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PDC Center for High Performance Computing

PDC Newsletter

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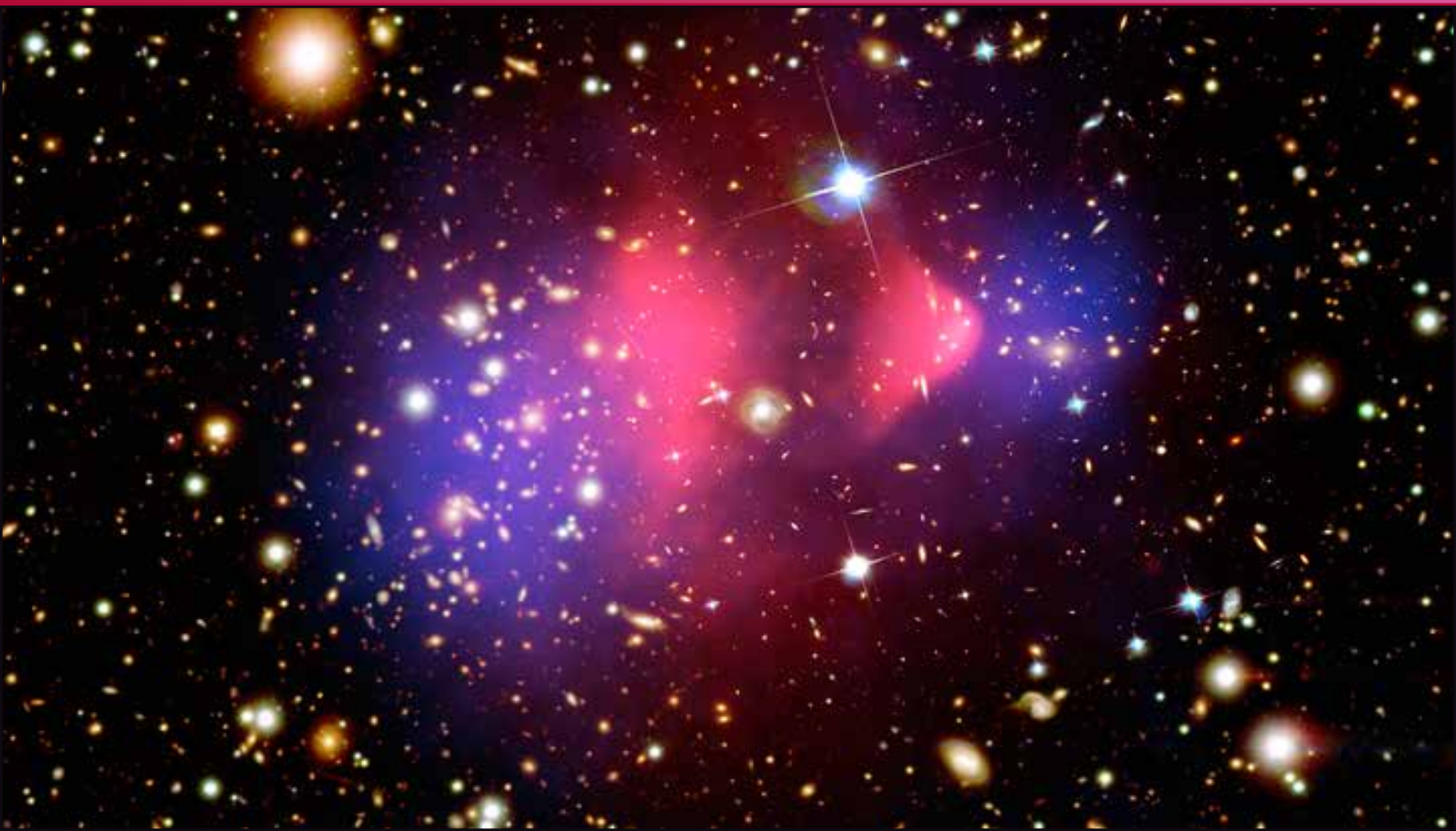
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Erwin Laure
Director PDC, and CST

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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).

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Cover

The matter of the Bullet Cluster with the blue hues showing the distribution of dark matter in the cluster - Source: [NASA](#)

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Editorial

Welcome to the Christmas Edition of the PDC Newsletter! At this time of year, one should reflect a bit on what happened during the year and also look forward to what the new year may bring.

2016 has been a productive year for PDC with all our systems in full production mode. Although we have not had any major new systems this year, we have still been engaged in major building activities: some offices on the 5th floor have been converted into an open space providing a relaxed environment where PDC users can interact with PDC experts. This open space is a key ingredient in the Swedish e-Science Research Council (SeRC) strategy to combine domain scientists and computer science researchers, as well as high performance computer centre experts, into multidisciplinary teams. We have also expanded our application expert team with new members focusing on fluid dynamics and graphics processing unit (GPU) programming, thanks to funds for research infrastructure fellows from the Swedish Foundation for Strategic Research (SSF).

Many international endeavours also made great progress in 2016. The Human Brain Project released the first version of their Information and Communications Technology (ICT) platforms, the Partnership for Advanced Computing in Europe (PRACE) is preparing to enter a new phase, called PRACE 2.0, and the Nordic e-Infrastructure Collaboration (NeIC) continued pooling Nordic competencies. In addition our Centre of Excellence for Computational Biomolecular Research, BioExcel, celebrated its first birthday!

Looking ahead into 2017, we will see a major change in the organisation and funding scheme for the Swedish National Infrastructure for Computing (SNIC). A task force is currently working out a new model for SNIC and the Swedish Research Council (VR) is expected to take a decision on this model during spring. This is happening in a timely manner for PDC as during 2017 we need to secure the funds for a system to replace Beskow. The new system is expected to be in place at PDC by early 2019, so initial technical planning for it has already started!

Finally, if you have ever wondered what our universe is made of, have a look at our cover article on Dark Matter, and find out about some of the fascinating research that our systems are being used for.

With this we wish all our users "Happy Holidays" and look forward to a great 2017!

Erwin Laure, Director PDC, and CST

The SeRC Open Space

A New Way of Interacting with PDC's Experts

Erwin Laure, PDC

During the past months several offices on the 5th floor of Teknikringen 14 (where PDC is based) have undergone a metamorphosis from standard PDC offices to an open space for informal interactions between researchers and PDC experts. The impetus for the Swedish e-Science Research Center (SeRC) Open Space has been driven by the original SeRC idea of bringing researchers from various scientific domains, computer scientists, and high performance computing (HPC) practitioners closer together; this space is the first step to providing an inspiring meeting place for such interactions.

The first major users of the space will be the researchers involved in the **SeRC Exascale Simulation Software Initiative (SESSI)** who will hold regular meetings there. But all PDC users are welcome to use the SeRC Open Space: desks will be available if you would like to bring your laptop over and work there, or grab a cup of tea or coffee in the kitchen and chat about your work with our experts – so just drop in. Further information about scheduling meetings and the availability of PDC application experts and advisors will be issued soon.

