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PDC Center for High Performance Computing

PDC Newsletter

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Erwin Laure
Director PDC and HPCViz

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Cover

Beskow, PDC's new Cray XC40, with Erwin Laure (left) and Gert Svensson (right), respectively PDC's Director and Deputy Director

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Editorial

After an extensive testing and pre-production phase with pilot users, our new flagship system, Beskow, was opened for general usage on the 15th of January and since then it has been providing Swedish scientists with unprecedented computational power. Beskow was officially inaugurated on the 27th of January with a well-attended ceremony and a scientific workshop. You can read more about this ceremony and the first user experiences with Beskow in this newsletter. With Beskow entering full production, we had to say goodbye to our previous system, Lindgren, which was decommissioned on the 25th of January after a migration phase where it was still running alongside Beskow. The Lindgren hardware will be returned to Cray during the summer. We are also happy to announce that we have finalised the procurement of the pre- and post-processing system for Beskow. The system, named Tegner, features 76 nodes, some of which have large memory configurations. It is equipped with both consumer and high performance graphics processing units (GPUs). Tegner is currently being tested and the first pilot users have already been granted access to the system. When Tegner comes into full production, which is expected to happen before the summer, we will gradually retire our current cluster systems, Ferlin and Povel; our previous GPU pilot system, Zorn, was retired earlier this spring. With these installations, almost all of PDC's hardware infrastructure has now been modernized and we look forward to the results of the great research that is now possible thanks to these updates.

Since the installation of Lindgren six years ago, PDC has been at the forefront of environmentally friendly computing thanks to our development of a system for re-using the heat generated by the supercomputer for heating purposes. KTH has recently invested in a new heat pump system so that now Beskow and the other PDC systems are contributing their heat to this campus-wide network. This new system also generated a lot of interest within the PRACE community that gathered for an infrastructure workshop organized by PDC in Stockholm this spring.

On the international front, the next phases of the large-scale European infrastructure projects PRACE, EGI, and EUDAT are starting, with PDC playing particularly important roles within PRACE and EUDAT – you can read more about our involvement in EUDAT in this newsletter. Other projects have come to an end, specifically the exascale flagship project CRESTA. The results from CRESTA are being carried forward into ongoing projects, such as EPiGRAM, as well as into completely new projects, and PDC has

been particularly successful in the first rounds of applications for the Horizon 2020 programme with funding being granted for four projects in the area of Futures and Emerging Technologies related to High Performance Computing (FET-HPC), as well as two Centres of Excellence. As a result, PDC will be coordinating a FET-HPC project, ExaFLOW, on new algorithmic approaches for fluid dynamics together with the Department of Mechanics at the KTH Royal Institute of Technology, and PDC will also be coordinating a Centre of Excellence for Biomolecular Research (BioExcel) together with SciLifeLab – we will tell you more about these projects in the next edition of the newsletter.

With this I wish you a relaxing, sunny and warm summer!

Erwin Laure, Director PDC and HPCViz

Above: Helene Hellmark Knutsson, Swedish Minister for Higher Education and Research, speaking at the Beskow Inauguration on the 27th of January 2015

Above: Peter Gudmundson, President, KTH, at the Beskow Inauguration

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Beskow Inauguration

Erwin Laure, PDC

The 27th of February saw about a hundred people gathered at KTH for the inauguration of the new petaflop Cray XC40 system, Beskow. The proceedings got off to a flying start with the President of KTH, Peter Gudmundson, who then introduced the Swedish Minister for Higher Education and Research, Helene Hellmark Knutsson. The program continued with a series of brief talks by speakers from organisations that are significant in the field of high performance computing (HPC) research, particularly in Sweden, such as Sven Stafström, the Director General of the Swedish Research Council and Mille Millnert, the Chair of the Board of the Swedish National Infrastructure for Computing (SNIC). Amongst other things, their talks stressed the importance of continued funding for the Swedish HPC infrastructure in order to maintain a vibrant research environment in Sweden. We were fortunate that Anni Hellman, Deputy Head of the e-Infrastructures Unit at the European Commission (EC) was also able to attend. Anni discussed the EC's strategy regarding HPC, which is built on three pillars – infrastructure, industry and applications. She also highlighted Sweden's role in the European HPC scene.

Beskow will be made available to researchers in other countries via the PRACE Research infrastructure, which was represented by Sanzio Bassini, the PRACE Council Chair.

Above: Mille Millnert, Chair of the Board, Swedish National Infrastructure for Computing (SNIC) at the Beskow Inauguration

Below: Sven Stafström, Director General, Swedish Research Council (VR) at the Beskow Inauguration

Dan Henningson, Director of the Swedish e-Science Research Centre (SeRC), then discussed the importance of a world-class HPC infrastructure for e-Science and gave some examples of leading research results obtained using PDC's infrastructure. Although Beskow is based at KTH, it will be used not only by academic researchers but also by some researchers from the industrial sector, which was represented by Sven-Åke Edström, Senior Vice President R&D, Scania, whose company has undertaken a lot of developmental research on PDC's earlier supercomputer systems, and which will be even more involved with research using Beskow. The introductory talks were concluded by two people whose companies were responsible for producing Beskow: John Josephakis, Vice President of Worldwide Sales, from Cray and Mark Spargo, Worldwide HPC Sales Director, from Intel.

Keynote speeches were given by Prof. Spencer Sherwin from the Department of Aeronautics at Imperial College London, who spoke about "Spectral/hp element, scale resolving modelling for high Reynolds number F1 Aerodynamics" and Prof. Bert de Groot from the Max Planck Institute for Biophysical Chemistry in Göttingen, Germany, who discussed "Exascale computing to explore nanoscale machines".

In addition, some of the researchers who participated in the pilot test phase of Beskow reported on the research project that their groups undertook during the pilot period. The following snippets give an overview of that work.

Below: The now empty Ytterby pit quarry where seven of the lanthanides were discovered

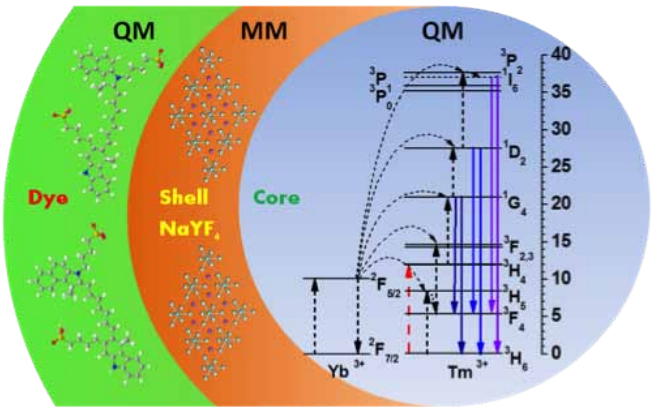
Beskow Pilot Research: DIRAC

Hans Ågren, KTH Theoretical Chemistry & Biology

In the Department of Theoretical Chemistry and Biology at the KTH Royal Institute of Technology we take an interest in the DIRAC program, which is the world's leading four–component quantum-relativistic code. The program implements the theory that was put forward by Paul Adrien Maurice Dirac about 80 years ago. It is a little brother of the non-relativistic program DALTON, which has been the main motor of molecular property calculations on the Swedish National Infrastructure for Computing (SNIC) supercomputers for a long time. The DIRAC program has gradually been assuming more and more of the functionalities of DALTON. During our pilot access project on Beskow, we worked on installing DIRAC so that it is now available on the Beskow computer system.

We use DIRAC for studying atoms and molecules where relativistic effects are important, namely in the heavier elements in the periodic table. One set of heavy elements that are of great importance in areas of applied technology is the group known as lanthanides. Out of curiosity we note that seven of the lanthanide elements were discovered in the small pit in Ytterby, just 20 km north of KTH. For example, yttrium, ytterbium, erbium and terbium all derive their names from "Ytterby". At the time of their discoveries in the mid 19th century, little could be known about their fantastic properties, which give rise to the versatility of their use and functionality in what we now call nanotechnology.

This is a circumstance that rather recently motivated us to enter lanthanide research, in particular, to undertake studies of the outstanding optical properties of lanthanides for the purposes of imaging and energy harvesting. In this research, we use the DIRAC program for modelling the properties of lanthanide complexes at a fully relativistic level, and to predict the dependence of their spectral response on chemical and electronic structure and the nature of complex environments. The project is formulated around some outstanding features of specifically designed lanthanide complexes that can sequentially absorb two or more photons via real intermediate long-lived electronic states to produce one shorter wavelength photon upon emission. Such light conversion materials in the form of nanoparticles can efficiently operate with incoherent light in the infrared wavelength region at low excitation power. These quite amazing features mean that these materials have great potential for use in high-contrast deep tissue bioimaging, optogenetics, photovoltaics and many other areas. The most effective upconversion nanoparticles contain rare earth lanthanide ions encapsulated into host matrices of inorganic crystals, which are thus the subject of our DIRAC project.



