PDC Newsletter

PDC Editorial

Lennart Johnsson
Director PDC

Erwin Laure
Director PDC-HPC

On the cover:
DFT-optimized structure of photo-system II placed into an experimental X-ray density.

The year 2011 started with a big bang at PDC: on January 19 the upgraded version of Lindgren was made publicly available. With this upgrade, the Swedish research community now has access to the most powerful computer in the Nordic region, offering 305 TFLOPS and the fast Gemini interconnect. This upgrade resulted in a busy month of December with installation of extra cooling capacity, 11 new Cray cabinets arriving on December 8, and the upgraded machine being made available to pilot users on December 22; needless to say, our staff really looked forward to Christmas break. But as science never sleeps, the system was available to pilot users throughout the holiday period and saw the largest job ever run on a Swedish system: a fluid mechanics simulation using some 34 000 cores. A big "thank you" is due to the system and application staff at PDC who made this quick and smooth upgrade possible! We collected a few experiences from early users in this newsletter and we are confident that Lindgren will be a great resource for Swedish scientists.

With Lindgren we are also starting a major exercise towards green computing in Sweden. The heat produced by Lindgren is captured and used to heat neighboring buildings on campus at KTH. This innovative system has successfully passed initial testing and is now being fine-tuned. We will report more on this in future editions of this newsletter.

While we are all proud of our flagship Lindgren, we are already preparing the next major investment which will be the replacement of our foundation-level resource, Ferlin, due early 2012. Ferlin is heavily used, for instance, in quantum chemical studies of respiration and photosynthesis, as illustrated in our front-cover article by Margareta Blomberg and Per Siegbahn.

Thanks to collaborations with VIC-Stockholm we are now able to offer access to a small GPU cluster with 12 NVIDIA C2050 Tesla Fermi cards. We are also offering a cloud prototype to SeRC and the Venus-C project. On another front, our work on energy-efficient computing is continuing with plans to provide more detailed measurement facilities for our SNIC-PRACE prototype, Povel; additionally, we are working on a new prototype for PRACE, this time based on DSPs and ARM processors together with HPC2N and Texas Instruments.

In the context of the PRACE project, we organized two high-profile events: a two-day scientific seminar with a program composed by a program committee including major Nordic HPC users, which we report on elsewhere in this newsletter, and the PRACE 3rd Industry Seminar with a program developed by a program committee with representatives from 14 PRACE partner countries, which was held while the newsletter was in print. For PRACE, we also coordinated the Swedish participation in the second implementation project that begins summer 2011. In this project phase, PRACE will also continue the successful DEISA Extreme Computing Initiative (DECI). During the last DECI round, three Swedish projects were funded and five European projects got awarded time on our resource Ekman.

With Lindgren, we now have a solid local base resource that is not only providing unprecedented capabilities to Swedish researches but also supporting Swedish scientists who are taking the step towards top-level European petaFLOPS resources. This movement is only possible with advanced support and—thanks to SNIC and SeRC—PDC can now offer more application expertise in a wide area of fields which will grow further during 2012; this is also thanks to our collaborations with NSC in the SeRC context.

We are delighted that, in PRACE's 2nd regular call for access to tier-0 resources, an application with Prof. Arne Johansson from the department of mechanics in the school of engineering sciences, KTH, as lead investigator, was successful. This is the first successful Swedish application for PRACE tier-0 resources with an allocation of 46 million core hours. PRACE Preparatory Access to the CURIE system provided by GENCI and hosted by CEA was also granted to a group of Nordita Researchers in Stockholm as part of a collaborative proposal submitted by Dr. Petri Käpylä, Docent in Astronomy and Academy Research Fellow, Department of Physics, Helsinki University. Such successes should encourage other Swedish researchers with need for tier-0 resources to prepare applications for future (twice yearly) PRACE calls for proposals. With this, we hope that 2011 will be a successful year for our users, and we are looking forward to many scientific breakthroughs enabled by SNIC and KTH investments, as well as our services.

Lennart Johnsson, Director PDC
Erwin Laure, Director PDC-HPC

Quantum Chemical Studies of Respiration and Photosynthesis

by Margareta R. A. Blomberg
and Per E. M. Siegbahn

Photosynthesis and respiration are two of the most important processes in nature, both connected to energy storage. In spite of extensive scientific efforts during many years, the detailed molecular mechanisms for these reactions are not known. Experimental studies are severely hindered by the complex nature of these chemical processes occurring in membrane bound proteins. Therefore, theoretical studies based on quantum mechanics, that allow detailed investigations of individual steps of electron and proton transfer, play an important role for understanding the mechanisms. Three important factors making such studies possible are the development of den-

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Staff Focus

ILJA LIVENSON

Ilja Livenson joined PDC in 2010 as a Ph.D. student after receiving his M.Sc. in computer science at the University of Tartu, Estonia <http://ut.ee/en>. At PDC, he works on data management issues in the VENUS-C project. His supervisor is Erwin Laure. Ilja has previous experience working as a developer, system administrator, and security analyst in several industry and academic projects, for example, developing medical health system (eHL), helping to extend EGEE to the Baltics (EU FP6/7 BalticGrid I and II), supporting the CERN CMS user community, and working on the peer-to-peer virtual-world platform (EU FP7 VirtualLife).

Apart from sitting a lot in front of the computer, Ilja also likes rock climbing, discovering new sorts of beer, and discussing Weltschmerz-problems.

sity functional theory (DFT) for solving the quantum mechanical equations, the advancement of modeling techniques for complex systems, and the access to faster and more efficient computers.