Over the coming months we will also start open discussions on specific topics of interest to the PDC user community – these will be held in the SeRC Open Space and you are all welcome to attend. Again, further details about these events will be available shortly.

We look forward to you passing by and help making this space a vibrant new environment for Swedish HPC.



Above: SeRC Room Housewarming, PDC, 9 November 2016

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Staff Focus



Evelyn Otero

Evelyn Otero obtained a double Master's degree in computational engineering from the Friedrich-Alexander University Erlangen (FAU) in Germany, and in scientific computing from KTH in 2009. Since then Evelyn has been contributing to the development of different national computational fluid dynamics (CFD) codes. She carried out her Master's thesis at the European Centre for Research and Advanced Training in Scientific Computation (CERFACS) in France where she worked with the ONERA elsA CFD code for Aeronautical applications. This led her to doctoral studies in Aerospace Engineering at KTH in 2010, which focused on computing time reduction of the Swedish CFD code Edge in collaboration with the Swedish Defence Research Agency (FOI). Evelyn performed her large-scale computations on PDC's supercomputers and appreciated the helpful and efficient support. After obtaining her Ph.D. degree in 2014, she joined the aviation company AVTECH where she worked on a wake vortex prediction algorithm for Air Traffic Management (ATM).

Evelyn is now back at KTH as a post-doctoral researcher based at the De-

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Reaching a New Level in Dark Matter Searches

Jan Conrad, Stockholm University

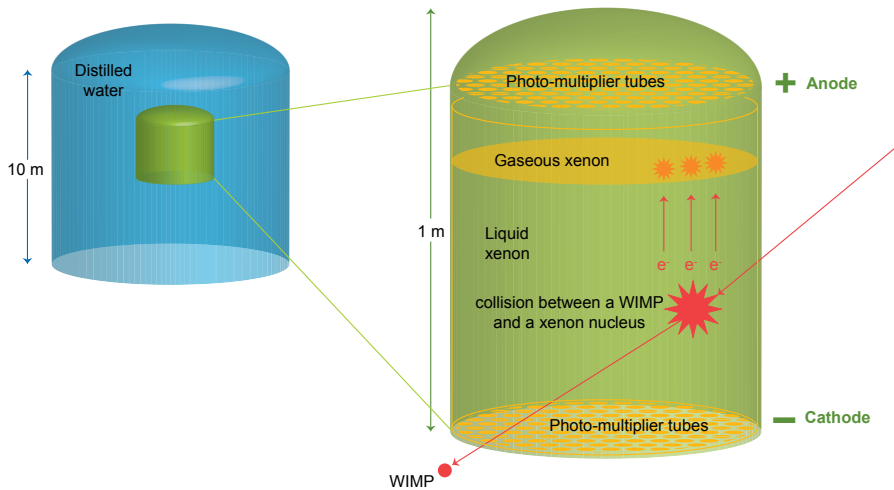
Over the last couple of years, the evidence for the existence of a significant component of matter in the universe that cannot be viewed with conventional telescopes has become indisputable – this component is known as Dark Matter (DM). Present measurements indicate that only a few percent of the total matter in the universe is made of particles that we know about. The nature of DM however is completely unknown, though many theoretically motivated explanations have been proposed. The most popular theory is that DM consists of a new type of elementary particle created in the early Universe, which has been dubbed the weakly interacting massive particle (WIMP). These particles would interact very feebly but would be a hundred to a thousand times heavier than a proton. Swedish scientists from Stockholm University are now participating in one of the leading experiments worldwide to search for these particles. This experiment is called **XENON1T** and is based at the Laboratori Nazionali del Gran Sasso (LNGS) in Italy. LNGS is one of the largest underground laboratories in the world. It is situated under about 1.4 km of rock which provides necessary protection against background interference induced by cosmic ray interactions as well as a unique infrastructure for the challenging search for WIMPs. The XENON1T dark matter xenon detector was built and is operated by a collaboration consisting of research groups from 21 institutes in France, Germany, Italy, Israel, the Netherlands, Portugal, Sweden, Switzerland, the United Arab Emirates and the USA. In total about 130 physicists are involved in the project.

Apart from leading a variety of tasks within the experiment, Sweden hosts the European analysis hub, a computer cluster provided by PDC, which is partly financed by the Knut and Alice Wallenberg Foundation.

The idea of the dark matter detector is to attempt to detect the recoil of nuclei that WIMPs interact with. The challenge is that, even in one tonne of heavy liquefied noble gas, we only expect one or two of these WIMPs to recoil per year. This would be alright, if it was not for the more than 100 billion other interactions that we need to filter out. These pose a formidable challenge in terms of computing, data handling and data reduction. The amount of data that is collected from the detector can, at times, be as much as 300 MB per second, and in total we expect to collect approximately 6 PB of data during the next few years.

The dark matter detector is made of xenon gas that is kept at $-95\text{ }^{\circ}\text{C}$, which means that the gas is liquefied. Any nucleus that recoils

Below: Schematic diagram of XENON1T dark matter detector



(due to colliding with a dark matter particle) causes ionization and excitation of the surrounding xenon atoms. The resulting freed electrons are drifted in an electric field to the top of the detector where xenon is kept in gas phase – as there they will cause an avalanche of electrons. Eventually in this way two signals should be produced: one from the interaction with the gas phase xenon and one from interacting with the liquid phase xenon. Both signals would be detected by arrays of photo-multiplier tubes (PMTs) which are light sensors that are sensitive to single photons. This concept is known as a time projection chamber (TPC). The fact that each such scattering produces two signals can then be used to separate the precious WIMP-induced recoils from all the noise that is caused by the much more abundant background consisting of cosmic rays and the radioactivity that is in the environment and in the detector components themselves. See the figure above for an illustration of the concept.

The XENON1T detector is about 30 times larger than its predecessor, consisting of about 3.5 tonnes of liquid xenon in total. The XENON1T TPC, which is a cylindrical shape 1 m high and 1 m in diameter that is laterally encased by highly reflective Teflon, is the largest liquid xenon TPC ever operated. The XENON1T TPC will host 2 tonnes of liquid xenon (LXe) in two arrays consisting of a total of 248 3" PMTs, with 121 PMTs at the bottom immersed in LXe, and 127 PMTs on the top in the gaseous phase xenon. The figure on the next page shows a picture of the TPC.

As we mentioned earlier, being able to separate out and reject the data relating to background events is the key to success for direct detection experiments. The backgrounds induced by the environment and cosmic rays can be minimized by exploiting the self-shielding capabilities of the xenon. Most external particles stop after a few centimetres in the heavy xenon material. In addition, the XENON1T detector is surrounded by a cylindrical water tank, 10 m high and 9.6

Staff Focus

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partment of Mechanics and PDC. She works as a developer of the CFD code Nek5000 from the Argonne National Laboratory, improving its robustness and performance on the path to exascale computations. Evelyn is also a member of the Swedish e-Science Research Centre Exascale Simulation Software Initiative (SESSI) group. In her free time Evelyn enjoys training and participating in social events. She also loves travelling and photography. Gaining knowledge and new experiences of other cultures and life in general is also of great interest to Evelyn.