Above: Schema of upconversion using Lanthanides

Below: Facing operation in stainless steel
Metal machining is indispensable to today's society. In the pilot project run on Beskow, the stability of cutting tool coatings was simulated under realistic conditions equivalent to what is experienced by the tools when in operation. Source: Ludvig Landälv

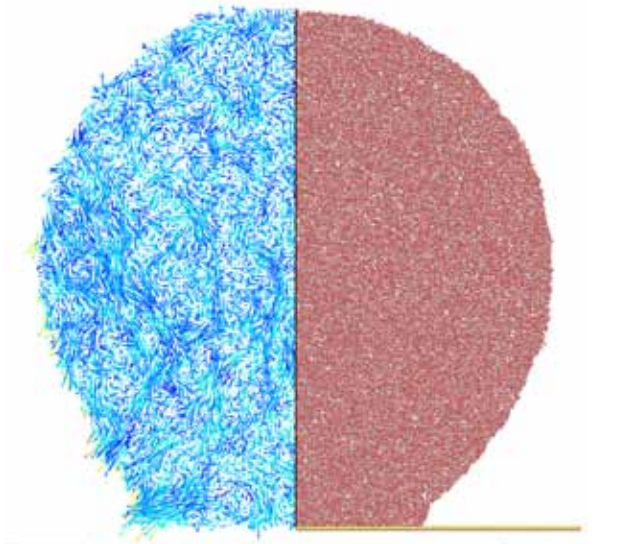
Beskow Pilot Research: Sharpening Sweden's Industrial Cutters

Igor Abrikosov, IFM, Linköping University

The Theoretical Physics Group at Linköping University is heavily involved in investigating and identifying novel materials and phenomena with high strategic potential for future technological applications. Much of this work is performed by means of state-of-the-art computer simulations, and hence we need the results of the simulations to be highly accurate. The main goal of the pilot project that we carried out on Beskow was to develop new theories and novel software to significantly reduce the number of approximations in our calculations while explicitly taking into account the external conditions at which such materials are considered, both in experimental settings and in real-life operation in technological applications. In this way, we make the accuracy of our predictions (from the simulation) comparable to, if not better than, the accuracy of physical experiments.

In particular, during the pilot access, we investigated titanium aluminium nitride or (Ti-Al)N alloys, which are a prototype system from the family of transition metal carbides and nitrides. These materials show a unique combination of properties: high hardness, high melting point and excellent electrical conductivity, which make them attractive in many technological applications. For instance, hard, wear-resistant thin films based on (Ti-Al)N alloys are used as coatings on cutting tools which are commercially available at present, and the business continues to expand rapidly. In real applications, the tools operate at temperatures above 1,000 °C and under stresses up to 50,000 atmospheres. Until we had access to the capabilities of Beskow, taking these extreme conditions into account in simulations would have been unrealistic.

Now, using Beskow and the temperature-dependent effective potential method developed in our group, we have been able to accurately and efficiently investigate the stability of the (Ti-Al)N alloys under realistic conditions equivalent to what is experienced by the cutting tools when in operation. We have demonstrated that, in fact, the alloy is significantly more stable at these conditions than one would have expected from earlier studies. These results should have a decisive influence on the development of new materials for hard coating applications, which is vital for competitiveness in one of the key Swedish industries.



Above: A 100 nm diameter water droplet (3.6 million atoms) spreading on a silica substrate with the flow-field representation on the left and the atomistic representation on the right

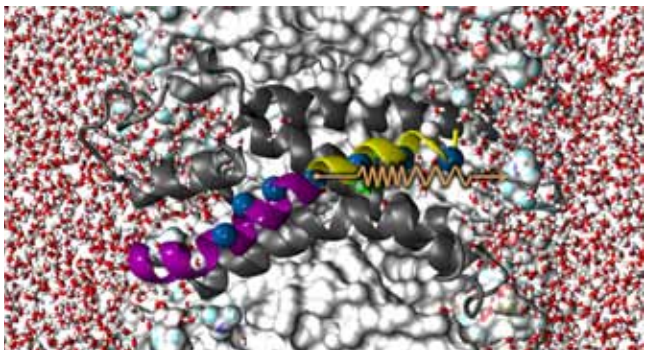
Beskow Pilot Research: Molecular Simulation

Berk Hess, KTH Theoretical Physics

In the Biophysics groups at the KTH Department of Theoretical Physics, we use large-scale molecular dynamics simulations to understand molecular processes, both in biological and technological systems. A lot of our effort goes into developing the molecular simulation package GROMACS, which focuses on high efficiency as well as parallelization. Although it is easy to parallelize molecular simulation, it is difficult to achieve good scaling, because there is not much work to do per particle for each time step. We took advantage of the pilot access to Beskow by running simulations that were more highly parallelized than we can usually do – this enabled us to achieve faster throughput for scientific projects where starting conditions or parameters for simulations often depend on the results from previous simulations. We ran two projects during the pilot phase: sampling conformational transitions in membrane proteins, and a study of water droplets wetting different substrates.

For bio-molecular applications we ran simulations over several ion-channels that reside in cell membranes. The channels are involved in signal transduction, as well as in the processes of opening and closing in response to the (un)binding of ligand molecules, either occurring naturally or induced by drugs, or in response to changes of the electric field over the membrane. The image on this page shows part of a voltage-gated ion channel where the purple/yellow helix moves in response to a voltage thereby opening and closing the pore (not shown). In reality this process occurs in a time span in the order of milliseconds. This is far too slow for our simulations, which can reach microseconds with billions of integration steps! Using an accelerated sampling method developed in our group, we were able to accelerate the transitions by several orders of magnitude and observe multiple transitions within a microsecond. GROMACS fully utilizes the AVX2 SIMD acceleration of the processors on Beskow to reach high peak performance and the fast network allowed us to scale up to 400 nanoseconds per day for these (relatively) large systems of 150,000 atoms.

In a completely different project, we studied how the molecular interactions between water and substrates affect the dynamics of how droplets wet surfaces. Here we used systems of up to 4 million atoms (see image on previous page) to simulate the wetting of a quasi-2D droplet with a radius of 100 nm. Although this might seem small, it is much larger than what has been simulated before and is also large enough to avoid finite size effects. We are mainly interested in the processes occurring close to the three-phase contact line, which is where the liquid meets the substrate and vapour, but we need to simulate the whole droplet to avoid boundary effects. We had run simulations of this system with truncated electrostatics interactions, which are computationally cheap, but they have the disadvantage of introducing some artefacts. On Beskow we have been able to use proper particle-mesh Ewald electrostatics, which is computationally far more expensive. By running on up to 16,000 cores, we were able to quickly get much more accurate results. Surprisingly the change in electrostatics treatment lowered the spreading rate by a factor of two. We are currently investigating what molecular interaction effects cause this large increase in effective friction. This will lead to a better understanding of what determines the rate of wetting of surfaces by water.



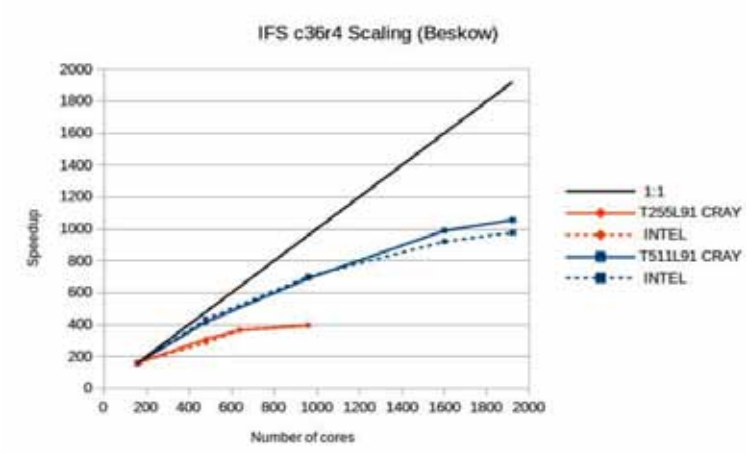
Above: A voltage sensor consisting of 4 helices embedded in a lipid bilayer membrane (white) - In vivo, the purple/yellow helix moves in response to a voltage across the membrane that works on the charged residues (blue). In molecular dynamics simulations, we pull on the helix with a spring to measure the force required to move the helix.

