PDC Newsletter

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PDC has seen very exciting summer months this year. Lindgren, our new Cray system arrived and was assembled in June. First users got access during July, and the system was officially inaugurated during our 20th anniversary celebration at the end of August. Many of you have certainly seen the press coverage of this major new Swedish system funded jointly by SNIC and KTH. While this system is now being used in production, we are busy upgrading the infrastructure for its expansion that will turn Lindgren into a 305 TeraFlops XE6 system, and thus to one of the major systems in Europe. The upgrade will take place in December and the expanded Lindgren is expected to be available early 2011.

Lindgren will also be available to European researchers through the PRACE infrastructure, and we are currently gaining first-hand knowledge by offering parts of Ekman to DEISA Extreme Computing Initiative projects.

SNIC has recently approved the prolongation of its support for Ferlin throughout 2011, so you will be able to enjoy another year of running on this resource before we aim for a SNIC replacement system in 2012.

On the international scene, a number of projects with PDC participation have started. This includes the first implementation phase of PRACE, where PDC coordinates the Swedish contributions provided by HPC2N, NSC, and PDC, and leads a few of the tasks; the Venus-C cloud infrastructure project; and the PDC-led ScalaLife project. A number of project proposals are also being submitted in November, most importantly the second implementation phase of PRACE where, this time, all six SNIC centers will contribute. With these projects, we put Sweden firmly on the European landscape and can ensure that Swedish scientists will have seamless access to the resources they need, whether in Sweden or on the European scale.

In the PRACE effort, Sweden will host a PRACE Scientific Seminar in February 2011, and PRACE’s 3rd Industrial Seminar in Stockholm, March 28-29, and co-organize PRACE’s 2011 Summer School together with CSC, Helsinki. Through PRACE’s 2nd regular call, researchers can now apply for time on two systems: the Blue Gene/P in Juelich provided by the Gauss Center, and a fat node x86 system provided by GENCI in Paris.

In this edition you will also read about INCF, the International Neuroinformatics Facility, located in Stockholm and supported by KTH and PDC as well as about our yearly summer school, which this time attracted a new record of applications.

With this, we wish you all the best for the upcoming holiday season and a successful 2011. We hope that with the recent developments at PDC we will continue to be a strong partner for your HPC needs.

Lennart Johnsson, Director PDC
Erwin Laure, Director PDC-HPC
INCF, Facilitating and Strengthening Neuroinformatics Research
by Mikael Djurfeldt

INCF AT A GLANCE
The International Neuroinformatics Coordinating Facility (INCF) fosters international neuroinformatics infrastructure, which promotes the sharing of data and computing resources within the research community. The INCF also facilitates development of applications that can be used by neuroscientists worldwide.

The INCF coordinates:
- the INCF programs
- the INCF workshops
- the annual Neuroinformatics Congress

The INCF has developed a web portal in order to make resources easily accessible. The portal contains research tools, listings of neuroinformatics-related events, training and jobs, and the neuroinformatics "People Directory."

WHAT IS NEUROINFORMATICS?
Neuroinformatics is a research field that encompasses the organization of neuroscience data and application of computational models and analytical tools. Neuroinformatics facilitates progress in all brain sciences and related fields.

INCF at a Glance

Core Activities
The INCF Programs represent long-term strategic undertakings to address issues of high importance to the neuroscience community. Establishing an INCF Program is a multi-step process. Each Program delivers products and services, and develops standards and guidelines for the particular field.

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The INCF Workshops focus on selected technical issues of importance to neuroinformatics, or research topics related to neuroscience databases, tool development, and modeling of the nervous system function. Each workshop delivers a report on current activities and recommendations to serve as the basis for further INCF activities. The recommendations may lead to the launch of an INCF program to provide products, services, standards, and guidelines.

The INCF Neuroinformatics Congress was established with the purpose to provide an international venue for interactions across academic domains. It also serves to facilitate dissemination of scientific results.

The Congress is held in one of the Member Countries: 2008 in Stockholm, Sweden; 2009 in Pilsen, Czech Republic; 2010 in Kobe, Japan; and 2011 in Boston, USA.

**Organization**

The Secretariat is the central office of INCF and is responsible for overall scientific and administrative activities.

The Governing Board is composed of representatives from the member countries, and makes collective decisions regarding INCF. The EU is represented on the Board.