Erica Carneiro

Erica Carneiro comes from Brazil where she received her M.Sc. degree in civil engineering at the University of Rio de Janeiro. Erica started to work at PDC last November and is currently studying for a second M.Sc. at KTH in fluid mechanics. To study what she likes and work with support for high performance computing (HPC) at PDC is a great opportunity for Erica. She gets the chance to learn more about Swedish academia, where she is aiming to work, and is making good friends in this cold land. In her free time Erica likes to go for walks with her husband and go camping in the forest.

Below: XENON1T experiment underground with the water tank on the left (partly covered by a poster showing what is inside) and the three-story service building on the right



m in diameter, that is equipped with PMTs as an additional shield against cosmic rays. For a detector the size of XENON1T, radioactive impurities in the detector parts and the xenon itself become the biggest challenge for reducing background noise. Extensive radiation screening campaigns, using some of the world's most sensitive germanium detectors, were conducted and high purity PMTs have been specially developed by the XENON1T collaboration. Contamination of the xenon by radioactive radon (mainly ^{222}Rn) and krypton (^{85}Kr) lead to the development of cryogenic distillation techniques, which mean that the abundance of these isotopes is suppressed to levels below a few parts per trillion (in the case of krypton).

The XENON1T detector was inaugurated on the 11th of November 2015 and we are about to finish work on commissioning and calibrating the detector. At the time of writing, we are about to start the first data collecting period looking for the rare dark matter interactions. After only about two months of continuous running, we will have probed the existence of WIMP dark matter with hitherto untested properties, which is predicted by the most favoured theories. A detection is clearly in the cards, especially

considering a relatively simple upgrade that we are already preparing, and that we expect will start operations by 2019. This upgrade will enlarge the detector to almost 8 tonnes of xenon.

In addition to the experimental work, the interpretation of the results requires advanced techniques from theoretical particle physics and nuclear physics. To provide this necessary progress to the international community, a consortium of researchers from Stockholm University and theorists from Chalmers Technical University has been formed. The consortium has been dubbed SweDCube and is supported the Knut and Alice Wallenberg Foundation. It is certain that this interpretation work will also require advanced numerical calculations where PDC's computing resources will be helpful.

Within the next five to ten years we should be in a position to detect dark matter if the current paradigm is correct. If not, we will face a paradigm shift and will have to rethink our approach to dark matter. With the help of PDC, Swedish scientists will be in the front line of this endeavour.

HBP Research Platforms Released

Mikael Djurfeldt, PDC

The Human Brain Project (HBP) is a ten year long project that started in 2013 and aims to create and operate a research infrastructure – based on Information and Communication Technology (ICT) – to help advance brain research in neuroscience, medicine and computing. Since the article in the PDC Newsletter (see [no. 2, 2013](#)) the HBP has been working on establishing its six ICT platforms, which were launched earlier this year on the 30th of March.

The six platforms are as follows:

1. the Neuroinformatics Platform, a web platform and application-programming interface (API) that will allow users to register, search for and examine large volumes of neuroscience data,
2. the Brain Simulation Platform, a suite of software tools and models that will allow users to construct and perform detailed simulations of the brain,
3. the High Performance Analytics and Computing Platform, a hardware and software infrastructure that will provide the high performance computing, storage, and data processing capabilities to analyse large sets of complex data and to run sophisticated, detailed brain simulations,
4. the Medical Informatics Platform, comprising innovative software that will allow users to access and analyse real patient data located in healthcare databases to help understand similarities and differences among brain diseases,
5. the Neuromorphic Computing Platform, consisting of two configurable, complementary neuromorphic computing systems that will be able to emulate the microcircuits of the brain and apply principles that are similar to the way the brain learns and understands to computers, and
6. the Neurorobotics Platform, a software and hardware platform that will allow users to connect virtual models of the brain to simulated robot bodies and environments.

The Neuroinformatics Platform

The Neuroinformatics Platform serves as the Human Brain Project's search engine for distributed data, curated data repositories, brain atlases and knowledge about the brain. The Platform consists of APIs for querying, plus a web-based platform and application programming interfaces for building software applications. Users can search and collate high quality neuroscience data generated within and outside the HBP. Data can be examined by species, contributing laboratory, methodology, brain region, and data type, thereby allowing functionality not currently available elsewhere. The data is predominantly organised into atlases (namely the HBP Strategic Rodent Brain Atlases and HBP Human Brain Atlases) and linked to the KnowledgeSpace – a collaborative community-based encyclopaedia linking brain research concepts to the latest data, models and literature.

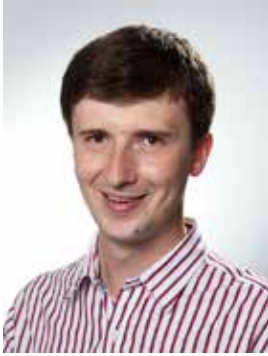
The Brain Simulation Platform

The Brain Simulation Platform provides scientists with powerful tools to reconstruct and simulate “scaffold models” of the brain and brain tissue in a data-driven fashion. Its development is embedded in one of the HBP subprojects on Brain Simulation, where a tight co-design loop between science and engineering ensures the required substantial technical and scientific innovations come to fruition. As a result, the unique functionality of the Platform allows novel questions to be addressed, which could not be investigated previously.

The High Performance Analytics and Computing Platform

The High Performance Analytics & Computing Platform comprises supercomputing capabilities at Forschungszentrum Jülich (Germany), the Swiss National Supercomputing Centre (CSCS) in Lugano, the Barcelona Supercomputing Center (BSC, Spain), and the Consorzio Interuniversitario del Nord-Est italiano per il Calcolo Automatico (CINECA, Italy) in Bologna. The Platform also provides access to high-fidelity visualisation systems at two locations in Germany (RWTH in Aachen) and Switzerland

Staff Focus



Roman Iakymchuk

Roman Iakymchuk works as a post-doctoral researcher at PDC and the Computational Science and Technology Department at the School of Computer Science and Communication at KTH. Roman is engaged with two EC-funded FET-HPC projects, namely INTERTWinE and AllScale. INTERTWinE is focused on the interoperability of programming models with a view towards exascale computing, while AllScale is concerned with an exascale programming, multi-objective optimization and resilience management environment based on nested recursive parallelism. Roman is contributing technically to both projects, and is also responsible for coordinating the KTH contributions to the INTERTWinE project. He verifies the interoperability of various programming models using the iPIC3D (implicit particle-in-cell simulator) application. Moreover, he applies task-based nested recursive parallelism in the iPIC3D application. That requires careful study of the 20,000 lines of the iPIC3D code with its complex algorithmic structure, as well as designing new task-based specific sparse iterative solvers.

Roman undertook his master's and
...continued on page 9

(EPFL in Geneva) and cloud storage with a dedicated capacity of 3 petabytes at the Karlsruhe Institute of Technology (Germany), which will also contribute research and development work to complement these resources.