Beskow Pilot Research: Porting of an Earth System Model

Gunilla Svensson, MISU, Stockholm University, and Klaus Wyser, SMHI

Swedish climate researchers are contributing to the sixth international Coupled Model Intercomparison Project (CMIP6) in a project know as S-CMIP. The S-CMIP consortium is collaborating on science problems that are studied with Earth System Models (ESMs) and involves scientists from universities in Stockholm, Lund, Gothenburg and Uppsala, as well as the Swedish Meteorological and Hydrological Institute (SMHI). During the pilot access phase for Beskow at PDC, the S-CMIP consortium was working on porting the EC-Earth global climate model onto the Cray XC40 architecture.

EC-Earth has been successfully ported onto Cray computers previously, but this was always done using the Intel compiler suite. Based on our experience of the performance of different computer platforms, we strongly suspected that Intel compilers gave a sub-optimal result on Cray architectures, and therefore we focused on compiling the model using the native Cray compilers instead. The model itself compiled without problems, but we encountered problems with gribex, the external library that reads GRIB files for the atmosphere. (GRIB is a file format often used for storing meteorological data.) The gribex library that comes with the atmospheric part of the ESM from the European Centre for Medium-Range Weather Forecasts (ECMWF) is outdated and is not supported any longer, yet it is still essential for the EC-Earth model. After many fruitless attempts, we finally had to give up on using the Cray compilers for gribex, and consequently we compiled that specific library with Intel compilers and then linked it to the rest of the model that was compiled with the Cray compilers. The resulting executable worked very well and has since been used for high-resolution simulations of a warmer climate state within the EU FP7 HELIX project.



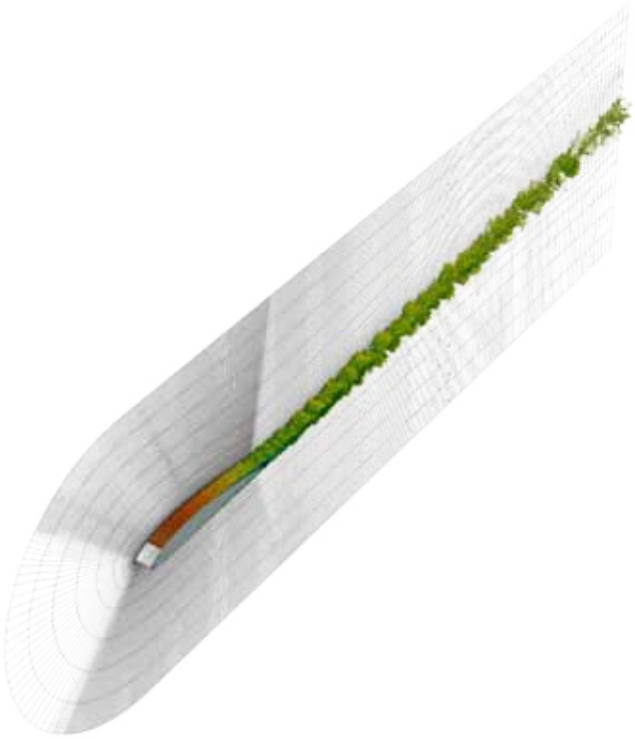
Above: The figure shows some of the results from the pilot project. The dashed lines indicate the performance of EC-Earth when it was compiled using only Intel compilers, whereas the coloured solid lines show how well EC Earth performed when most of it was compiled using the Cray compiler, with the Intel compiler being used for the gribex library. Note that all the curves are normalized to the 1:1 line at 160 cores; at this point the version compiled mainly with the Cray compiler is already approximately 20% faster. The experiments were performed at two different resolutions for simulations using only the atmospheric part of EC-Earth.

Was all the work needed for compiling EC-Earth with Cray compilers really worth the effort? Are the native Cray compilers really generating faster code than the Intel compiler suite? We are pleased to report that the answer to these question is a resounding "yes", as the code is about 20% faster and also scales better with a higher number of cores (which you can see in the figure). So far, the work we have done has focused on the atmospheric component of the EC-Earth model. The complexity of the optimizing work increases as more Earth System components are invoked. The investigation of scaling and performance with Cray and Intel compilers is continuing as we have now entered a demanding phase of updating the model system to get ready for the intensive modelling activities that are planned within the S-CMIP consortium as the Swedish participation in the internationally-coordinated CMIP6 project that will run from 2015 to 2016. The next step involves including the new updated versions of the ocean and ice models, which will be followed by adding the models for atmospheric chemistry, dynamic vegetation, and biogeochemistry in the ocean.

Beskow Pilot Research: Wind Tunnel Simulations

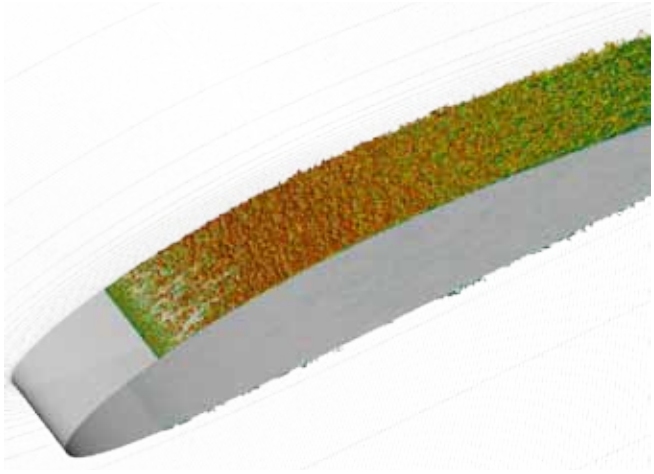
Mohammad Hosseini, Ricardo Vinuesa, Ardeshir Hanifi, Dan Henningson & Philipp Schlatter, Linné FLOW Centre and Swedish e-Science Centre (SeRC), KTH Mechanics

The project we chose for our pilot access to Beskow was the virtual wind tunnel, since it suits the capabilities of the new machine in terms of high performance computing (HPC). Within the context of the virtual wind tunnel, we set up a direct numerical simulation (DNS) of the flow around a wing section represented by the cambered NACA4412 profile. The Reynolds number, based on the airfoil length and the incoming velocity, is 400,000, which is comparable with academic wind tunnel experiments of this kind of geometry, and four times larger than any other existing numerical simulation of similar characteristics. Therefore, these simulations constitute a large step forward, not only in terms of usage of HPC resources, but also due to the use of high-order spectral methods to simulate turbulent flows around complicated geometries of industrial interest.



Above: View of the complete mesh, with the wing section located in the lower left part
The turbulence on the wing surface, and the fine flow structures in the developing wake region is clearly visible. The spectral-element mesh is shown in grey.

Below: Zoomed-in view of the front part of the wing section The flow is tripped to turbulence at 10% of the chord length, similar as in a typical wind-tunnel experiment.



A recent report by NASA discusses a number of findings and recommendations regarding the present and future role of CFD (computational fluid dynamics) in aircraft design. The focal points highlight the necessity of accurate predictions of turbulent flows with significantly separated regions, more robust, fast and reliable mesh generation tools and the development of multidisciplinary simulations (such as fluid-structure interaction, conjugate heat transfer or aeroacoustics) for both analysis and optimisation procedures. Our virtual wind tunnel project, where we consider fully-resolved simulations to further understand the characteristics of the flow in complicated configurations, exactly targets the topics discussed in the report by NASA.

We started our pilot access around mid-December 2014, and initially prepared a case with a Reynolds number of 500,000 which required around 5 billion grid points. The selected code for the project was Nek5000, which is based on the spectral element method (SEM). In this approach, the domain is divided into so-called spectral elements, and the solution is expanded in terms of Legendre polynomials evaluated at the Gauss-Lobatto-Legendre (GLL) points within each element. The case required 3.4 million spectral elements, and when running it on Beskow for the

Staff Focus

Mattias Claesson

Mattias Claesson finished a two-year electrical engineering degree at the Jakobsberg campus of KTH before entering the masters program in computer science in 1994 here at the KTH main campus. Mattias started developing "intelligent homes" technology at a small company called Easy-Living in 1995 and then also started working at PDC in 1996. After a couple of years he started working full time at PDC, mainly with virtual reality in connection with "VR Kuben". For the last couple of years Mattias has been working almost exclusively with storage, focusing primarily on parallel file systems (mostly the Lustre file system).

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first time we obtained the following error: **`ABORT: MPI_TAG_UB too small!`** In Nek5000 the inter-node communication is done via MPI, and some of the messages are identified by the number of the destination element. For the Cray XC-40 system Beskow, the maximum number of tags is 2,097,152 (21 bits); however, we had a total of 3.4 million elements! This was a small flaw in the code: it was possible to use tags to identify the elements when simulations were smaller, but as the size of the domains becomes bigger, a better strategy must be considered.

Our immediate first solution was to reduce the Reynolds number to 400,000, which led to there being 1.85 million spectral elements and 3.2 billion grid points. Afterwards we were able to completely remove the limitation in the Nek5000 code – we basically replaced the unique global element number **`eg`** with the unique pair:

- destination process number, **`mid`**, and
- local element number at the destination process, **`e`**.