Proton pumping in cytochrome oxidase

In respiration, the oxygen molecules that our bodies extract from the air we are breathing are reduced into water molecules in a process involving a series of proteins located in the mitochondrial membrane. In this process, electrons and protons are taken up from different sides of the membrane, which makes one side of the membrane positive and the other side negative, leading to an electrochemical gradient across the membrane. This gradient is a way to store the energy in the food that we eat, and is used to synthesize ATP (adenosine triphosphate), the energy currency of our bodies. To further build up and maintain the gradient there is also a transport of protons across the entire membrane, against the gradient. This is referred to as proton pumping. The motion of these protons will therefore be uphill in energy, and there must be specific mechanisms preventing the protons to go in the wrong direction back to the negative side of the membrane. Those mechanisms, referred to as proton gating are far from understood, and they are now studied using DFT calculations.
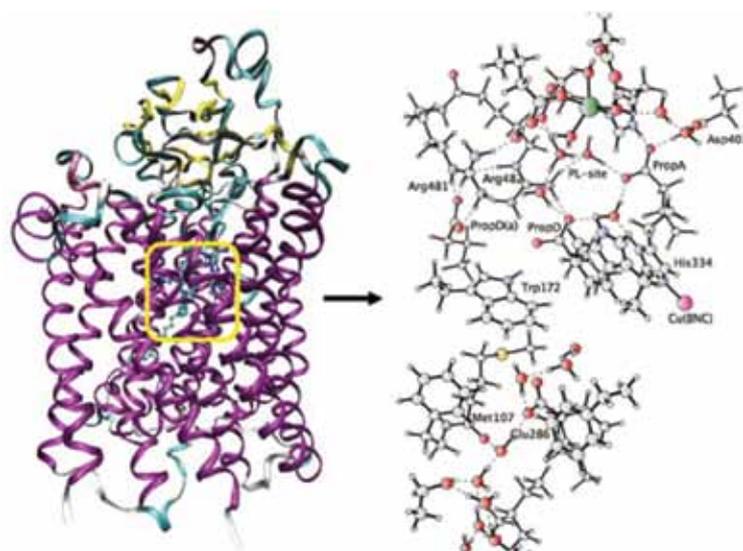

Figure 1: The left part of the figure illustrates the X-ray structure of the enzyme cytochrome oxidase in the respiratory chain. The right part shows a model used in the calculations on the pumping mechanism, and represents one of the larger systems ever used in DFT studies (almost 400 atoms).

Despite the developments mentioned above, it is still not possible to perform quantum mechanical calculations on entire enzymes. Therefore, the first step is to select the part of the protein where the reaction under study occurs, and build a model based on the X-ray structure. This is illustrated for cytochrome oxidase, the final enzyme in the respiratory chain, in Fig. 1. The general approach is to calculate the relative energies for different molecular structures along a reaction path, and construct an energy profile for the

chemical reaction under study. This is illustrated by the calculated DFT energy profile for the catalytic cycle for the reduction of molecular oxygen into water in cytochrome oxidase shown in Fig. 2, where the model used in these calculations is also given. From these calculations conclusions could be drawn about the detailed structure of the different intermediates, in particular their protonation states which are difficult to determine experimentally. The energy profile also hints at some problems remaining to be solved concerning the distribution of the released energy over the steps in the catalytic cycle, since it is required that all steps should be equally exothermic for the proton pumping to work.

It has only very recently become possible to perform DFT calculations on models for proton pumping, since this is a process occurring over a long distance and therefore very large models have to be used. It should be noted that to study chemical reaction mechanisms implies performing not only a few, but a large number of calculations with the model used, including optimizations of the structures for each of the different stationary points along the reaction path. A few years ago a model size of 50-100 atoms was the practical limit. With the upgrading to the Ferlin cluster with eight-processor nodes at PDC, models of the size shown in Fig. 1 with 400 atoms are now feasible. Using the DFT results obtained for the model in Fig. 1 and other similar models, together with experimental results and rather simple electrostatic considerations based on the crystal structure, it has been possible to suggest a mechanism for the main gating problem, where the protons being pumped are prevented from leaking back to the negative side of the membrane. An important ingredient in this mechanism is that the transition state for proton uptake is positively charged, implying that the proton pumping occurs by uptake of an extra proton rather than by dissociating a proton from a glutamic acid, which has previously been suggested.

Water oxidation in photosystem II

Photosystem II (PSII) is the only system in nature capable of forming oxygen gas from water and sunlight. The catalyst for the O-O bond formation is the oxygen evolving complex (OEC) containing four manganese and one calcium. Oxygen is formed after oxidizing the OEC in four steps, each one after absorption of a photon. After four photon absorptions, two water molecules have lost four protons and four electrons and the two remaining oxygens can then form an O-O bond. To understand this process is one of the main challenges in biochemistry.

A theoretical study of the mechanism for oxygen formation in PSII is different in character from those discussed above for respiration. The reason is that the experimental information on the structure of the OEC has been quite vague due to a rather low X-ray resolution (3.0-3.5 Å). With that resolution, rough positions of the metal atoms could be suggested, and also which amino acids that are probably directly bound to the OEC. However, many significant parts of the structure were still unclear, such as the critical positions of the oxygen ligands. Using the information available, the under-

Staff Focus

JOHNNY ERIKSSON

Johnny Eriksson studied mathematics a long time ago, before stumbling over a computer, which changed his life forever. He has been working with a lot of things, both computer-related and real-life hands-on things, and might be regarded as a jack-of-all-trades. His computer-related jobs include being a systems programmer at QZ (Stockholms Datamaskincentral) a long time ago, working for ten years at KTHNOC in the '90s, working as a developer/tester for a Swedish router vendor, and working for several ISPs.

Johnny's initial job at PDC was to handle infrastructure extensions for the new Cray system, Lindgren. This will likely morph into a more normal system administrator position when all else settles down.

Personal operating systems of choice are FreeBSD and Tops-10.