All of these systems are connected logically through UNICORE (Uniform Interface to Computing Resources) and physically through the high-speed PRACE (Partnership for Advanced Computing in Europe) network, with a bandwidth of 10 Gigabits per second, and other secure connections. These high-speed connections mean that the users can run larger and more complex workflows than previously possible, and will increase the speed at which research work can be performed.

The Medical Informatics Platform

Hospital and other medical databases contain vast amounts of data about health and disease that represent an enormous asset to researchers. Many such databases and repositories are largely underused due to issues of data privacy and patient confidentiality, or because it is not possible for researchers outside these institutions to access the material.

The Medical Informatics Platform is an innovative data analysis system that provides an interface through which clinicians, neuroscientists, epidemiologists, researchers, health managers and even the general public can access and analyse imaging and clinical data currently locked in hospital and research archives and public databases. The identifying details for the patients in the data have been removed (in other words, the data has been de-identified) and the resulting information has been aggregated before working out the overall results so the privacy of the patients is completely protected. Users can explore ontologies and variables, configure and apply statistical methods on clinical and research data, and visualize and dynamically interact with the results.

The Neuromorphic Computing Platform

The Neuromorphic Computing Platform consists of two complementary and configurable neuromorphic computing systems, based on custom hardware designs. These systems are designed to emulate neural microcircuits and apply brain-like principles in machine learning and cognitive computing, that is, principles that will allow the machine to learn in the way that the brain does rather than being programmed like a normal computer. To do this, the Neuromorphic Computing Platform uses state-of-the-art electronic component and circuit technologies and incorporates new knowledge gained from other areas of neuroscience research, such as experimental neuroscience, theoretical neuroscience and brain modelling.

The Neuromorphic Computing Platform provides remote access to large-scale neuromorphic computing systems based in Manchester, UK and Heidelberg, Germany. Together with the TrueNorth system by IBM these constitute the only neuromorphic systems in the world capable of running simulations of neural circuit systems with state-of-the-art models of neurons, synapses and plasticity in either real time or accelerated time (which, in this case, is equivalent to 10,000 times faster than real time).

The Neurorobotics Platform

The Neurorobotics Platform is an internet-accessible simulation system that lets users simulate robots and environments controlled by spiking neural networks.

The Platform enables simple virtual closed-loop experiments in cognitive neuroscience to be performed using brain models developed within the HBP, with the capability to customise several variables, such as the environmental and physical parameters, using a Robot Designer, an Environment Builder and a Closed Loop Engine.

These six HBP Platforms embody the key objectives of the HBP: to gather and disseminate data describing the brain, to simulate and build models of the brain, to develop brain-inspired computing and robotics, and to create a global scientific community around the developing research infrastructure. The development of the six platforms has been the result of an unprecedented multidisciplinary effort involving more than 750 scientific collaborators and engineers from 112 institutions in 24 countries.

Swedish Participation in HBP

The Swedish partners in the Human Brain Project are Uppsala University (Kathinka Evers), the Karolinska Institute (Sten Grillner and Kevin Grimes), KTH (Jeanette Hellgren Kotaleski and Erwin Laure) and the Linnaeus University (Abdul Mohammed). Anders Lansner was also part of the KTH participation during the start-up phase. Swedish researchers are participating in various areas of the project such as ethics, neuroinformatics and computational neuroscience.

During the start-up phase, Anders Lansner's group was part of the neuromorphic subproject of HBP. Their activities included the development of benchmark models, such as a detailed model of layers two and three of the cerebral cortex, which can run on both supercomputers and neuromorphic hardware. The PDC Cray XC30 Milner was extensively used in this work.

Jeanette Hellgren Kotaleski from the Department of Computational Science and Technology at KTH is the deputy leader of the Brain Simulation Platform. Her group is currently using Milner

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bachelor's studies in applied mathematics at the Ivan Franko National University of Lviv, Ukraine. He obtained a Dr. rer. nat. (which is equivalent to a Ph.D.) in Computer Science from RWTH Aachen University, Germany. During his Ph.D., Roman did an internship at the National Institute of Informatics, Tokyo, Japan.

Roman enjoys spending his spare and free time with his family, reading books to his child, watching movies with his wife, walking in the forest and hiking. He also likes to visit new countries and cities, discovering their traditions, heritages and, of course, cuisines. In addition, Roman is interested in visiting conferences and speaking with scientists as, for him, those conferences are springs of new ideas, as well as new opportunities for building his scientific networks.



Above: SeRC Room Housewarming, PDC, 9 November 2016

at PDC for computer simulations of the basal ganglia and for the development of cell models for the Brain Simulation Platform (see the article “[Milner Update](#)” elsewhere in this newsletter).

Mikael Djurfeldt who is based at PDC is a member of the neuromorphic subproject in HBP. He uses Milner for the development of two software tools for large-scale neuronal network simulations, MUSIC, which facilitates co-simulation of neuronal network models (see the “[Milner Update](#)” article in this newsletter), and CSA, which is a library implementing a mathematical method for describing neuronal network connectivity. CSA is used to facilitate the setup of such connectivity in large-scale models.

PDC has also offered computer time on Milner, as well as access to neuromorphic hardware to the Human Brain Project – an offer which has been appreciated by the project and which may be taken up later.

The HBP Contribution to the Neuroscience Community

The six HBP Platforms will enable new kinds of collaborative research to be performed in neuroscience, medicine and computing. The prototype tools, hardware systems and initial data sets are designed to make faster and more efficient research techniques possible in areas such as modelling, in silico experimentation, or data analysis. Users are encouraged to explore the Platforms and to build interactive “collabs” as part of the HBP Collaboratory, a scientific research hub that is accessible via the web and that serves as the main entry point to the Platforms.

The HBP Collaboratory and the HBP Platforms are subject to restrictions on their use. In most cases these restrictions are due to limited computing or storage capacity powering the Platform service offerings. For example, supercomputing time and an account with a high performance computing centre are required by the High Performance Analytics and Computing and the Brain Simulation Platforms. The Neurorobotics Platform has a limited number of servers that can

be used concurrently, and the initial data sets in the Neuroinformatics and Medical Informatics Platforms are limited. If you are interested in using the HBP Platforms, please see <https://www.humanbrainproject.eu/platform-access> for more details and guidance about accessing the platforms, as well as the terms of service and conditions of use for each of the platforms.

Below: BioExcel Workflow Training, Barcelona Supercomputing Center, Barcelona, 20-21 October 2016



Below: BioExcel All Hands, Barcelona, 3-4 November 2016



Below: BioExcel webinars (see <http://bioexcel.eu/webinars>)

BioExcel's First Birthday

Rossen Apostolov, PDC

It is now officially a year since the BioExcel Center of Excellence for Computational Biomolecular research started! We have made great progress with improving the performance and extending the functionality of the main codes that we support, extending the automation workflows further; developing the training programme and undertaking extensive outreach to the biomolecular research communities. The training events and the interest group activities have also picked up speed.

In October we held two major research community events in Barcelona: the **workflows workshop** and the **GROMACS hackathon**.