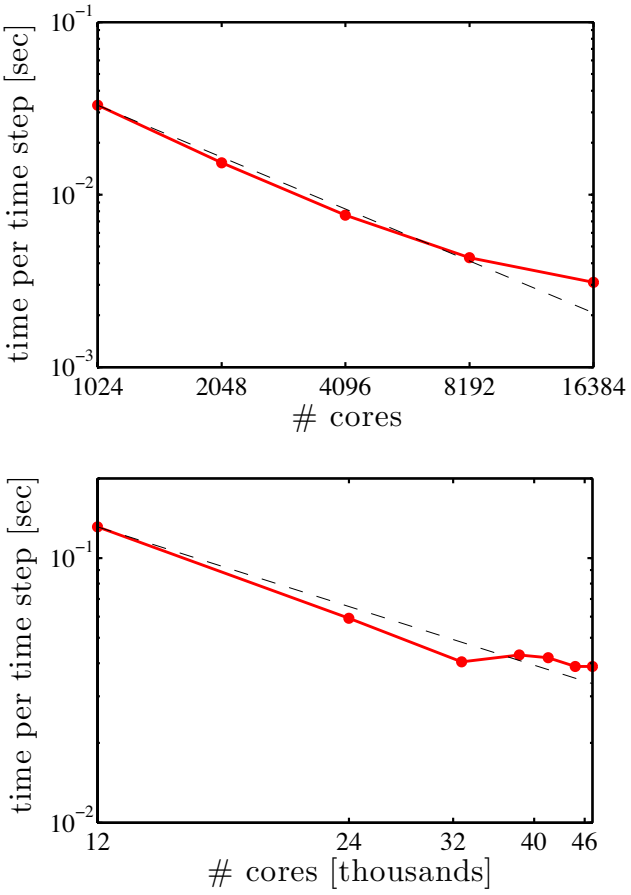
```
      do eg=1,nelgt              ! sync NOT needed here

         mid = gllnid(eg)
         e   = gllel (eg)
!     tag for sending and receiving changed from global (eg) to local (e) element number
!     to avoind problems with MPI_TAG_UB on CRAY
#ifdef DEBUG
         if (nio.eq.0.and.mod(eg,niop).eq.0) write(6,*) eg,' mesh read'
#endif
         if (mid.ne.nid.and.nid.eq.0) then              ! read & send

            if(ierr.eq.0)
              call byte_re     (buf,nwds,
              call csend(e,ierr,len1,mid
              if(ierr.eq.0) call csend(e,buf,len,mid,0)
            else
              call csend(e,ierr,len1,mid,0)
            endif
```

Even though these changes appear simple, they were buried deep in the code, and were thus quite difficult to identify.

We also performed scaling tests of our large case (3.2 billion grid points) and a smaller similar configuration (120 million grid points) – these are illustrated in respectively the lower and upper graphs on the next page. Our results show very good scaling on up to 16,384 cores in the large case. In addition to that, our tests indicate that Beskow is 3-4 times faster per core than Lindgren was and around 1.4 times faster than Triolith (which is based at the National Supercomputer Centre in Linköping).

With respect to the flow case under consideration, the graphs on the opposite page show the high quality of the simulation, where the mesh is meticulously designed to capture the smallest turbulent scales. Note that in both figures we visualise coherent vortices found in the turbulent flow fields. This case is of great interest due to the various interacting physical phenomena: transition to turbulence,

Below: Scaling of Nek5000 on Beskow for a smaller case (120 million grid points, upper graph) and larger test case (3.2 billion grid points, lower graph) with the virtual wing The dashed line indicates perfect linear scaling.



wall-bounded turbulence subjected to pressure gradient and wall curvature, flow separation and turbulence in the wake. The Reynolds numbers based on friction velocity and momentum thickness are 960 and 3,200 respectively, and the total cost of the simulation is estimated to be around 30 million CPU core hours. At the time of writing, we had completed around half of the projected simulation time.

Above: PDC Pub tours of the computer hall, 19 May 2015

Beskow Pilot Research: Simulating Materials

Olle Eriksson, Department of Physics and Astronomy, Uppsala University

During our pilot usage of Beskow, we investigated several specific topics. The first of these considers the influence of finite temperature effects on phase stability. This is basically an experimentally known and investigated phenomenon, for which there is currently very little theory available. This is partly due to a lack of suitable methodology, but also because the existing simulation methods are computationally very demanding. In this sub-project, the main advantage of using of Beskow was that it was possible to run jobs that were very demanding computationally, such as efficient molecular dynamics simulations, as well as highly accurate total energy calculations for large super-cells, thus allowing us to perform further post-processing with other methods.

In the Beskow pilot study we also investigated correlated electronic structures, which go beyond standard methods as described by density functional theory. These new methods are referred to as density functional theory combined with dynamical mean field theory (DFT+DMFT). For these investigations, supercomputing facilities are also absolutely crucial. First of all, DFT+DMFT calculations are computationally intensive. Second, in order to test the DFT+DMFT method within the Hubbard I approximation, many calculations have to be performed. A large computer system is therefore of great value. Especially in the testing phase, it is valuable to have short queuing times, which make it possible to perform the tests in a sensible order. During the pilot access on Beskow, jobs were started within a day after submission, which was important.

Finally, our pilot study on Beskow also involved functional surfaces. These three pilot projects are described in further detail below.

Finite temperature investigations of phase stability

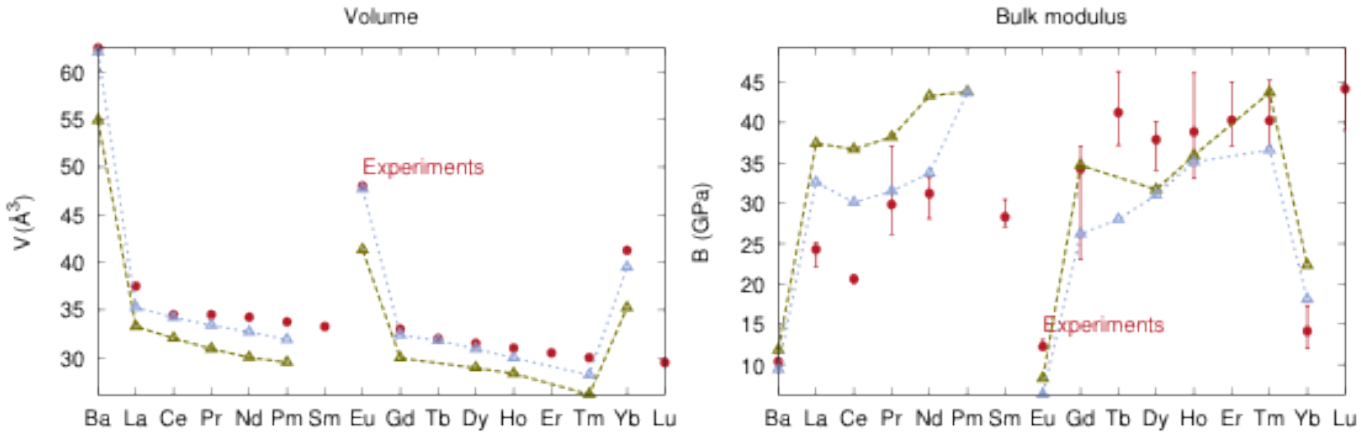
One of our main research interests here is to understand phase stability and phase competition at finite temperatures. This is important from the technological point of view, since it makes it possible to describe phase diagrams, and, in addition, from the fundamental point of view, it enables us to understand the underlying mechanism of phase transitions. Two of our ongoing projects include studies on phase competition in the VN binary alloy, which is a hard material that can be used as a cutting tool, and ferroelectric-like transitions in the metallic perovskite LiOsO3. This perovskite, LiOsO3, is the first known metallic system that undergoes ferroelectric-type phase transitions. Thus our studies of this system are of fundamental interest and we are looking for the explanation of such phenomena.

Our molecular dynamics simulations coupled to the temperature-dependent effective potential method (TDEP) show that the two possible structures of VN, cubic NaCl-type and hexagonal WC-type, are both dynamically stable at temperatures above 200 K. However, the hexagonal WC-type structure has not yet been observed experimentally. Therefore, free energy calculations are required in order to estimate the free energy between these phases at a set of temperatures which we are currently working on. This will require highly accurate total energy calculations for further post-processing within the TDEP technique.

In addition, we found that finite-temperature lattice dynamics calculations for metallic LiOsO3 in its low-temperature phase show continuous softening of the optical phonon mode around the Gamma point as the temperature increases. The soft mode manifests the instability of the low-temperature phase with respect to the high-temperature phase, which is in agreement with experimental results. Our results also answer the much-debated question regarding the type of the phase transition in this material (displacive or order-disorder type), and we have been able to conclude that the transition has a displacive nature.