Each INCF member country establishes a "National Node" to further the development of neuroinformatics and to interface with the INCF Secretariat.

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Staff Focus: Mattias Chevalier

Mattias Chevalier received a M.Sc. in engineering physics at Uppsala University and a M.Sc. in mechanical engineering at University of Houston, both degrees with emphasis on numerical analysis in general and on computational fluid dynamics (CFD) in particular.

When returning from the US, Mattias started to work at the Aeronautical Research Institute of Sweden (FFA) and at the same time he enrolled as an industrial Ph.D. student at the department of mechanics at KTH. His Ph.D. studies focused on how to optimally control, prevent, and delay the transition from laminar to turbulent flow. In parallel, at FFA (later Swedish Defence Research Agency), Mattias worked on many different aspects of CFD, everything from running simulations, to developing software tools, to compute and analyze fluid flows—mostly applied to airplane and rocket configurations.

In 2008, Mattias started to work at Scania CV AB as a CFD engineer, naturally with less focus on the high-speed flow regime and instead more focus on flow phenomena in combination with heat transfer on trucks and buses. Beginning in August 2010, Mattias work part... continuing on page 5.
The Community consists of research groups, consortia, funding agencies and publishers in the field.

**INCF Member Countries**

Belgium, Germany, Korea, Sweden, Czech Republic, India, The Netherlands, Switzerland, Finland, Italy, Norway, United Kingdom, France, Japan, Poland, and United States

**LEARN MORE: www.incf.org**

The INCF was established through the Global Science Forum of the OECD to develop an international neuroinformatics infrastructure. The proposal to create the INCF was endorsed by the OECD science ministers in 2004 and the INCF was officially established in 2005. The Secretariat is located in Stockholm, Sweden. Karolinska Institutet and the Royal Institute of Technology are its host institutions.

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**C!C, Promoting Cloud Technologies in Academia and Industry**

by Åke Edlund

KTH-SICS Cloud Innovation Center (C!C), <http://www.pdc.kth.se/research/cloud-computing> founded by KTH and SICS, is an open consortium promoting cloud technologies in academia and industry. Specifically, C!C will:

- Provide a forum to disseminate and discuss cloud initiatives in Sweden
- Foster research collaborations in national and international projects
- Coordinate education activities in cloud technologies
- Interact with industry through agile business driven projects
- Contribute to Swedish seed accelerator programs

C!C will host the annual Cloud Computing Day, which will be in spring 2011 (stay tuned!)

C!C started on October 14 and is coordinated by Åke Edlund (PDC).

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Rossen Apostolov obtained his Ph.D. in computational chemistry at the Institute for Protein Research at Osaka University, Japan. His work was on optimizing the molecular dynamics package "myPresto" and porting it to special-purpose processors such as MDGRAPE <http://www.peta.co.jp/index-en.html>.

...continuing on page 6,

**Staff Focus: Rossen Apostolov**
ScalaLife, Scalable Software Services for Life Science

by Lilit Axner

A new project, ScalaLife, Scalable Software Services for Life Science, was successfully launched on September 1, 2010. On September 27-28, PDC organized the project's kick-off meeting, during which the partners discussed the general planning and implementation structure of ScalaLife.

ScalaLife is a pan-European project funded by the EC's 7th Framework Programme. The six European partners of the project are the Institute for Research in BioMedicine (IRB) and the Barcelona Supercomputing Center (BSC) from Spain, Leibniz-Rechenzentrum (LRZ) from Germany, Oxford e-Research Centre (OeRC) from the United Kingdom, Synective Labs (SYN), and the Royal Institute of Technology (KTH) from Sweden.

Summary: Life science is developing into one of the largest e-Infrastructure users in Europe, in part due to the ever-growing amount of biological data. Modern drug design typically includes both sequence bioinformatics, in silico virtual screening, and free-energy calculations, e.g., of drug binding. This development will accelerate tremendously, and puts high demands on simulation software and support services. e-Infrastructure projects such as PRACE/DEISA have made important advances on hardware and scalability, but have been mostly focused on theoretical scalability for large systems; on the other hand, typical life-science applications concern small- to medium-
Xavi Aguilar received his M.Sc. in Computer Science at the Universitat Politecnica de Catalunya in Barcelona (<http://www.upc.edu/eng/> in 2003. He worked as a research collaborator at the university in the Computer Architecture Department (<http://www.ac.upc.edu>) while he finished his studies. After obtaining his M.Sc., he started to work at the European Center for Parallelism of Barcelona (CEPBA) as a developer in the CEPBA-tools team. There, he worked developing software to analyze application behaviour on supercomputers. In 2005, he began to work at the Barcelona Supercomputing Center (BSC) (<http://www.bsc.es>) as a researcher and developer, working in the field of performance tools and developing analysis and simulation software (<http://www.bsc.es/plantillaF.php?cat_id=52>). During this time, he also participated in collaboration projects with some research centers such as Lawrence Livermore National Laboratory, NASA Ames, and IBM.