At the workflows workshop we presented several of the most popular platforms and managers for workflow automation (Galaxy, KNIME and Taverna) and two powerful managers for large-scale deployment (Copernicus and pyCOMPS). Our new friends, the core developers of the Common Workflow Language (CWL) and the Nextflow platform, came and gave invited talks. After the tutorials, the participants were given the opportunity to bring up their own problems and to get help from our experts.

The hackathon brought together the core GROMACS team and many external developers for three days of productive hacking. (We will do it again next year, so stay tuned!) And if you have not updated your favourite Molecular Dynamics engine yet, we have two patch releases for GROMACS: **2016.1** and **5.1.4**!

We have also continued with our **webinar series**. If you have ever wondered how to squeeze the most out of your HPC cluster with GROMACS, this **webinar** is the definitive guide! Predicting binding affinities is not a trivial task but the **PRODIGY server** makes it much more simple. Large-scale analysis on cloud infrastructure is not usually something one would do lightly, but we have it covered with this **webinar** in case you really want to. We also have a **special webinar** on defining the training needs of researchers in the field of computational biomolecular research. Many of the core aspects of the training programme, which was presented at the webinar, will be useful for training professionals (such as lecturers and application experts) in other fields of computational research.

And remember that if you ever hit a roadblock with any of the biomolecular codes that we support, we also have a range of support forums at <http://ask.bioexcel.eu>.



Aleksei Lupinov

This year Aleksei Lupinov finished a two-year master's programme in scientific computing – it was an Erasmus Mundus Computer Simulation for Science and Engineering (COSSE) master's course undertaken at KTH and the Technical University of Berlin.

Aleksei's master's thesis project was about implementing a particle mesh Ewald (PME) method (that is, a long-range electrostatic interaction algorithm) on graphics processing units (GPUs), which is something that may help to improve the performance of molecular dynamics (MD) simulations on GPU-abundant hardware configurations.

After completing his thesis, Aleksei joined PDC as a full-time research engineer; his current goal is to fully integrate the PME GPU implementation into GROMACS, the open-source MD software.



Above: SeRC Room Housewarming, PDC, 9 November 2016

PDC Summer School 2016

Apostolos Vasileiadis, CST

This year was the 21st time that the PDC Summer School has been held. A total of 41 researchers attended the school, which was held at the KTH Royal Institute of Technology main campus in Stockholm during the last two weeks of August. For many years we have had wonderful sunny weather during that period. This means that the picnic on the first day – which is a great chance for the participants to meet each other and the staff involved in the course – usually also gives people a chance to work on their suntans while sitting on the grass in the main KTH quadrangle. This year, despite positively hot weather earlier in the summer which dried much of the normally verdant Swedish grass to straw, we had drizzly weather for the first day of the school and only just managed to take a group photo before the rain started.



Many of the participants at the Summer School were “locals” from KTH but there were also attendees from other Swedish universities (Uppsala University, Chalmers University of Technology and Lund University) and from SAAB Electronic Defence Systems. We were also glad to welcome researchers and inventors from further afield who came from Inria (Inventors for the Digital World), France, and from the Institute for Theoretical Physics (IFT) which is based at the Autonomous University of Madrid in partnership with the Spanish Scientific Research Council (UAM-CSIC), Spain.



Above: PDC Summer School lectures and labs, August 2016

Below: PDC Summer School labs, August 2016



During this intensive fortnight, the researchers at the Summer School are introduced to the fundamentals of programming supercomputers, and also learn how to improve programs for parallel scientific applications so that they run more efficiently. Because the aim is for people to be confident in using high performance computing (HPC) systems by the end of the course, participants do not just attend lectures, but also take part in plenty of practical guided hands-on lab sessions.

There are also tours of the PDC computer hall so that attendees can see Beskow, the fastest academic supercomputer in the Nordic countries, and the other systems at PDC, as well as getting an idea of the complex infrastructure that is required to run such high performance systems continuously and reliably.



Above: Tours of PDC computer hall, August 2016

neic Nordic e-Infrastructure
Collaboration

Pool Nordic Competencies!

Michaela Barth, PDC

The national e-infrastructure providers in the Nordic countries possess a wide range of competencies within the operation and development of services if we consider their combined resources. However, this competence is partially fragmented and is not coordinated between the different countries. Thus, for NeIC – the Nordic e-Infrastructure Collaboration – to make the Nordic countries capable of tackling e-infrastructure challenges beyond what is currently possible on individual national scales, pooling competencies from the five membership countries has become imperative in order for the collaboration to succeed.

Pooling competencies was therefore selected as one of the four focus areas in the **NeIC strategy implementation plan** with the other imperative focus areas being:

- sharing resources,
- securing long-term funding, and
- strengthening dialogues with stakeholders.

Each of these focus areas (“Pool competencies, Share resources, Secure long-term funding, and Strengthen stakeholder dialogue”) has its own set of activities and milestones.

The NeIC strategy implementation plan seeks to implement the strategy for the years 2016-2020 that the NeIC Board updated in 2015. This NeIC strategy update was in response to five of the ten concrete actions involving e-infrastructure in the revised **Nordic eScience Action Plan** which was delivered to the Nordic Council of Ministers back in June 2015.

The Nordic Council of Ministers responded by directing NordForsk to facilitate the implementation of the plan and consequently NeIC – which is organisationally hosted at NordForsk – was seen as the natural body to coordinate

the implementation of the corresponding e-infrastructure actions.

The pooling of competencies is being pursued through the following activities:

- a) mapping skills, as well as identifying and prioritising needs,
- b) establishing Nordic cross-border training programmes, and
- c) making NeIC more attractive for competent personnel.

Working group members, initially just for activity b), were nominated by the national e-infrastructure providers. In addition, the working group decided to combine activities a) and b) by defining the focus on training as a pilot case and by defining a common work plan for those two activities. The first step in this process was to get a deeper understanding of the training status in the different countries so the group could make comparisons and have a fruitful exchange of ideas. A series of one-to-one interviews with the national training coordinators, along with face-to-face group meetings and biweekly video calls, were all part of the process used to establish a common basis for the discussions and then produce a document giving a more or less complete training status overview.

The group's work plan and the first deliverable (that is, the document that was produced outlining the training status) are available on the NeIC Pool Competencies wiki page: wiki.neic.no/wiki/Pool_competencies.