Correlated electronic structures

During the pilot access on Beskow, we studied the cohesive properties and spectroscopic features of the lanthanide series. These elements are very interesting, both from the technological point of view – as they show useful magnetic properties – as well as from the theoretical point of view. From the theoretical perspective, the lanthanides are characterized by extremely localized 4f electrons,

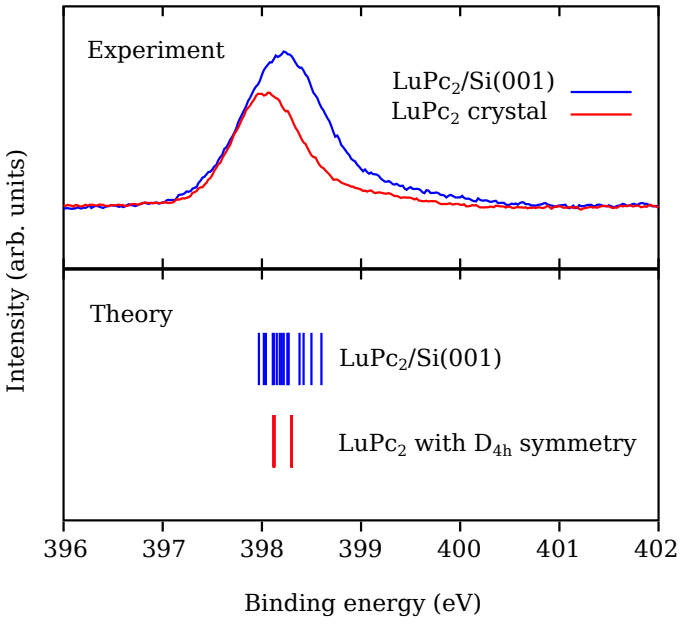


Above: Comparison of the volumes and bulk moduli of the rare earth elements
The green and blue points correspond to DFT+DMFT calculations within the Hubbard I approximation using different functionals. The red points are experimental values taken from K. A. Gschneidner, Jr., Bull. Alloy Phase Diagrams 11, 216 (1990) and W. A. Grosshans and W. B. Holzapfel, Phys. Rev. B 45, 5171 (1992)

which are impossible to describe properly with standard density functional theory (DFT). Within the standard model of the lanthanides (where the 4f electrons are treated as chemically inert, localized electrons), the structural properties can be described, but the spectral properties are not accessible. The spectral properties can be accurately calculated with many body methods, such as DFT+Dynamical Mean Field Theory (DFT+DMFT) within the so-called Hubbard I approximation. This method has also been shown to be successful for calculating the structural properties for similar materials, such as TbN and cerium pnictides. We therefore used Beskow to perform DFT+DMFT within the Hubbard I approximation to describe the following physical properties for the whole series of the rare earth elements: structural properties (such as equilibrium volume and bulk modulus), spectroscopic properties, magnetic moments and the effective exchange parameters for interatomic exchange, for example, as used in a Heisenberg model. During the pilot access on Beskow, we mainly focused on the first two. The first results for the equilibrium volumes and bulk moduli are shown in the figure on the previous page. From these we can see that the theory-based calculations reproduce the observed volumes and bulk moduli with excellent accuracy. For most of the crystals of elements in the series, we also calculated the spectra and found good agreement with experimental data.

Functional surfaces

Understanding molecule-substrate interaction is crucial to understanding the complex mechanisms that lead to the formation of domains in molecular films, self-organizations in ordered structures and complex changes of the electronic properties in molecules and in substrates. We performed detailed investigations regarding the adsorption of functional organo-metallic molecules, such as Lutetium-Bis-Phthalocyanine (LuPc2), onto substrates. This was a collaborative effort where experiments using soft X-ray spectroscopy (including X-ray Photoemission and Photoelectron spectroscopy) were performed in conjunction with Density Functional Theory (DFT) calculations. This gave us insights into the electronic properties that were beyond normal experimental capabilities via a detailed analysis of the surface registry dependence. Large-scale simulations employing the final state approach were used to simulate the XPS spectra. This technique computes the 1s binding energies and also accounts for small shifts in the energy mediated by the chemical environment. The calculations resolve different adsorption sites and structures from which the XPS spectra were calculated. The theoretical spectra resolve the contribution of each atom to the total XPS spectrum. Calculations as demanding as these can only be conducted using high performance computing facilities, like Beskow, with efficiently parallelized DFT codes, for instance VASP. Some of our results for the N1s XPS spectra of LuPc2 adsorbed on Si(001) are shown in the figure below, as an example. They demonstrate that adsorption onto the substrate causes discernible changes in the chemical environment.



Above: Comparison between the experimental and the theoretical N1s binding energies of LuPc2 in crystalline form and adsorbed on Si(001)

What's on in Exascale at PDC/HPCViz?

Stefano Markidis, HPCViz

It may be a few years yet till PDC gets its first exascale computer - the slight delay being due, if nothing else, to the fact that no one has actually built a computer system that fast to date – but we are nevertheless busy with work preparing for the advent of the exascale era.

The EPiGRAM project has now entered its second year. During the first year, the project focused on designing and implementing new concepts in message passing and PGAS programming models, and as a result produced three design documents for MPI, GPI-2 and a PGAS-based MPI. In the second year, EPiGRAM is concentrating on integrating the three approaches into one hybrid approach combining the best features of the three programming models. KTH is leading the work on proving the advantages of this approach by using the new programming model concepts in the Nek5000 and iPIC3D applications. In addition, a new communication kernel, based on GPI-2, has been developed for the both of those applications.

You may remember that EPiGRAM has been organising workshops on Exascale MPI at the annual International Conferences for High Performance Computing, Networking, Storage and Analysis (SC) for the last two years. This year we have again been successful with the ExaMPI15 workshop being accepted as part of SC'15. These ExaMPI workshops are designed to bring

Above: Ivy Bo Peng presenting at EASC2015

Below: Daniel Holmes presenting the MPI endpoints proposal at EASC2015

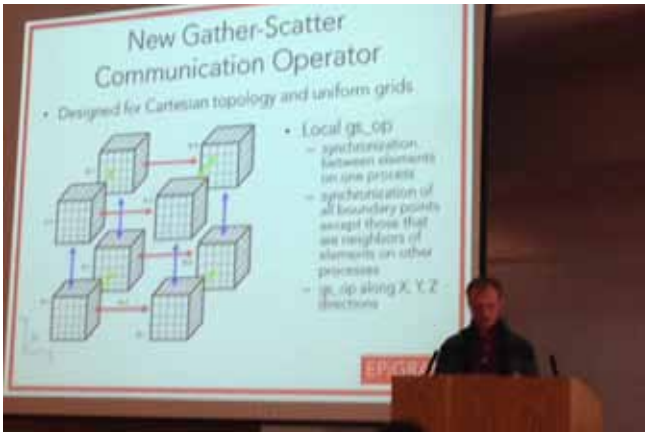
developers and researchers together to discuss innovative algorithms and concepts in message passing programming models, particularly in relation to MPI. If you would like to join us in Texas later this year, you can find more information about the workshop here: https://www.pdc.kth.se/exampi15.

ExaMPI is not the only place you will find PDC/HPCViz represented – our researchers have been, and will be, out and about at a range of exascale events this year. Ivy Bo Peng and Ilya Ivanov presented their work in the EPiGRAM project at the Exascale Applications and Software Conference (EASC2015) in Edinburgh this spring. Erwin Laure has been invited to speak at a workshop that is part of the ISC High Performance conference this summer. The workshop addresses the topic "Is Europe ready for Exascale? A Summary of Three Years of European Exascale Research" (http://www.isc-hpc.com). Meanwhile Stefano Markidis is one of the invited speakers at the PRACE Scientific and Industrial Conference 2015 (also known as PRACEdays15) where he will participate in the workshop "Enabling Exascale in Europe". In addition, Stefano has been invited to speak at ASTRONUM 2015, which is one of the most important conferences in computational astrophysics (http://irfu.cea.fr/ASTRONUM2015).

As a final note, we can assure you that the PDC/HPCViz researchers and doctoral students have not just been travelling the world – one of

their papers, “Idle waves in high-performance computing”, has been selected as “Editor’s choice” in the Physical Review E journal. see https://www.kth.se/en/csc/forskning/hpcviz.

Juris Vencels and Ivy Bo Peng, two of the students who contributed to that paper, are also in the running for the best paper award with two papers at the International Conference on Computation Science (ICCS), which is conveniently close in Reykjavik this summer.