QZ
http://sv.wikipedia.org/wiki/QZ
KTHNOC
http://www.noc.kth.se/

JOHANNES MARKSTRÖM

Johannes Markström joined PDC in September 2010. He is working part-time as a system administrator focusing on the Ferlin and Ekman clusters. When he is not at PDC, he is studying for a M.Sc. in Aerospace Engineering at KTH. Johannes has formerly been working in the IT business, and has more than 10 years experience with UNIX system administration. He was born in Linköping and moved to Stockholm in 2000. Johannes is interested in many things, including programming, photography, and aviation. Aviation has always been a strong interest and it attracted him to KTH and the Vehicle Engineering program. His future plans are to work with a combination of computing and aviation and of course, whenever it is possible, enjoy life above the clouds.
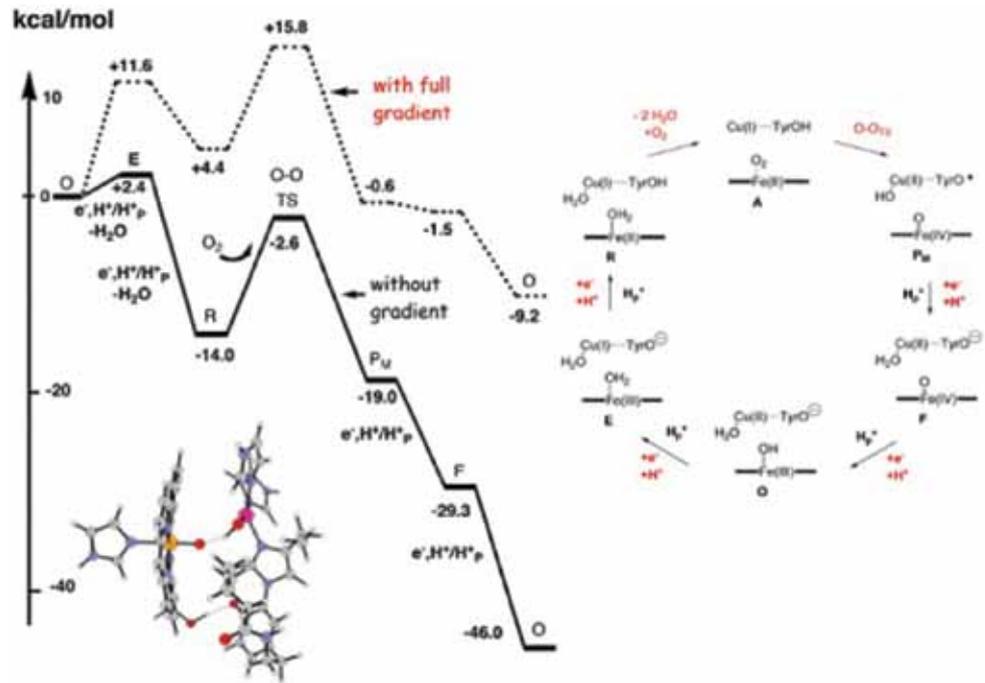

Figure 2: The right part of the figure illustrates the catalytic cycle for reduction of molecular oxygen to water in cytochrome oxidase. The left part illustrates a calculated energy profile for this catalytic cycle, with and without the presence of the electrochemical gradient across the mitochondrial membrane, together with the model used in the DFT calculations.

standing of the mechanism and the structure of the OEC has gradually increased during the past decade based on DFT model calculations. A few years ago, the computational investigations converged to a structure which has similarities to, but also significant differences from, the structures suggested based on X-ray crystallography and various spectroscopies. The largest model used so far in the DFT calculations, containing 190 atoms, is shown in Fig. 3.
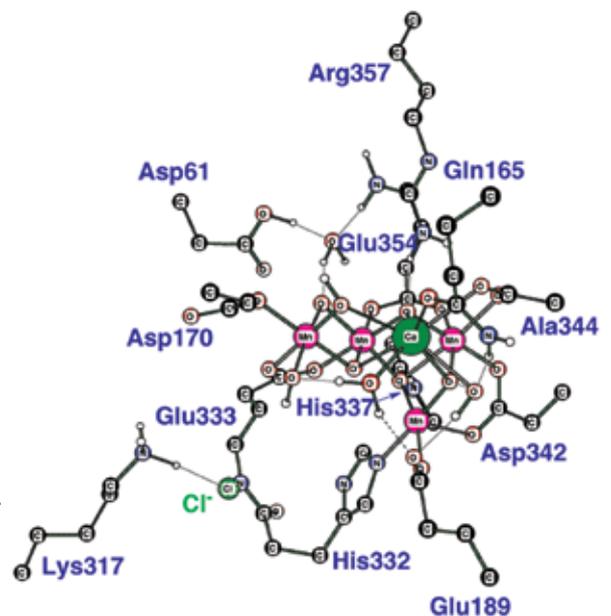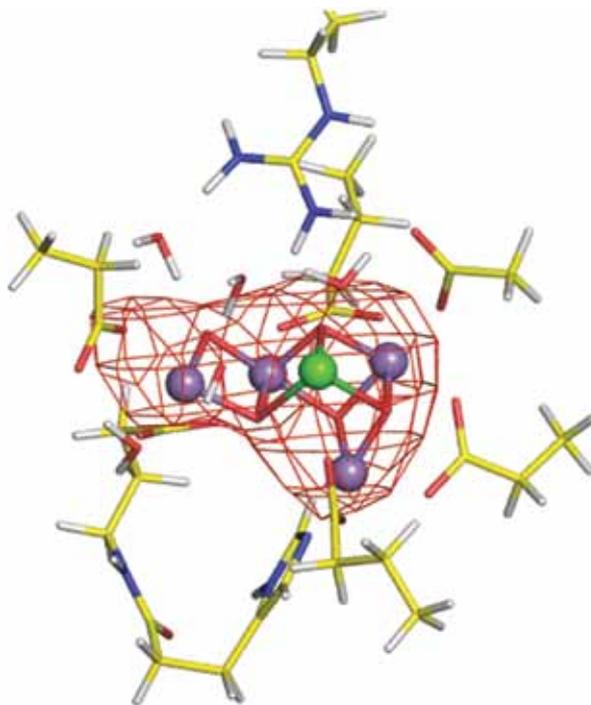

Figure 3:
The largest model used so far for the catalytic center for oxygen evolution in photosynthesis.

The model in the figure was based on experimental information, but also – to a major extent – on an understanding of what is required for oxygen formation. It was realized 5-10 years ago, that an oxygen radical is necessary for formation of the O-O bond, which occurs at the final stage of the process. Later on it was found in another DFT study, that the oxygen radical should ideally be at the center of the OEC. Working backwards by DFT modeling, a structure was reached for the dark-stable resting state by adding protons and electrons. The central structure of the DFT model turned out to fit the experimental low-resolution density very well; see Fig. 4. An interesting development occurred half a year ago, when the results of a new high resolution experiment was described by Shen and coworkers on a conference in Beijing. The results are not published yet, but from pictures that have been distributed, it appears that the new structure agrees in detail with the one suggested by the present DFT modeling. At the same time, it differs significantly from all other previous suggestions of the structure.