Additionally, the pooling competencies “PoCo” working group agreed on a set of quality assured questions about training that were designed to be included in the national user surveys – both to improve the usefulness of the information that the national organizations get from these surveys, and to assess the willingness of Nordic e-infrastructure users to travel in order to benefit from training opportunities in other countries. A further achievement is the establishment of a joint training calendar (which can be plugged in to the national training websites) and a training metaportal. (This was celebrated with a big [press release](#).) The calendar is used for coordinating

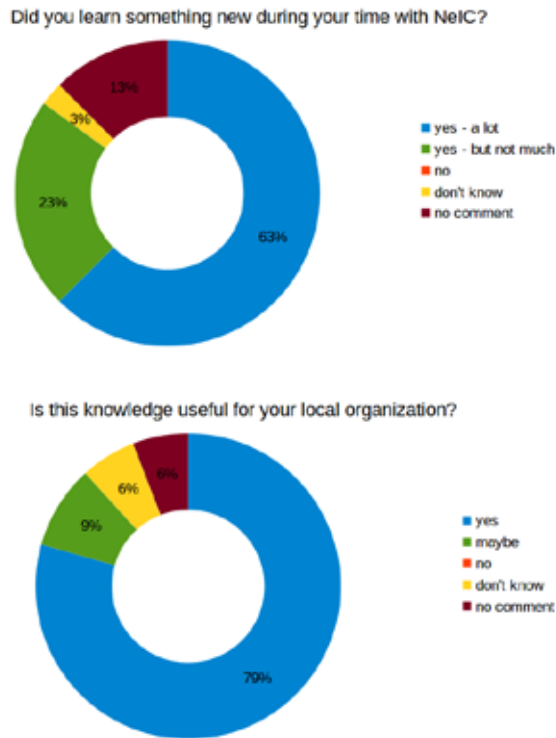
and surveying the present training offerings in the Nordic countries. Findings from this calendar will be used as the basis for decisions on funding new training. A corresponding mailing list (which is not explicitly intended for the end users) is currently under testing.

A NeIC training policy (and recommendations for corresponding national training guidelines on opening national training activities for other Nordic participants) is in progress. Furthermore, there will also be a NeIC mobility enhancement programme enabling Nordic participants to get travel grants to participate in training events in other Nordic countries. In the course of developing the training programme – which is the final goal of activity b) – the working group sketched the scope of the activities to be handled by a future training programme manager.

The other side of the coin when it comes to making training more readily accessible – namely moving the courses closer to the participants – is being achieved by creating transferable courses along the lines of the concept that NeIC is also adopting in the [CodeRefinery scientific software project](#). To this end, the “PoCo” working group also acts as a logical reference group for proposals for additional training money available through NordForsk.

The NeIC training programme manager is taking a proactive role in finding people willing to make their courses more transferable and will eventually also coordinate the online training efforts. The NeIC mobility enhancement training programme will be run in a manner that is similar to a small NeIC project with the current “PoCo” working group as the logical steering group. The [training programme manager position](#) is currently being advertised so the training programme can start in 2017. Two people would be needed to perform a peer review of applications for the mobility enhancement grants (to travel to courses abroad within the Nordic countries), so the training programme manager and the chair of the steering group for the training programme could take care of the peer reviews. The cut-off dates for applications for the mobility enhancement grants are planned to be on the 1st and 15th of each month.

Below: Some results from NeIC employee survey



For activity c) a NeIC employee survey with about 25 questions was created and conducted (see above). The survey took about 20 minutes to complete and received 40 responses (that is, about 85% of the NeIC staff at the time responded to the survey). The ongoing analysis of the answers will provide input to the final formulation of the corresponding employer survey. The next milestone in activity c), namely developing a NeIC Human Resources Policy, will be tackled in early 2017.

NeIC is in the process of become a driving force to further the development of competence across the entire Nordic e-infrastructure community. To achieve this, the current skills distribution needs to be mapped and matched with the current state-of-the-art within the field, and, of course, also with the needs of the e-infrastructure user communities in the Nordic countries.

In addition to the current efforts related to training, competencies will also need to be pooled in other fields. For that the NeIC Board members were asked to provide a ranking of suggested hot topics (like security or procurement) where further pooling of competencies could yield significant benefits. Data management was chosen as the number one priority

where more competence mapping and pooling is clearly needed. The different Nordic countries are in different states of maturity in this field. A Nordic platform where stakeholders meet and discuss the entire life cycle of research data, as well as becoming familiar with each other's terminology and interests, will be useful. NeIC has taken the first steps to populate such a platform by accepting nominations for suitable representatives from the individual national e-infrastructure providers.

If you have further questions about NeIC activities, please contact Michaela Barth (caela@pdc.kth.se) who is the main person responsible for the NeIC "Pool Competencies" focus area.

Parallel Programming Workshop with NVIDIA

Henric Zazzi, PDC

NVIDIA visited PDC on the 19th of September and ran a workshop demonstrating parallel programming with their open standards. About fifteen researchers and developers from the Stockholm area attended the meeting. The programme focused on developing software for the mixed architecture of future supercomputers while maintaining a single code base and covered topics like PGI Accelerators, OpenACC, and libraries for C++/Fortran and Python.



Above: NVIDIA Parallel Programming Workshop, KTH, September 2016

The CodeRefinery Project

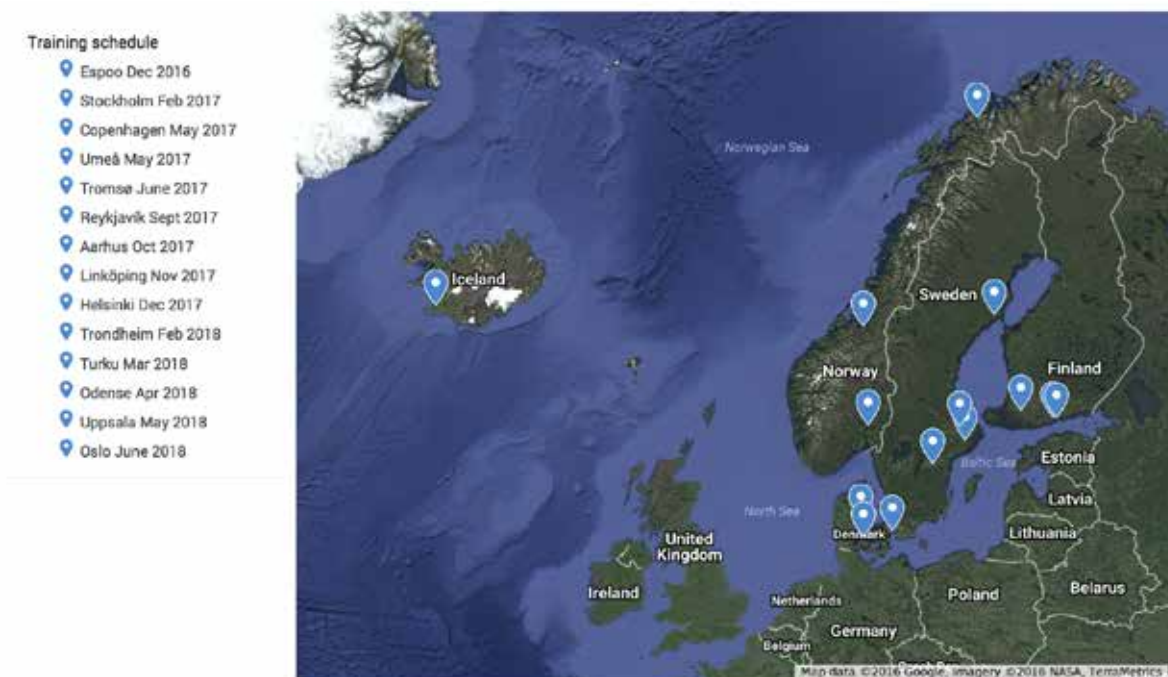
Thor Wikfeldt, PDC

PDC is participating in the new **CodeRefinery project** that was launched this autumn - the project aims to promote better software development practices in scientific communities across the Nordic countries. Funded by the **Nordic e-Infrastructure Collaboration (NeIC)**, the CodeRefinery project will initially run for a two-year period. Software lies at the heart of research projects across a wide range of disciplines, but many common practices in the development and maintenance of scientific software are inefficient and/or outdated. Core developers have, in many cases, never received training in modern software development methodologies because their main training and interests are in their respective scientific domains.