Above: Ilya Ivanov presenting the work on the new communication kernel for Nek5000 at EASC2015

HPC Infrastructures Workshop

Gert Svensson, PDC

PDC was the local organizer for the 6th European Workshop on HPC Centre Infrastructures, which was held in Stockholm from 10-13 May 2015. The number of attendees at these workshops has steadily increased over the last six years and this year we reached a record of 73 people, some of whom came from as far afield as the USA and Australia. Everyone really enjoyed the great atmosphere and gourmet food at Såstaholm, which is a lovely old mansion north of Stockholm that used to be a home for retired actors and actresses.

A main focus of the conference was the topic of increasing energy demands from HPC systems and the implications of this for HPC infrastructures. Thanks to the Swedish climate and the consequent need for good heating during our cold winters, which has led to the existence of city-wide district heating and cooling networks, we have a unique possibility

Below: Såstaholm mansion

to re-use heat energy from HPC systems. Included in the workshop were visits to the PDC computer hall, where the heat is re-used locally at KTH, and a visit to the data centre of Bahnhof, an internet and co-location company that is based in a nuclear bomb safe bunker under central Stockholm. The heat from this data centre is completely recovered and re-used in the Stockholm district cooling and heating networks.

Attendees are unlikely to forget what happened on the way back from visit to Bahnhof! When one group came out from the data centre bunker, they could not get into the bus, as it was locked with no sign of the driver. They waited… and finally the other bus turned up. The driver of that bus explained that the other driver was locked in the toilet of the first bus and could not get out, but he said that he would be able to unlock the bus and unjam the toilet door. However he was unable to free the driver of the first bus, after much wrestling with the jammed door. The conference participants were then asked if anyone would like to volunteer to try to break the door apart. One of the men volunteered and eventually he succeeded in breaking the door down so an amused, and possibly slightly bemused, group was glad to finally get back to Såstaholm for the evening meal.

Above: Såstaholm survivors

Staff Focus

Hannes Leskelä

Hannes Leskelä joined PDC in June 2014 and is currently working in the support group, where he helps users to debug problems and make the most of the PDC resources. He is studying computer science at KTH and is currently completing an M.Sc. in that field. In his "leisure" time (which is often extremely busy), Hannes likes to do stuff that involves not sitting still in one way or another, preferably while being outdoors.

Staff Focus

Daniel Ahlin

Daniel Ahlin joined PDC in 2000. Since then he has worked in and coordinated various development and applied research projects. Currently he is leading the Systems group and acting as PDC's technical director.

EUDAT Extended

Damien Lecarpentier, CSC – IT Center for Science, Finland

In late March, the CSC - IT Center for Science in Helsinki played host to people from all over Europe who gathered for the kick-off meeting for the next phase of the EUDAT project, which will run until early 2018. EUDAT is now a bit over three years old. While this is still young for a pan-European infrastructure seeking to provide data management solutions across research disciplines and national boundaries, much has already been achieved. EUDAT is already providing a suite of common data services supporting multiple research communities and individuals. These services are offered through a geographically distributed, resilient network connecting general-purpose data centres and data repositories for specific research communities. EUDAT's shared services and storage resources are distributed across 15 European nations with data stored alongside some of Europe's most powerful supercomputers.

Above: EUDAT kick-off, Helsinki, March 2015

In practical terms, EUDAT connects to and interoperates with data e-infrastructures driven by research communities to steward data for the whole community of European researchers. This is important where there is no single underlying organisation that deals with the full complexity of managing such data. EUDAT provides IT solutions that would be difficult for some research communities to provide on their own, thereby reducing their costs and enabling the communities to make investments in community-specific services and developments. It is important to emphasise that EUDAT operates in a European landscape of developing research infrastructures. These infrastructures often have ready-developed solutions and tools for managing their data. The goal of EUDAT is not to replace these infrastructures but to support and enrich them by providing strong underlying components and generic services on which they can rely to build up their data management strategies and e-infrastructure capacity.

EUDAT's ultimate objective is to create a sustainable pan-European Collaborative Data Infrastructure (CDI); much remains to be done to achieve that. EUDAT recently received a further €19 million to continue laying the foundations for that data infrastructure. In the first project phase (which ran from 2012 to early this year), our priority was to determine which common data services were needed most and to build those services and get them running as soon as possible. Technically, we've made very good progress! The priorities for the next few months are to consolidate these services and also to develop the necessary policies and business models, as well as the organizational framework, that will make it possible to provide these services in a cost-efficient and sustainable way.

We want to create a CDI that is open to all and which addresses the different needs of its users. Many users are researchers who just wish to share data with colleagues or collaborators, or to discover and re-use data as part of their ongoing research. These users can come from many different walks of life – researchers (from

Below: EUDAT kick-off, Helsinki, March 2015

academia and industry), citizen scientists, policy makers, and members of the public. EUDAT is there for anyone wanting to share or re-use European research data in simple, powerful ways. Other EUDAT users are concerned with the management of research community data repositories and wish to join their repositories formally with the EUDAT CDI network, thus instantly benefitting from the persistence and resilience offered by the EUDAT partners. Users who are interested in joining the CDI are primarily interested in archiving, replicating, processing and cataloguing data on behalf of a particular research community.

In the new project phase we will also reach out beyond our traditional sphere of influence to engage with a wider range of stakeholders and research communities. To this end, EUDAT has brought ten new organizations on board and plans to issue two calls for collaboration to engage effectively with research communities that are not presently part of the project consortium. Currently EUDAT interacts and serves 29

research communities and plans to increase this interaction to over 50 communities in the next three years. EUDAT has, since its inception, been working on the principle that the research communities should not only be in the driving seat for selecting the main services, but that they should also directly participate in the design and development of these services. We expect that new requirements will emerge from these calls for collaboration and that we will consequently be able to foster new lines of activity. At present, we see a lot of interest in the area of semantics and big data analytics and we encourage all stakeholders interested in these topics to partner us in building new components on top of the CDI.

EUDAT is in the process of creating an infrastructure that can act as a key pillar of the European Research Area. Additionally, by identifying and proposing solutions to barriers to the development of an efficient e-infrastructure ecosystem, research e-infrastructures like EUDAT make concrete contributions to reinforcing the level playing field for researchers and data managers and eliminating barriers to investment in the proposed European connected Digital Single Market.

There are many reasons to be interested in EUDAT and to become concretely involved in this outstanding initiative! Follow us for more regular news and updates on our activities on http://www.eudat.eu, and on social media such as Twitter and Facebook. If you or some members of your research community would like to take up one or more of the EUDAT services, or join our pool of experts, please get in touch with us at eudat-info@postit.csc.fi.

PDC in the Extension of EUDAT

Erwin Laure, PDC

PDC initially became involved with EUDAT because PDC is a national Swedish high-performance computer (HPC) service provider under the auspices of the Swedish National Infrastructure for Computing (SNIC). Consequently PDC has a mandate to provide efficient and easy-to-use HPC and storage services to Swedish academia. As research is becoming more and more international, it is of growing importance to PDC's users to be able to easily share their data with their peers in other countries and in return gain easy access to data provided elsewhere. The common policies and services provided by EUDAT are of benefit as they are a perfect tool to ensure that PDC's infrastructure is compatible with other European research infrastructures, which means that PDC's users can easily share data and collaborate with their peers. At the same time, as EUDAT is prototyping new services that are potentially of interest to Swedish users, the whole Swedish research community can profit from the experiences gained in other countries in evolving our infrastructures.

In addition, it is becoming increasingly more important to have a strategic approach to data handling that includes not only storage, but also data management – including metadata handling, replication, persistent identifiers (PIDs) and so forth. EUDAT provides data centres with a perfect forum to ensure that their efforts are not happening in isolation but in sync with similar efforts elsewhere, which has certainly been PDC's experience with EUDAT.

PDC has had multiple roles within EUDAT since the project started. First, as national Swedish high performance computing centre, PDC functions as a resource node in the common data infrastructure (CDI) offering the EUDAT services – that means that PDC makes the EUDAT services available to researchers on our systems. PDC will continue to do this in the extension of the EUDAT project as, after all, one of the primary goals of EUDAT is providing persistent storage so that data continues to be available in the long term.

PDC has also participated actively in the development of the EUDAT services, in particular B2SHARE, where PDC will continue to lead the development efforts in the new phase of the project. The reason PDC focussed on B2SHARE is that it was a new service with a high potential for uptake within PDC's user communities.

The persistent identifiers (PIDs) offered by the European Persistent Identifier Consortium (EPIC) are another example of where PDC has been actively contributing to EUDAT, and PDC can now offer this service on a national basis.

In addition, PDC has been engaging with research communities and exploring the potential of EUDAT services to serve their needs. PDC has been working with the Swedish Museum of Natural History in Stockholm. They are a national node in the Global Biodiversity Information Facility (GBIF) and have participated in testing storage for the EUDAT iRODS service, as well as being involved with B2SHARE. The Biobanking and Biomolecular Resources Research Infrastructure (BMRI) has been working with PDC on biobanking using B2SHARE – this work initially came out of their participation in the B2SHARE Nordic project. The International Neuroinformatics Coordinating Facility (INCF) is running a B2SAFE node at PDC, which they use for storage. And we are also having discussions with the Integrated Carbon Observation System (ICOS), which just joined EUDAT very recently.