At the end of summer of 2009, Xavi decided to change his life and moved from warm Barcelona to Stockholm in order to join PDC as a system specialist. He is currently working on scalable performance tools for upcoming HPC systems and collaborating in the European project, Scalalife (<http://www.scalalife.eu>), as well.

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**Objectives:** We have identified three main objectives for ScalaLife:

1. We will develop new hierarchical parallelization approaches explicitly based on ensemble and high-throughput computing for new multi-core and streaming/GPU architectures, and establish open-software standards for data storage and exchange.

2. We will implement, document, and maintain such techniques in pilot European open-source codes such as the widely used Gromacs and Dalton, a new application for ensemble simulation, DISCERTE, and large-scale bioinformatics protein annotation software called PredictProtein.

3. We will create a competence centre for scalable life-science software to strengthen Europe as a major software provider and to enable the community to exploit e-Infrastructures to their fullest extent. This competence network will provide training and support infrastructure, and establish a long-term framework for maintenance and optimization of life-science codes.

**Competence Center:** A competence centre for scalable life-science software to strengthen Europe as a major software provider and to enable the community to exploit e-Infrastructures to their fullest extent will be established. This competence centre will provide training and support infrastructure, and establish a long-term framework for maintenance and optimization of life-science codes.

For pilot applications, the focus will be concentrated on a number of widely used European open-source codes: Gromacs, which does classical molecular dynamics simulation; Dalton, which does quantum chemistry; a newly developed meta-application, DISCERTE, designed to make full use of clusters with millions of cores through a database approach to modeling; and finally, PredictProtein, which provides data management of large-scale automated protein annotation using a number of the most important bioinformatics programs.

...continuing on page 8, ScalaLife
The main impact of the competence centre will be to break the barriers between hardware, software, and application research; this unified community of computational scientists will be an essential element of underpinning next-generation e-Infrastructures, and have a significant structuring impact on the European research area.

**Service activities:** The service activities in ScalaLife are aimed to offer an integrated service to the life-science software community, providing software integration and maintenance, application validation, and the life-science competence centre, which is in the centre of the project. We will maintain world-leading life-science software packages and integrate new scalability techniques as well as interfaces and data formats. This will be a part of producing deployable releases of software packages. We will offer these packages on European e-Infrastructures and validate them with real application cases. The life-science software competence centre will act as “one-stop-shop” for groups seeking advice and help with life-science software through providing documentation, best practices, and expert advice.

Simulating the dynamics of large proteins such as voltage sensors or other membrane proteins depends on advances in scaling and performance enhancements to enable simulations of tens of microseconds by scaling to thousands of processors on next-generation supercomputers.

**Joint research activities:** We will explore scalability techniques for life-science software starting with pilot applications and will develop and push standards for handling both storage and exchange of the ever-increasing amount of simulation data in life science. In the context of ScalaLife, an incremental route for existing applications will be formulated. We will also investigate the usage of ensemble computing techniques to overcome the scaling limitations inherent in some applications and investigate the usage of acceleration technologies. We will help to establish the standards in the field and act as a driving force in order to avoid humans from becoming the limiting factor in modeling/bioinformatics projects.

**User communities:** Apart from the four pilot applications, ScalaLife will interface to the life-science software community through the life-science software competence centre. The centre will be distributed to make best use of the different competences available with the partners involved in the centre and to provide a good geographic coverage over Europe. The competence centre will be the key vehicle to ensure the project results will be taken up widely by the life-science software community, and – by working with different groups – help overcome the fragmentation of knowledge in this field. Communities receiving expert support will be selected on their expected impact to the European life-science community judged using factors like user base, geographic spread, potential for improvement, etc.