Various other similar projects have clearly demonstrated the value of scientific software development training, such as the **Software Carpentry project** which has taught efficient computing skills – ranging from basic to advanced level – to thousands of researchers since 1998. Drawing inspiration from such projects, CodeRefinery focuses on intermediate-level training and is directly aimed at assisting

research groups in the Nordic countries. A major component of the project will be to develop course material and to teach topics such as collaborative distributed version control, managing code complexity, automated testing and code documentation approaches. Workshops based on interactive and type-along types of presentations will be organised in various locations (see map below), starting with a workshop in Espoo, Finland, from the 14th-16th of December 2016, and followed by one at KTH from the 20th-22nd of February 2017. (For further information about the workshops and for registration details, see the **CodeRefinery website**). In addition to delivering a dozen training workshops in two years, CodeRefinery also aims to provide tools, systems and infrastructure to Nordic researchers for web-based hosting of open source as well as proprietary source code. This hosting service will be connected with an automated testing service. A final aspect of the project will be to build an active and interconnected community of researchers, software developers and application experts, leading to an environment for the exchange of expertise within the Nordic region.

Follow us on Twitter (@coderefine) and the project website: <http://coderefinery.org>!



Above: CodeRefinery Workshops 2016-2018

PRACE 2.0 on Its Way

Michaela Barth, PDC

New times may be in store for scientists and researchers from academia and industry who regularly set out to address society's grand challenges by carrying out excellent quality experiments and simulations; PRACE – the Partnership for Advanced Computing in Europe – is entering its second phase, still following a clear mission to facilitate high-impact scientific discovery, as well as engineering research and development, across all disciplines for the benefit of society and to enhance European competitiveness. PRACE seeks to realize this mission by offering world-class computing resources and services through a series of calls with time allocations being awarded via a peer review process. After a successful first phase of PRACE, which ran from 2010-2016 and offered over ten billion core hours in 13 calls, the second phase of PRACE, PRACE 2.0, will officially start in 2017 together with PRACE-5IP. In actual fact the 14th call is part of PRACE 2.0, even though it was closed in November 2016, as it is offering over two billion core hours to be used from April 2017 onwards. PRACE 2.0 will run for three years until 2020 offering a total of six calls.

PRACE has been established as an international non-profit association based in Brussels and currently has 25 members and two observers. However, the number of full members may change with the new funding model that will be put into place by the start of PRACE 2.0.

In Sweden the Swedish Research Council (VR) is the official PRACE member with the Swedish National Infrastructure for Computing (SNIC) being its representative. Because of planned structural changes within SNIC (which include a new funding cycle starting in 2018), at the moment Sweden can only commit to join PRACE 2.0 in 2017; the formal decisions for the following years need to wait until the new model for SNIC is in place. While this leaves some uncertainty in the meantime, we hope that this will not impinge on Swedish PRACE users and their access to PRACE resources.

The PRACE regular project access call 14 has already been opened under the new PRACE 2.0 framework and closed on the 21st of November 2016, with time allocations for standard single-year access starting on the 1st of April 2017 for a period of 12 months. Multi-year projects based on a 24- or 36-month schedule are also possible. Additionally, the call reserves 0.5% of the total resources available for Centres of Excellence (CoE) as selected by the European Commission (EC) under the E-INFRA-5-2015 call for proposals. The Swiss National Supercomputing Centre (CSCS) will be the new fifth PRACE hosting partner in PRACE 2.0 and they are making their system PizDaint available. The other hosting countries are, as usual, France, Germany, Italy and Spain. Altogether the five PRACE hosting partners are offering seven systems with more than 2000 million compute core hours, and a cumulative peak performance of 50 petaflops was offered in this call, which is three times more than in previous calls. Final decisions on the proposals will be made by the PRACE allocation committee in mid-March 2017. For further information about the Tier-0 calls, see <http://www.prace-ri.eu/prace-project-access>.

While the 14th Tier-0 call was open, the latest PRACE Tier-1 call (which interestingly was also the 14th call in its series) was also open for researchers affiliated with a Swedish institution and the deadline was synced with the Tier-0 call. The PRACE Tier-1 calls are traditionally known as DECI calls – meaning Distributed European Computing Initiative – and they now constitute an optional programme within PRACE that was adopted from DEISA in 2011. For DECI-14 Sweden is again providing 5% of PDC's local flagship system, Beskow, which is still the largest academic supercomputing resource in the Nordic countries. Traditionally, we in Sweden do well in DECI applications.

The DECI-14 call features some changes compared to previous DECI calls.

- Up to 30% of the computing time has been reserved for projects from countries that are not providing resources to the call.

- Individual projects have been limited to a maximum of 5 million core hours. (The average award per project is expected to be around 2.4 million core hours; the maximum limit was set partly to give a better idea of realistic project sizes and to mark the difference between Tier-1 and Tier-0 projects.)

As was the case with the previous DECI-13 call, for DECI-14 researchers could apply to participate in the popular joint pilot programme with EUDAT. In DECI-13 half of the applications expressed interest in taking part in the joint EUDAT pilot activities and, out of those, five projects were selected. This time the EUDAT storage offerings were again set to about 150 TB per project and up to 1 PB of total storage capacity in the hope that there would be more suitable projects that could be selected for the joint EUDAT pilots. For more information about the joint pilot activity, see

- www.prace-ri.eu/dec14-call and
- <https://eudat.eu/collaboration/prace>.

The new Type D preparatory access project type, referred to as "Tier-1 for Tier-0" (which was presented in the last issue of the PDC newsletter), has unfortunately been delayed due to some of the uncertainties with PRACE 2.0, but has finally come to light for real in the latest December cut-off. Eight Tier-1 centres have agreed to participate, with most of them being able to host one or two projects with a typical size of 150 000 core hours. Keep watching <http://www.prace-ri.eu/prace-preparatory-access> to find out more!

The current implementation phase of PRACE (PRACE-4IP) will come to an end on the 30th of April 2017. The next implementation phase PRACE-5IP has had its EC funding confirmed and will officially start in January 2017, although in practical terms it will begin on the 1st of May 2017, and then run until the 30th of April 2019. The suggested distribution of person months (PMs) for Sweden's contributions to PRACE-5IP in the proposal submitted to the EC was as follows: 19 PMs for the KTH Royal Institute of Technology, 6.5 PMs for Umeå University and 8.5 PMs for Linköping University, giving a total of 34 PMs.

New PRACE Training Centres will be established in PRACE-5IP. A fair and transparent selection process and an open call for becoming a PRACE Training Centre will be prepared. The plan is to open this call just after the PRACE-5IP project starts.