Finally, EUDAT is also important in the evolution of the Swedish national SNIC data service, SweStore, as EUDAT provides best practices and guidelines that help shape SweStore into an interoperable infrastructure supporting Swedish researchers.

Above: PDC Pub tours of the computer hall, 19 May 2015

CRESTA Comes to a Close

Stefano Markidis, HPCViz

The CRESTA project ended in December 2014 on a positive note when the European Commission reviewers awarded the results of the project an "excellent" final grade. CRESTA showed for the first time that the co-design approach truly is effective for exascale computing with non-trivial code applications. Within the project, PDC led the work on programming models, runtime systems, compilers and auto-tuning systems. Scilab and the Linné FLOW Centre, which is one of the centres at the KTH Mechanics department, implemented new code for exascale in the GROMACS and Nek5000 codes.

Below: SNIC Cloud Spark course held at Uppsala University and given by Åke Edlund and Izhar ul Hassan, 21 April 2015

Clouds All Up in the Air

Åke Edlund, PDC and HPCViz

Much has been happening on the cloud front here at PDC and in the HPCViz Data-Intensive Computing Group, with the SNIC Cloud now in its second year and the PDC Cloud itself being successively adapted to the needs of "Big Data". The SNIC Cloud is currently running a smaller set of prioritized use cases - something that we will share more about in the next newsletter. Since late 2014 we have also been involved in the NeIC Cloud project, "Glenna", where we are leading the work package on PaaS (Platform as a service) and SaaS (Software as a service), again with a focus on data analytics platforms (which, in this case, is mainly Apache Spark).

NeIC Conference 2015

Dejan Vitlacil, PDC

Around 185 scientists and technical experts from the Nordic countries attended the Nordic e-Infrastructure Conference 2015 that was held in Espoo, Finland, on the 7th and 8th of May 2015, with additional workshops being held earlier on the 5th and 6th of May. This NeIC conference and also the previous one (which was held in Trondheim, Norway, in 2013) were enriched by participants and speakers coming from various European countries, as well as from the USA.

NORDUnet (which is a collaboration between the national research and education networks in Denmark, Iceland, Norway, Sweden and Finland) was in charge of streaming all the plenary sessions from the NeIC 2015 Conference. The two days offered a large number sessions and speakers that provided a variety of views on e-infrastructures, including a very interesting panel discussion that rounded off the event at the Hanasaari Swedish-Finnish Cultural Centre in Espoo. The recordings can be viewed on the NeIC 2015 Conference website.

The aim of the conference was to couple Nordic user communities with the skills base that exists within the national e-infrastructure organisations in order to develop ideas, and to elicit opportunities for cost-efficient common solutions and joint e-infrastructure services.

Above: Dan Reed at the NeIC Conference 2015

Below: Riitta Maijala at the NeIC Conference 2015

During the workshop sessions that were held on the 5th and 6th of May, David Simonsen, the head of WAYF - Where Are You From, a publicly funded electronic identification (eID) federation from Denmark, gave a general introduction and deeper insights into Authentication and Authorisation Infrastructures. Lots of people had a good time and gained new skills during the Security workshop that was held by the well known "Nordic Security Officer" Leif Nixon. Another noteworthy workshop was one that was rather unusual for our community, but very much appreciated – it was a workshop of a more philosophical nature on Bioethics that was chaired by Janne Nikkinen from the Nordic Committee on Bioethics.

The conference events on the 7th and 8th of May were opened with a welcome from Riitta Maijala, who is Director of the Science Policy Division within the Department of Higher Education and Science at the Finnish Ministry of Education and Culture. Paul Messina then gave an insight on Trends in HPC Environments while Dan Reed talked about how Big Data Meets HPC.

In addition, during the NeIC Conference 2015 two important documents had their first public presentation: the Cognitus report and the Nordic eScience Action Plan 2.0.

The Cognitus report was prepared for the NeIC Board to facilitate future decisions in the Nordic region in the area of high performance computing and related topics. An external expert, Dr. Robert Pennington, Deputy Director of the

National Center for Supercomputing Applications at the University of Illinois Urbana-Champaign, was engaged as a special advisor to NeIC for the project. He consulted with Nordic researchers, Nordic HPC systems staff and NeIC staff, as well as other researchers who have been engaged in similar activities in other countries. A copy of the report can be downloaded here: http://www.nordforsk.org/en/publications/publications_container/cognitus-a-science-case-for-high-performance-computing-in-the-nordic-region/download.

The first version of the Nordic eScience Action Plan was presented in November 2008, comprising ten concrete actions in three different action lines for implementing an integrated Nordic strategy covering higher education in e-science, e-science research and e-infrastructures. At the end of 2012 following the successful implementation of many actions in the first version of the action plan, the Nordic Council of Ministers for Education and Research (otherwise known as the MR-U) under the Swedish presidency of the Nordic Council of Ministers, appointed a project leader and an ad hoc expert group to produce an updated version of the plan, the Nordic eScience Action Plan 2.0. This can be downloaded here: http://www.nordforsk.org/no/publikasjoner/publications_container/nordic-escience-action-plan-2-0-escience-and-einfrastructure-in-an-international-context/download.

These are just some of the excellent contributions from the workshops and the conference sessions at the NeIC 2015 Conference that made it so successful, and also created a challenge for the organisers of the next NeIC conference (which is planned for 2017 in Sweden) as they try to line up an equally stimulating array of speakers.

Meanwhile, for more information on NeIC, see http://neic.nordforsk.org or contact Dejan Vitlacil (vitlacil@kth.se) and Michaela Barth (caela@kth.se), the NeIC Coordinators for Generic Technologies.

PDC Pub and Open House

Jonathan Vincent, PDC

Good company and great beer!
Why weren't you there?

Tours of the PDC computer rooms with Gert Svensson

Listen well, my children, while Uncle Gert tells you a tale of how a supercomputer works...

In which Uncle Gert demonstrates how to tango with a supercomputer...

Beskow brings out the inner child...

Tegner

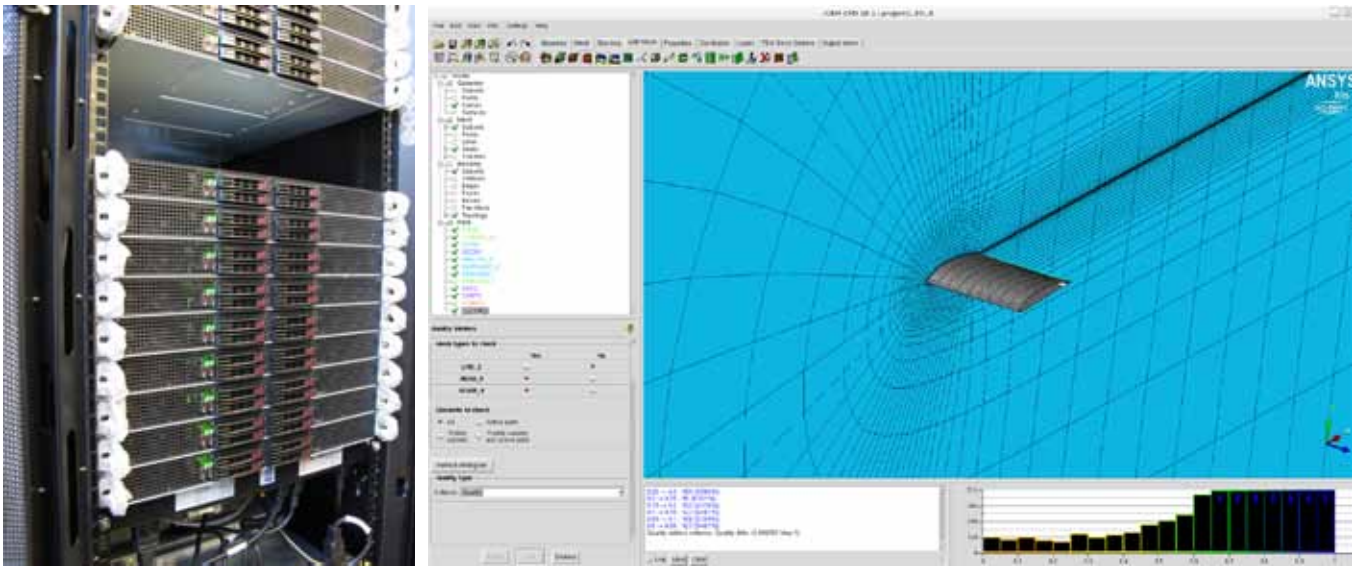
Gert Svensson, PDC

PDC is excited to announce that the new pre- and post-processing system we have all been waiting for has arrived at PDC and should be available to users before the summer. For the last few months since the arrival of our new supercomputer Beskow, which is currently the fastest academic supercomputer in Scandinavia, PDC has been working to find a suitable pre- and post-processing system for Beskow. The pre- and post-processing system is needed to prepare the data that is used in the large simulations that run on Beskow (for example, preparing a grid of points to represent the surface of an aeroplane wing), and to analyse the data that results from the calculations performed on Beskow (for example, creating an image with different colours to indicate the different levels of air resistance around the wing of a plane after Beskow has calculated the air resistance values for all the points in a grid representing the surface of the wing).