For more information please refer to www.scalalife.eu.
**Record Interest in HPC Summer School**

by Mike Hammill

More students than ever applied for the "Introduction to High-Performance Computing" course offered at PDC this summer. For the last five years, interest in the course has gone up every year, with applications in 2010 increasing 17% over 2009 and 97% over the level five years ago. The number of students participating this year, 70, was up 26% over average. Two important contributing factors were the increased number of students from the National Graduate School in Scientific Computing (NGSSC), and the KTH Computational Science and Engineering Centre (KCSE) Graduate School. The 11 NGSSC students nearly double the number participating the year before, and the 16 KCSE students were the most that have ever participated in the school’s 15 year history.

Being at the leading edge of high-performance computing is what the class is all about. The students get both a strong conceptual foundation in state-of-the-art HPC as well as experience with practical aspects through lab work and projects.

To help the students make the most of the two-week course, a seasoned cadre of professors and professionals from around Sweden are joined by world-famous practitioners to cover various topics. These include parallel programming (OpenMP, MPI), modern computer architectures, parallel algorithms, efficient programming, and case studies. Lecturers included such well-known leaders in the field as David Black-Schaffer, Uppsala Univ.; Iris Christadler, Leibniz Computing Centre, Munich; Björn Engquist, KTH/Univ. of Texas at Austin; Thomas Ericsson, Chalmers; Erik Hagersten and Sverker Holmgren, Uppsala Univ.; Lennart Johnson, KTH/Univ. of Houston; Pavel A. Korzhavyi, KTH; and Anders Ynnerman, Linköping Univ./NVIS.

Each student is expected to complete a project, which is often related to his or her research area. This year’s projects include titles such as "A Molecular Dynamics simulation of Liquid Argon", "Solving and Visualizing Incompressible Newtonian Navier-Stokes Equations Using GPGPU," and "Computational Study of Electronic Structure of Graphene."

To help the students complete this work, a tutor is assigned. In addition to helping answer students’ questions, the tutor reviews the work in conjunction with the course examiner, Jesper Oppelstrup, a numerical analysis professor at KTH.

For PDC, the course is a win-win situation. Not only do the students gain valuable knowledge that will help them with their research, but PDC also benefits by encouraging more efficient use of its resources by the next generation of its users.

What do the students think? They gave the overall course a 3.5 score out of 4.0 with 4 being "very good" and 1 being "poor." Here are some quotes from this year’s course evaluation.

"I enjoyed the two weeks very much (even though I noticed that I had quite some background), and I’ve not only taken knowledge with me, but also some friends, a tentative research idea, and more practical information than I expected."

"I love the courses very much, and the lab is also designed such that every student can follow and learn what they need."

"The course is very good. It is in fact much better than what I anticipated. Also very good speakers. The lab exercises were very clear and were made easy to understand and implement. [Those in charge of labs] were really very tolerant and helpful. Overall it’s all positive."

The course, which is given the last two weeks in August, receives support from NGSSC, KCSE (both of which receive funding by the Swedish Research Council (Vetenskapsrådet), and of course KTH. It is open to local and international students as well as those outside of academics.

This is the 15th year the course has been given since the first summer school in 1996.

For more information, see the course Web page at <http://www.pdc.kth.se/education/summer-school/>.
On January 15, 1990, the President of KTH Royal Institute of Technology, Janne Carlsson, inaugurated what was to be called PDC. The center started to take shape two years before that official inauguration day, back in 1988, when a group of scientists at the KTH School of Computer Science and Engineering applied for a grant to buy a massively parallel computer. The money was granted, and during the fall of 1989, Thinking Machines Corporation installed an 8K Connection Machine, (CM2) at KTH.

On August 30, 2010, PDC Center for High Performance Computing celebrated its 20th anniversary with a two-day symposium at Tammsvik Konferens och Herrgård. During the symposium, the new Cray XT6m system was inaugurated by Prof. Erwin Laure, director of PDC-HPC; Ulla Thiel, vice-president of Cray Europe; and Prof. Sverker Holmgren, Director of SNIC and professor in Scientific Computing, Uppsala University.

At the anniversary symposium world-leading scientists gave speeches on high-performance computing in Europe and Sweden, and science done using such high-end computing power.

The event was opened with a welcome speech of Prof. Gunnar Landgren, vice-rector of KTH. He gave a historical overview and emphasized the importance of high performance computing in the world of science.