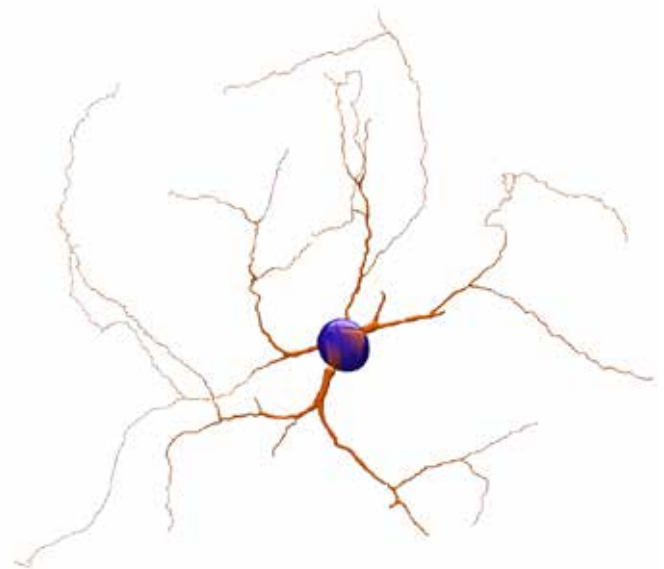
If you would like to understand more about PRACE and what it could help you to achieve with your research, please contact Michaela Barth (caela@pdc.kth.se) straight away!

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.

Sweden's participation in the EU-funded Human Brain Project (HBP) involves research using Milner. Jeanette Hellgren Kotaleski is the deputy leader of the HBP Brain Simulation Platform, which provides software, workflows and models for brain simulation. One of the long-term



*Above: A medium spiny neuron (MSN) from the striatum, part of the motor system in the brain
Johannes Hjorth uses Milner to determine experimentally unknown parameters through optimization.*

goals of the HBP is to simulate the entire human brain. As a step towards this goal, accurate models of the different types of neurons in the brain need to be created. Some of the model parameters can be measured directly, but other parameters are as yet unknown. Johannes Hjorth, who is a postdoctoral researcher in Jeanette's research group at the SciLifeLab, based at the Karolinska Institute in Stockholm, is developing and using a workflow where optimization techniques are employed to determine appropriate values for unknown parameters. Johannes says that "The goal of the optimization is to make our models behave similarly to what we observe in experimental data. The parameter space we investigate is so large that we need to use supercomputers for our parameter search. For this project we are using the PDC supercomputer Milner".

PDC also participates as a partner in the Neuromorphic Computing Platform in the Human Brain Project, where the Multisimulation Coordinator (MUSIC) is being developed. MUSIC is a software tool that works as a communication bridge between brain simulation software tools and/or hardware, allowing larger simulations to be built from components. MUSIC has recently been integrated into the Closed Loop Environment (CLE) software from the HBP Neurorobotics Platform.

One of the projects in the Swedish e-Science Research Centre (SeRC) community known as Brain-IT is a "Scalable systems level simulator" – this project is being run by Anders Lansner, Örjan Ekeberg and other researchers. Here the interaction between a running neuronal network simulation and the environment, as well as interactive visualization, is being explored. This project, as well as the "Scalable brain-like cognitive architectures for virtual agents" project which is based at the KTH Department of Computational Science and Technology (CST) and run by Anders Lansner, Örjan Ekeberg, Pawel Herman and Christopher Peters, use MUSIC to connect simulations running on Milner with the outside world.

SNIC User Forum 2016

Gert Svensson, PDC

The Swedish National Infrastructure for Computing (SNIC) User Forum was held on the 24th and 25th of October 2016 in Lund and hosted by Lunarc – the Center for Scientific and Technical Computing at Lund University – which is the SNIC centre in Lund. The purpose of these user forums is to disseminate information about SNIC to the researchers using the SNIC systems, to give those researchers a chance to meet the staff of the SNIC centres, and for SNIC to listen to the opinion of the researchers using the SNIC computing resources. This was more important than usual this year as the Swedish Research Council (VR) is planning to change the funding model for Swedish research infrastructures, including SNIC. This was reflected in the large number of attendees at this year's meeting: over a hundred people attended the meeting including researchers from difference disciplines.

Two keynote speakers gave an international perspective on high performance computing (HPC) and eScience. The first keynote speaker was Michael Uddstrom who described the **New Zealand eScience Infrastructure** (NeSI). In the second keynote talk, Allison Kennedy, Director of the **Hartree Centre** in the UK, gave an overview of the British national infrastructure for HPC and big data. Another important point on the agenda was the presentation of **this year's SNIC User Survey**. (Interestingly the largest number of responses from researchers came from the bioinformatics area.) Other highlights were a **presentation** by Dejan Vitlacil from PDC who (together with Jens Larsson from NSC, the National Supercomputer Centre at Linköping University) talked about the future of the SNIC storage services, and an inspiring **talk about providing better user guides** for the software at the different SNIC centres given by Cristian Cira from PDC.

The SNIC User Forum ended with a discussion in smaller groups between researchers, SNIC centre staff and SNIC decision makers. Each of the groups summarised their conclusions which are being used to provide input for an improved SNIC.

Below: Introduction to PDC Systems course, 13 September 2016



Learning How to Use the PDC Systems

Cristian Cira, PDC

The Introduction to PDC Systems course that was held on the 13th of September 2016 at PDC brought together 20 supercomputer users from various scientific backgrounds (most of whom were postdoctoral researchers, assistant professors or professors) for a three-hour course that covered an overview of the PDC computer systems. The course focused on describing the hardware of PDC's systems, along with PDC's programming environments (including the running and queuing policies). Participants were also given comprehensive information about the size of Swedish National Infrastructure for Computing (SNIC) time allocations and a brief description of the application process. The main goal of the course was to give attendees a good grasp of the workflow and requirements when it comes to using PDC facilities. The course ended with a tour of the PDC machine room where each of the researchers was given the opportunity to walk around Scandinavia's fastest academic supercomputer.

If you would like to learn how to use PDC's supercomputer systems, please keep watching the [Events section](#) of the PDC website where the date of the next introductory course will be advertised – the next course is likely to be held in February 2017.

PDC-Related Events

CodeRefinery Workshop

20-22 February 2016, KTH, Stockholm

<https://www.pdc.kth.se/events/event-repository/coderefinery-workshop-on-sustainable-scientific-software-development>

PRACE Spring School 2017 - HPC in the Life Sciences - in collaboration with BioExcel

10-13 April 2017, KTH, Stockholm

The school is being organised as a collaboration between the Swedish National Infrastructure for Computing (SNIC), represented by KTH, and the BioExcel Center of Excellence for Computational Biomolecular Research. For details see: <https://events.prace-ri.eu/event/502>.

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

<https://www.egi.eu/category/events>

HPC University

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

HPCwire

<http://www.hpcwire.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 2017

Umeå, Sweden

29 May - 1 June 2017!

After being in Norway and Finland, the NeIC Conference will be held in Sweden for the first time in 2017. Further details about NeIC2017 are available here:

<http://neic2017.nordforsk.org>.