Figure 4:
The DFT optimized structure placed into the experimental X-ray density.

During recent years, the DFT modeling has been extended to the description of different types of spectra, such as from EPR, EXAFS, XANES, FTIR, and to studies of other types of experiments such as water exchange. The computed spectra are in very good agreement with the direct experimental measurements, but the interpretations differ sometimes strongly from those made directly from the experiments. The overall DFT mechanism for O-O bond formation is largely different from anything suggested previously. A major advantage of DFT model studies is that very short-lived species can be studied with equal ease as long-lived ones. Some of the critical short-lived species may, in fact, never be amenable for spectroscopic studies, at least during the next several decades.

Staff Focus

GILBERT NETZER

Gilbert Netzer was born in Linz, Austria. After studies in computer science at the University in Linz and KTH he started working at PDC in 2006 developing grid software for the OMII Europe project. Today he works as system administrator mostly responsible for the local SweGrid resources. Furthermore, he is involved in the development of prototype hardware to study energy efficient HPC solutions in the context of the PRACE project. His personal interests include computer architecture, computer hardware, low-level software development and operating system design.

OMII Europe
http://www.omii-europe.org/

SweGrid
http://www.snic.vr.se/projects/swegrid

PRACE http://www.prace-project.eu/

PDC/KTH – An Associate Partner of DEISA Pan-European project

In 2009 PDC/KTH became an associate partner of the DEISA2 (Distributed European Infrastructure for Supercomputing Applications) project. DEISA2, the successor of DEISA, is a consortium of leading national Supercomputing centres that aims at fostering pan-European world-leading computational science research. DEISA2 is funded by the European Commission in FP7.

The DEISA Extreme Computing Initiative (DECI) is a scheme through which European computational scientists can apply for single-project access to world-leading computational resources in the European HPC infrastructure, for a period of up to 10 months (see http://www.deisa.eu). Since 2005, DEISA has opened six DECI calls.

The last one, the DECI6 call, was opened in December 2009 and the number of proposals the DEISA consortium received for this sixth call shows its popularity: 122 applications were submitted from 30 countries; of these 30 countries, 22 were from Europe and eight from other continents. The total requested compute time was over half a billion compute hours, causing oversubscription by a factor of ten. All the projects went through thorough scientific and technical evaluation by the DEISA executive committee.

Three Swedish projects are among the accepted 56 applications that got nominated for access to pan-European supercomputing infrastructure. These projects are:

• **BRAINCOR** (http://www.deisa.eu/science/deci/projects2010-2011/BRAINCOR), principal investigator: Prof. Anders Lansner, Head of Department of Computational Biology at KTH/CSC.

• **SIVE** (http://www.deisa.eu/science/deci/projects2010-2011/SIVE), principal investigator: Prof. Erik Lindahl, Professor of Computational Structural Biology at KTH/CSC.

Distributed
European
Infrastructure for
Supercomputing
Applications

• **WALLPART** (http://www.deisa.eu/science/deci/projects2010-2011/WALLPART), principal investigators: Dr. Luca Brandt and Dr. Philipp Schlatter, Department of Fluid Mechanics, Linné FLOW Centre, KTH.

As an associate partner within DEISA2, PDC provided Swedish resources to the DEISA infrastructure and welcomed its first European users from the DECI6 call. Five accepted European projects from Italy, Finland, Germany, UK, and France started their computations on Ekman in October 2010 (http://www.deisa.eu/science/deci/projects2010-2011). These projects will continue to run their simulations until May 2011 for a total of 5,000,000 standard CPU hours. The applications are from different disciplines, comprising plasma and particle physics, materials science, earth sciences, and bio sciences.

Annually, DEISA, together with the PRACE (Partnership for Advance Computing in Europe) project, organizes DEISA/PRACE symposia where scientist using DECI resources can present their scientific achievements and computational results. This year, the DEISA/PRACE symposium is organized in Helsinki, Finland on April 13-14, 2011.

PRACE Scientific Seminar: HPC Boosts Science

PRACE organized a three-day scientific seminar "HPC Boosts Science" in Stockholm. The seminar was hosted at Royal Institute of Technology (KTH) and was organized by SNIC/PDC - Center for High Performance Computing at KTH with the help of CSC - IT Center for Science Ltd. in Helsinki, Finland.

The aim of the seminar this year was to tackle different aspects of HPC within multiple scientific disciplines. During the seminar, prominent researchers from a wide range of scientific communities presented their achievements and gave their opinions on the current and future trends of HPC. They addressed many advantages

of, and possible needs for improvement in, adapting HPC systems to different scientific areas. A large range of disciplines was covered, such as neuro-informatics, biotechnology, computational chemistry, astrophysics, theoretical physics, mechanics, and more.

The first day of the seminar was concluded by a poster session. Several participants submitted posters describing their research. One of the posters was submitted by a DECI 6 applicant of the DEISA project, Philipp Schlatter from the mechanics department at KTH.

The culmination of the seminar was the panel discussion where PRACE HPC experts, together with researchers, discussed possible improvements to the services that the current HPC ecosystem provides. The members of the panel were Prof. Lennart Johnsson (The University of Houston and PDC - Center for High Performance Computing, KTH), Prof. Igor Abrikosov (University of Linköping), Dr. Berk Hess (KTH) and Prof. Kari Laasonen (Aalto University).

One of the points of the discussion was that in order for scientific community codes to scale well on petascale, and in the future, exascale machines, hardware-tuned codes and low-level libraries are needed. Developers need to know more details about topology as well as hardware components of systems, which is currently one of the aims that PRACE is pursuing.

For scientists to have easy access to systems, a common submission environment is an absolute necessity. It was pointed out that such an environment has already been in use by DEISA and is in the development stage in PRACE.

