer School 2016

Last 2 weeks in August 2016, KTH, Stockholm

Registration for the summer school will open around May and be accessible from <http://www.pdc.kth.se/education/summer-school>.

HPC Sources

We recommend the following sources for other interesting HPC opportunities and events.

CERN

<http://cerncourier.com/cws/events>
<http://cds.cern.ch/collection/Forthcoming%20Events?ln=en>

EGI

<http://www.egi.eu/about/events>

HPC University

<http://www.hpcuniversity.org/events/current/>

HPCwire

<http://www.hpcwire.com/events>

Linux Journal

<http://www.linuxjournal.com/events>

NeIC

<http://neic.nordforsk.org>

PRACE

<http://www.prace-ri.eu/HPC-access>
<http://www.training.prace-ri.eu>
<http://www.prace-ri.eu/events>
<http://www.prace-ri.eu/news>

SeSE

<http://sese.nu>

SNIC

<http://www.snic.vr.se/news-events>
<http://docs.snic.se/wiki/Training>

XSEDE

<https://www.xsede.org/conferences-and-events>

NeIC Conference News

Join us in Sweden in 2017!

The 2017 NeIC Conference will be held in Sweden - further details will be available from <http://neic.nordforsk.org> and also in the PDC newsletter nearer the time.