Prof. Lennart Johnsson, director of the PDC research center, and director of the Texas Learning and Computation Center, The University of Houston, presented the history of PDC during its existence of 20 years. He highlighted the important steps in the early life of PDC and the major events and projects that PDC participates in nowadays. PDC is one of six SNIC centers and represents Sweden in the rapidly developing high performance computing world.

Swedish research and innovation were discussed by Prof. Dan Henningson, head of the department of Mechanics, KTH, who presented the Swedish e-Science Research Centre (SeRC) and Prof. Sverker Holmgren, SNIC, who explained the SNIC infrastructure and presented HPC developments in Sweden. Prof. Göran Sandberg, director of Lunarc, presented the eSSENCE project.

PDC was also honored by the presence of several representatives from leading European high performance computing centers and research Institutes. Within the invited speakers were Prof. Petros Koumoutsakos, Eidgenössische Technische Hochschule Zürich (ETHZ), who highlighted the recent advances in the development of wavelet-based adaptivity for particle methods, the coupling of atomistic and continuum descriptions, and discussed the implementation of these methods in massively parallel computer architectures.

Prof. Thomas Schulthess, Swiss National Supercomputing Centre (CSCS) at Manno, presented simulations software developments for next generation supercomputers, specifically, discussing the Swiss platform for high performance and high productivity computing, a program that could
serve as a model for European contributions toward exascale computing.

Dr. Kimmo Koski, IT Center for Science (CSC) in Finland, presented the pan-European project PRACE and Europe on the road to Exascale Computing. He emphasized that under the umbrella of PRACE, a first implementation project has started and a second and third one are intended to follow in 2011 and 2013, respectively.

Among the guests were also Mario Mattia, Cray, Europe, and Leif Nordlund, AMD, who have discussed the trends in microprocessor design and developments within supercomputing in Europe and the world in general.

Dr. Lilit Axner, PDC, KTH, and Dr. Per Öster, CSC, Helsinki, presented three pan-European projects: DEISA, PRACE, and HPC-Europa. They announced the current open application calls and explained the general procedures of the selection processes.

SNIC Interaction complemented the 20th anniversary with a poster session highlighting accomplishments by high performance computer users in Sweden.

A lively panel discussion wrapped up the 20th anniversary. Kimmo Koski, CSC; Jacko Koster, Norwegian research network (UNINETT); Sverker Holmgren, SNIC; and Lennart Johnsson, PDC/KTH; discussed Nordic supercomputing and the need for increased collaboration within Scandinavian supercomputer centers and research institutes.

During the anniversary dinner, PDC, as represented by its director, Erwin Laure, received many presents from its guests. Dr. Ingrid Melinder, Dean of the KTH School of Computer Science and Communication, gave PDC Kosta Boda glassware called "Brain" by Bertil Vallien. Prof. Bengt Persson, director of NSC, gave PDC a painting depicting NSC’s initial location at Linköping University. Tomas Pålsson and Jakob Sandgren, from Southpole, presented PDC with three surrealistic photographs of PDC’s Ekman computer. PDC has AMD and SNIC to thank for sponsoring the event. Additionally, AMD provided PDC anniversary t-shirts. There were also anniversary coffee mugs and espresso cups. At the end of the program, Erwin Laure presented his staff with a certificate for a hot-air balloon adventure, noting that, as far as PDC is concerned, "the sky is the limit!"
We can recommend the following sources for other interesting HPC opportunities and events:

**CERN**
http://cerncourier.com/cws/events
http://cdsweb.cern.ch/collection/Conferences?ln=en

**DEISA**
http://www.deisa.eu/science/deci

**EGI**
http://www.egi.eu/about/events/

**HPC UNIVERSITY**
http://www.hpcuniv.org/events/current/

**HPCwire**
http://www.hpcwire.com/events/

**Linux Journal**
http://www.linuxjournal.com/events

**Netlib**
http://www.netlib.org/confdb/

**PRACE**
http://www.prace-project.eu/prototype-access
http://www.prace-project.eu/hpc-training-events
http://www.prace-project.eu/news

**SNIC**
http://www.snic.vr.se/news-events

**TeraGRID**
https://www.teragrid.org/web/events/tg10

**US DEPARTMENT OF ENERGY**
http://hpc.science.doe.gov/