In order to foster the enthusiasm of researchers for applying for compute time, the current waiting periods between application submission and acceptance should be shortened. Current procedures from a scientist's perspective require too much paperwork and appear bureaucratic. It would be ideal if the grant applications for funding scientists also included both requests for Ph.D. students as well as compute hours that would be needed for the given project.

As for the number of cores vs. compute time, it was clear that for some disciplines the codes can scale to many thousands of cores while for the others, several hundred will do, but more compute time is needed to conduct several simulations. For the latter type of disciplines, queuing and prioritizing systems can become a bottleneck and thus new approaches are needed.

It was also discussed how to motivate communities to work with application experts. Currently, most of the community codes are 10 to 20 years old. Codes are huge and researchers tend to not touch the old parts of it. In this situation, the assistance of application experts is essential. However, more methodological code development is needed rather than hardware specific tuning. For a researcher to hire a programmer is a lot more expensive than to hire a Ph.D. student. Thus initiatives such as PRACE are helping to fill the gap of knowledge in the area of computer science that research communities have. Moreover, there is an urgent need for a greater number of committed work hours by application experts on community codes.
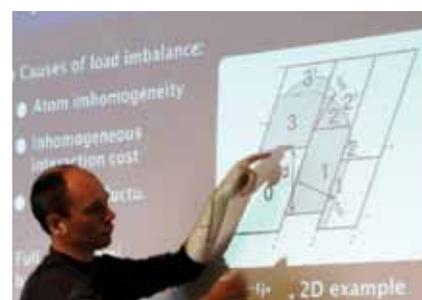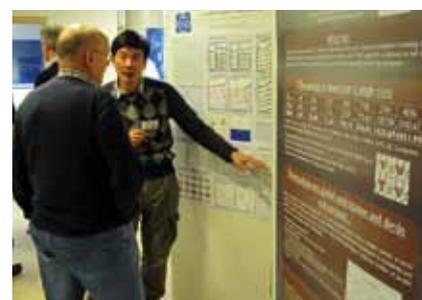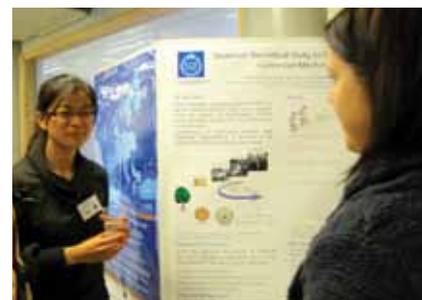
Cray Early User Experiences

**Much has been written about Lindgren's hardware and software, but how do the researchers experience using PDC's new Cray?
Below are some quotes from a cross section of some of Lindgren's early users.**

"Early use of Lindgren for jet in crossflow stability analysis" by Milos Ilak, FLOW Postdoc, co-investigator with Philipp Schlatter and Dan Henningson, on grant SNIC 014/10-10 "Large-scale simulations in Stability, Transition, Turbulence and Control"

The jet in crossflow is a close relative of the flow one typically observes when watching smoke coming out of a chimney, but also occurs in fuel injection in turbine burners, cooling of turbine blades, vertical takeoff in aircraft, and many other important applications. An effort to study the dynamics of this complex flow has been going on at the Linné FLOW Centre for about four years now. To the best of our knowledge, we are the first group to attempt a fully three-dimensional stability and sensitivity analysis of a jet in crossflow, with the goal of using the knowledge gained to manipulate such jets to our advantage.

We simulate the jet in crossflow using our SIMSON code that has been developed at KTH Mechanics over the past two decades. The simulations need to be very accurate and are therefore demanding in terms of CPU time (on the order of several days walltime each on 1024 cores). The capabilities of Lindgren have allowed us to expand significantly upon earlier work and investigate the flow more in-depth; our code scales very well up to 16384 cores. The modules implemented by PDC on the system make compilation and linking a breeze, and the queuing system is very responsive, which makes running and restarting jobs very easy too. The amount of good data that we have been able to generate during the early use phase will keep us busy for a while!

A volume rendering of the hairpin vortices that are characteristic for a jet in crossflow in the flow regime. The yellow regions indicate the 'cores' of the vortices.
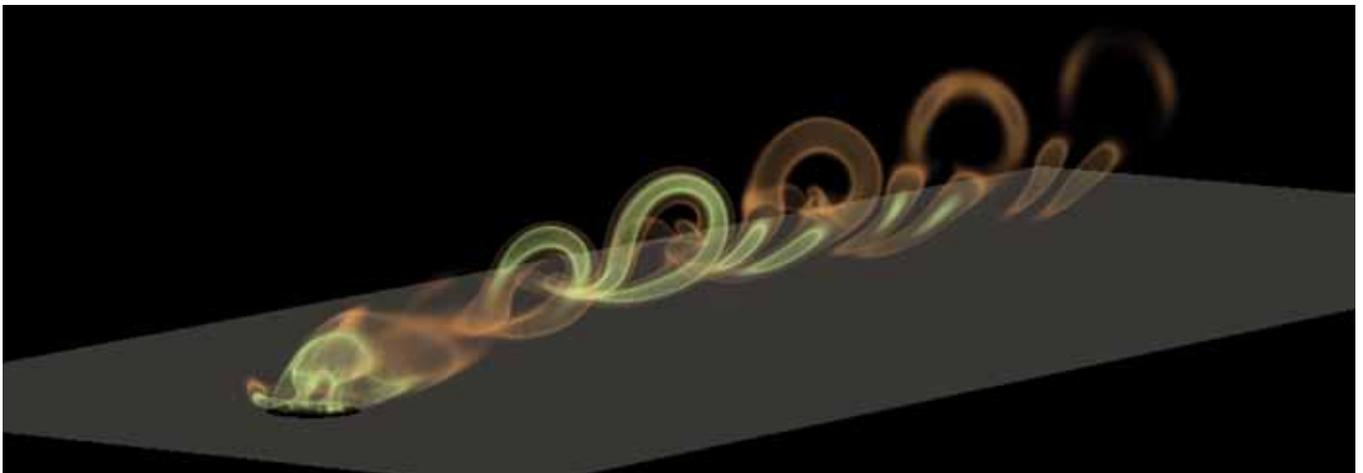
Niclas Jansson, co-investigator with Johan Hoffman, on grant SNIC 014/10-22 "High-performance adaptive finite element methods for turbulent fluid flow" with additional funding provided by SSF, VR, ERC, and Energimyndigheten.