The increasing exchange rate of the US dollar against the Swedish krona, along with the fact that PDC's requirements for a pre- and post-processing system were highly demanding overall, made it extremely hard for the vendors who were involved in the procurement process to give us bids that complied with all of our requirements. The good news is that, after tough negotiations, PDC was able to sign a contract with Data Access Sweden (a company that specialises in providing high performance computing and mission critical systems) and its distribution partner Nextron to provide the pre- and post-processing system. The system will be called Tegner in honour of Alice Tegnér who wrote many Swedish songs for children. (We leave out the accent in the computer name for practical reasons.) In the first

Facts about Tegner

- 5 nodes with 2 TB of memory - each with quad 3.0 GHz Ivy Bridge 12 core CPUs
- 5 nodes with 1 TB of memory - each with quad 3.0 GHz Ivy Bridge 12 core CPUs
- 57 nodes with 0.5 TB of memory - each with dual Haswell 12 core CPUs
- 9 of the 57 nodes are equipped with nVIDIA Tesla K80 GPUs
- All other nodes in the system have nVIDIA Quadro K420 KEPLER GPUs



Above: Tegner's 0.5 TB nodes (left) and a screen shot of pre-processing to generate a mesh to represent a section of a wing (right) The mesh above is used for the simulation of a section of an aircraft wing, and has a total number of 3.2 billion grid points. The mesh was produced by KTH Mechanics using ANSYS ICEM CFD, a powerful meshing tool with unique capabilities for both structured and unstructured meshes. It can read and export multiple CAD geometries, and can produce meshes for various solvers, including one suitable for use with the spectral-element method Nek5000.

half of last century Alice Tegnér collaborated with Elsa Beskow to create many charming song books for children, with Alice composing the music and Elsa illustrating the books. Both Alice and Elsa lived in Djursholm in Stockholm, and now, almost a century later, the computer systems Tegner and Beskow will be cooperating in a similar manner a little farther south at PDC in Norra Djurgården.

The system Tegner will consist of 67 Intel Super Micro nodes with 9 NVIDIA Tesla GPUs and 40 terabytes of main memory and will have a maximum processing speed of about 100 teraflops. The system will cost ten million Swedish krona over four years, with financing coming from SNIC, KTH and other partners.

Anyone who already has a time allocation on Beskow is welcome to start using Tegner. Researchers from the Stockholm region who are interested in using Tegner as a general cluster, or other users interested in using GPUs, are welcome to apply directly to PDC – just send an email to support@pdc.kth.se.

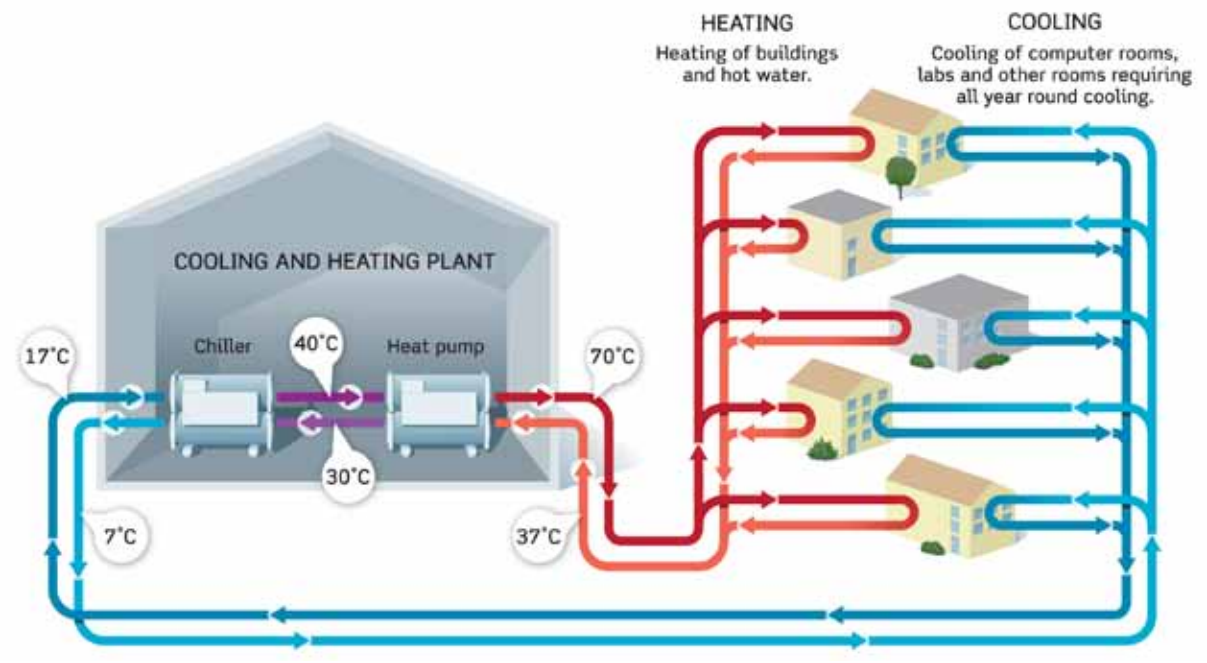
The system will have an EDR Infiniband interconnect in its final incarnation after the summer. Until then, Tegner will use existing FDR Infiniband equipment from one of PDC's earlier systems, Ekman.

Below: The new heat re-use facility was officially opened by Sten Wetterblad, the Regional Director of Akademiska hus, Peter Gudmundson, the President of KTH, and the Mayor of Stockholm, Karin Wanngård.

New Heat Re-Use Facility at KTH

Gert Svensson, PDC

On the 4th of May, KTH inaugurated a new heat re-use facility. For a long time KTH has been using a local network of hot and cold water pipes to supply heating and cooling to the university buildings, however the networks were just being used as an extension of the city-wide district heating and cooling networks within Stockholm. But now Akademiska hus (which is the company that owns the KTH buildings, and indeed most university buildings in Sweden) has invested in a huge heat pump for the KTH campus. The heat pump will be used to increase the temperature of



Above: Schematic diagram of the heat re-use system

Below: The new heat pump at KTH

the water from the cooling loop (which is normally around 18 °C) to a level that is useful for providing hot water, both for taps and also for the hydronic radiators in the buildings at KTH (which are heated by circulating hot water). PDC's supercomputers are the single largest sources of heat for the new heat pump.

PDC-Related Events

PDC Summer School 2015

17-28 August 2015, KTH, Stockholm

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

Introduction to PDC Systems

17 September 2015, PDC, KTH, Stockholm

https://www.pdc.kth.se/events/event-repository/introduction-to-pdc-systems-september-2015

Advanced GPU Programming

5-6 November 2015, KTH, Stockholm

https://www.pdc.kth.se/events/event-repository/advanced-gpu-programming-november-2015

Performance Optimisation of Numerical Simulation Codes

9-13 November 2015, KTH, Stockholm (PhD course, 5.0 ECTS)

http://sese.nu/performance-optimisation-of-numerical-simulation-codes

Introduction to Programming the Xeon Phi Processor

24 November 2015, KTH, Stockholm

https://www.pdc.kth.se/events/event-repository/introduction-to-programming-the-xeon-phi-processor-november-2015

Code Optimisation and Performance Tuning

26-27 November 2015, KTH, Stockholm

https://www.pdc.kth.se/events/event-repository/code-optimisation-and-performance-tuning-november-2015

Introduction to GPU and Accelerator Programming

14-18 December 2015, PDC, KTH, Stockholm (PhD course, 5.0 ECTS)

http://sese.nu/introduction-to-gpu-and-accelerator-programming-for-scientific-computing-2015/

EXAMPI15: Workshop on Exascale MPI

16 November 2015, Texas, USA (in conjunction with SC15)

https://www.pdc.kth.se/exampi15

HPC Sources

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

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

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

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

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

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

NeIC
http://neic.nordforsk.org

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

SeSE
http://sese.nu

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

XSEDE
https://www.xsede.org/conferences-and-events

NeIC Conference News

Join us in Sweden in 2017!

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