Simulating turbulent fluid flow using adaptive finite element methods often requires several adaptive iterations until convergence in a chosen output is achieved. For each iteration the problem size as well as the needed simulation time increases. The large number of available cores on Lindgren has significantly reduced our needed simulation time from weeks to days. With shorter simulation times we can run iterations covering longer time periods on larger problems which makes us reach our research objectives faster.

Working with Lindgren is a nice and enriching experience. Cray provides a great environment for developers, with optimized compilers and excellent performance analysis tools. It took us less than a day to get our code up and running in production on Lindgren. With the fast interconnect our code now shows strong linear scaling to 3072 cores, an increase by a factor of three compared to other SNIC systems.
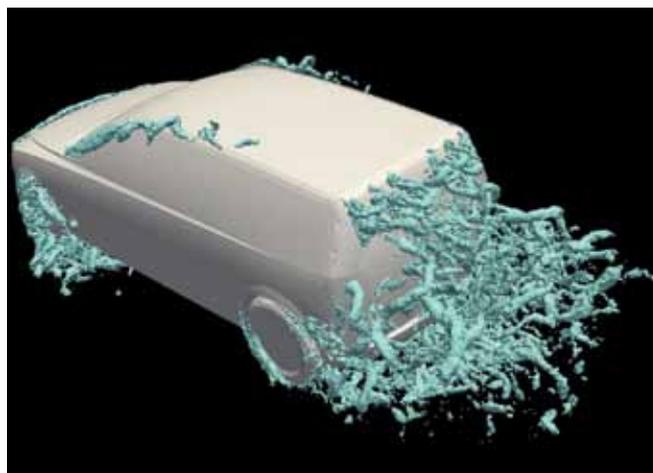
Visualizations from a currently running simulation on Lindgren showing isosurfaces of Q-criterion for turbulent flow past a full car model, with geometry provided by Volvo. Simulation time is less than 48 hours using 1032 cores.

Peter Kasson, co-investigator with Erik Lindahl on grant "Stockholm University: Centre for Biomembrane Research"

Lindgren has certainly shown its power in early testing. The fast Gemini interconnect has allowed extremely good scaling, making this machine ideal for extremely large jobs (thousands of CPU cores) that have extensive interprocess communication. We have used it for large molecular simulations of membrane fusion, where the capability of both rapid turnaround and extremely long simulations has been particularly useful. Large, tightly-coupled clusters of this sort have been critical for our work in this area, and having a state-of-the-art machine at PDC is particularly exciting.
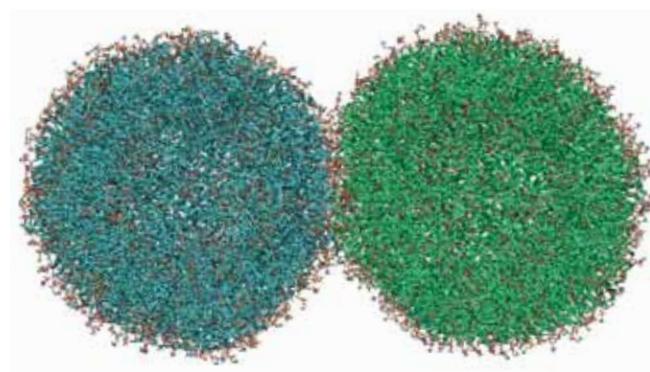

Image from our n-1 simulations, mostly pre-Lindgren; published in two recent papers: Kasson, Lindahl, Pande. PLoS Comput. Biol 2010 Jun 24;6(6):e1000829. Kasson, Lindahl, Pande. J Am. Chem. Soc. 2011 Feb 25.

Andreas Skyman (skymandr) co-investigator with Pär Strand and Hans Nordman on SNIC 014/10-6 "Turbulence and transport in multi ion species fusion plasmas"

The performance of a fusion plasma relies fundamentally on the turbulent transport of energy and particles. Simulating turbulence is already a challenge, but further complications arise in a plasma because of long-range interactions causing collective behavior. In general, many different plasma phenomena of varying frequency and wavelength coexist in a fusion plasma. They interact non-linearly and non-locally, and resolving their interplay places high demands, not just on the implementation, but also on the hardware. Simulations regularly require thousands of cores running for extended periods of time, and thus access to supercomputers, such as Lindgren, is essential for this kind of research. With the upgrade of the Lindgren computer, we have observed a speed-up of 30-50%

compared to before Christmas; further scaling studies, comparing GENE's [http://www.ipp.mpg.de/~fsj/gene/] performance on Lindgren to that on the HPC-FF supercomputer in Jülich are currently under way.

Getting a program up and running on a new supercomputer is rarely trivial, but PDC's flexible implementation of the module system on Lindgren – along with prompt and helpful support – made the setup very smooth. During the campaign of 2011, we look forward to continuing this collaboration, as we venture from thousands of cores into the ten thousands, marking our first steps toward true multi-scale plasma simulations, including global phenomena. Though this will require challenging amounts of computer power, the fact that it is even an option is testament to the fact that, with access to new modern supercomputers, non-linear phenomena is turning from an obstacle, into a field of scientific opportunity and discovery.
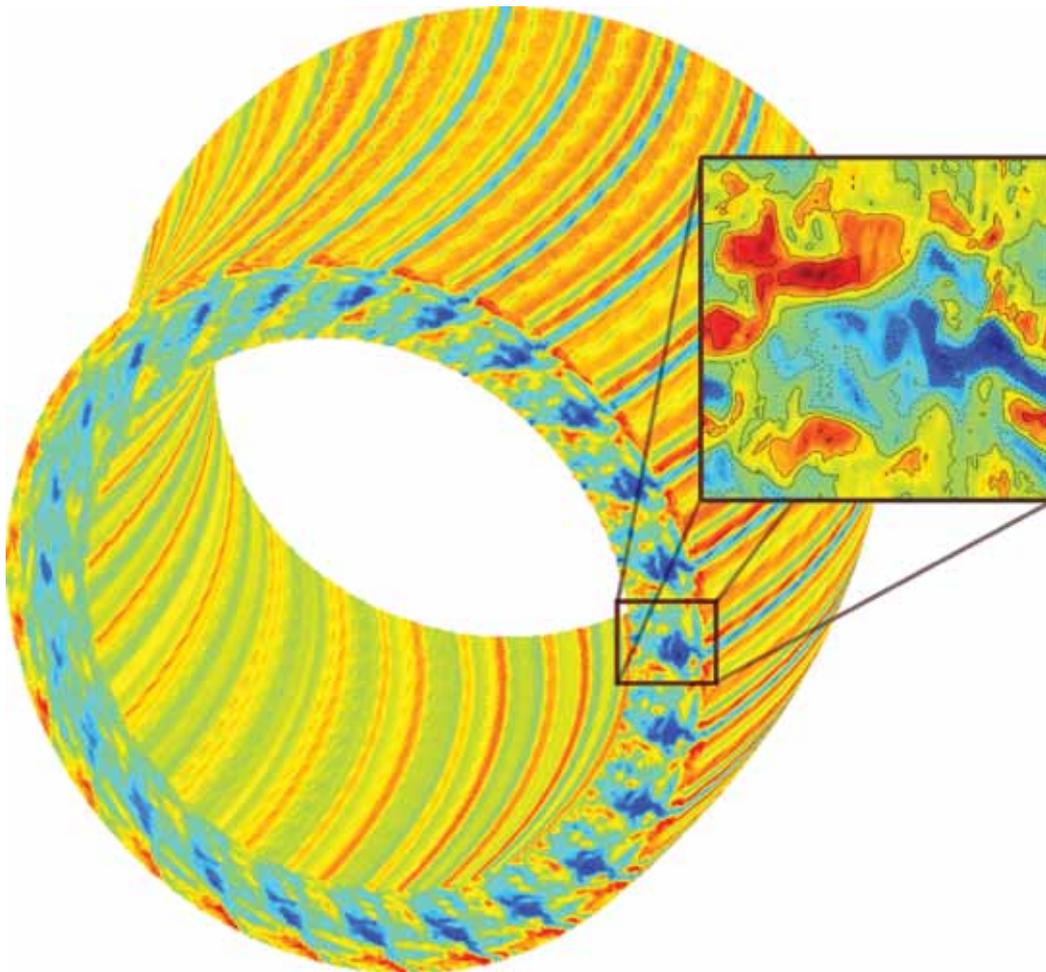

...s made up of the flux tube ...ving the magnetic field. ...: in the density of fuel ions. ...s been indicated.

Sander Pronk, co-investigator with Erik Lindahl on grant SNIC 014/10-31 "Simulations of membrane proteins and influenza vesicle fusion"

In my experience, Lindgren has at the same time been the fastest machine I've worked on, and the most user friendly in the sense of effortless scaling: it is just as easy to use one node as it is to use one hundred. The run-time system provides a consistent, very high-bandwidth parallel environment. The fast interconnects allow us to scale the individual runs up to larger numbers of cores than on any other system.

We've been able to scale up even further by going beyond individual molecular dynamics runs by sampling in protein configurational space, mapping both the dynamics and the static properties of its characteristic states in one massively parallel run.
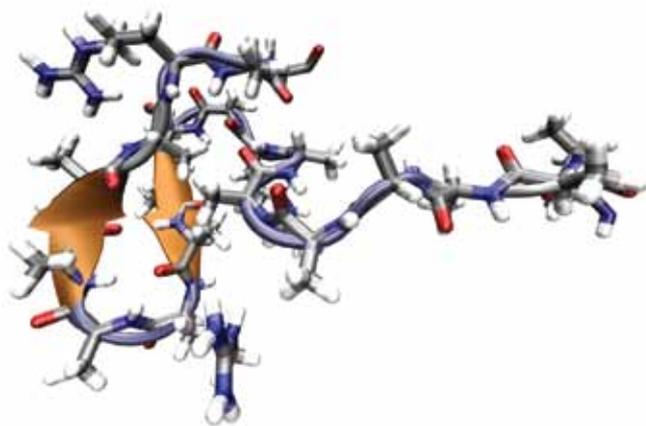
This is currently being simulated on Lindgren: a small protein on its way to being folded in its native conformation.

Petros Souvatzis, co-investigator with Olle Eriksson on grant SNIC 006/10-3 "Theoretical simulations of materials"

Large scale materials calculations at PDC

Ever since computational materials set sail in the early sixties, the predictive power and efficiency of materials calculations have developed in close connection with the hardware evolution.

A good example of what this marriage between hardware evolution and science has accomplished is the work I have been doing on the PDC's Lindgren simulating the thermo-electric materials PbTe and PbS. The computations made on these two compounds showed that the lattice distortion found in PbTe and PbS at finite temperatures could not be global but rather had to be local. These findings where recently published in Science 330, 1660-1663 (2010).
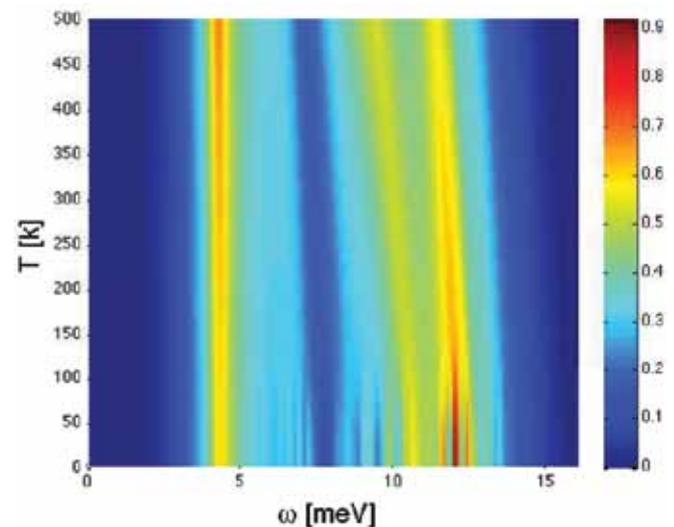
The phonon spectra of PbTe calculated on Lindgren at different finite temperatures.

PDC Summer School:
Introduction to High-Performance Computing
Stockholm, Sweden, August 15-26, 2011

The class of 2010

MATMUL competition prize

Lennart Johnsson, Univ. of Houston and PDC

Invitation

You are invited to register for the class "Introduction to High-Performance Computing" being held at PDC on the KTH main campus. To register, and find out more about the class, visit the course Web page at http://www.pdc.kth.se/education/summer-school/.

Background

The PDC Summer School in High-Performance Computing is an annual offering to researchers to improve on their skills in scientific computing. The course is held for its fourteenth consecutive year at KTH, Stockholm, Sweden.

During two intensive summer weeks at the KTH campus students will be able to learn and improve their skills in writing efficient programs for serial and parallel scientific applications.

The course carries 7.5 ECTS (European Credit Transfer and Accumulation System), where 1.5 ECTS credits are equivalent to one week's workload of 40 hours. The student receives these credits on successful completion of the post-course project. Participants are strongly encouraged to bring their own problems or programs for discussion and to possibly use as the basis of the post-course project. Participants are provided with remote access to the PDC's new Lindgren (Cray XE6) system. Industrial participation is welcome. The number of seats for all participants is limited.

Computer Laboratories

Roughly half of the class time will be spent hands-on in the lab. The lecturers and the PDC staff will assist in the computer labs. Students who do not already have an account at PDC will receive one. These accounts will stay active after the course so students may work on the post-course project.

Outline

A number of topics will be covered in overview lectures given by international experts and in-depth technical lectures followed by hands-on computer lab sessions. The course will consist of about 35 hours of lectures and 35 hours of computer lab sessions.

Registration opened March 15 and closes June 1.

Among the topics:

Programming Environments at PDC
Parallel Programming
Modern Computer Architectures
Parallel Algorithms
Efficient Programming
Case Studies

These topics will be covered both in lectures and labs by the following teachers:

Scott Baden
(University of California, San Diego

David Black-Schaffer
(Uppsala University)

Iris Christadler
(LRZ - Leibniz-Rechenzentrum)

Björn Engquist
(KTH and the University of Austin

Thomas Ericsson (Chalmers)

Erik Hagersten (Uppsala University

Michael Hammill (PDC)

Sverker Holmgren
(Uppsala University and SNIC)

Niclas Jansson
(CSC - KTH School of Computer Science and Communication)

Lennart Johnsson
(PDC and University of Houston)

Erwin Laure (PDC)

Dag Lindbo
(CSC - KTH School of Computer Science and Communication)

Elisabet Molin (PDC)

Jesper Oppelstrup
(CSC - KTH School of Computer Science and Communication

Michael Schliephake (PDC)

Anders Ynnerman
(Linköpings Universitet)

PDC Related Events (Sponsored/Associated)

SeRC Second Annual Meeting
May 10-11, 2011, Tammsvik, Sweden

The Swedish e-Science Research Centre (SeRC) has now been formally running for slightly more than a year, and the involved research groups are in full action with strategy planning and starting up activities. The meeting is an opportunity to get updated on ongoing and planned activities related to SeRC.

Organized by SeRC. Mattias Chevalier is coordinator.

http://tinca.pdc.kth.se/article/invitation-second-annual-meeting-10-11-may-2011-tammsvik

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CSC Summer School in Scientific and High-Performance Computing
May 23 - June 3, 2011, Espoo, Finland

The school is aimed for graduate students working with computational sciences, e.g. computational chemistry, physics, biosciences, or engineering; but also undergraduates as well as post-docs will find the school very useful.

This course will be co-organized by PDC and CSC, Helsinki. Lennart Johnsson and Lilit Axner are PDC's lead organizers.

http://www.prace-project.eu/hpc-training-events/gpu-computing-courses-at-csc-october-28-29-and-november-3-5-espoo-finland

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PDC Summer School 2011:
Introduction to High-Performance Computing
August 15-26, 2011, KTH main Campus, Stockholm

This course will give an introduction to the skills needed to utilize high-performance computing resources. The course is intended for Ph.D. and Masters students with interest in the application of High-Performance Computing.

http://www.pdc.kth.se/education/summer-school

7th IEEE International Conference on e-Science
December 5-8, 2011, Stockholm City Conference Centre, Sweden

Conference Scope: Interdisciplinary research communities, developers, and users of e-Science applications and enabling IT technologies. The conference serves as a forum to present the results of the latest research and product/tool developments and to highlight related activities from around the world.

Organized by SeRC in collaboration with eSsence. Erwin Laure is the general co-chair.

http://www.escience2011.org/

Sources

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

CERN http://cdsweb.cern.ch/collection/Conferences?ln=en

DEISA www.deisa.eu/news_press/deisa-latest-news
www.deisa.eu/science/deci

ECEE
www.scientific-cloud.org/events.html

EGI www.egi.eu/about/events/

GRDI2020
www.grdi2020.eu/Pages/DocumentList.aspx?id=40&nome=Events

HPC University
www.hpcuniv.org/events/current/

HPCwire www.hpcwire.com/events/

INCF http://incf.org/Events

Linux Journal
www.linuxjournal.com/events

Netlib www.netlib.org/confdb/

PRACE
www.prace-ri.eu/hpc-access?lang=en
www.prace-ri.eu/Calls-for-Proposals
www.prace-project.eu/hpc-training-events
www.prace-project.eu/news

ScalaLife www.scalalife.eu/activities
www.scalalife.eu/trainings

SeRC http://tinca.pdc.kth.se/communityevents/all

SNIC www.snic.vr.se/news-events

TeraGrid www.teragrid.org/web/events/tg11/

US Department of Energy
http://hpc.science.doe.gov/

Venus-C www.venus-c.eu/Content/Events.aspx