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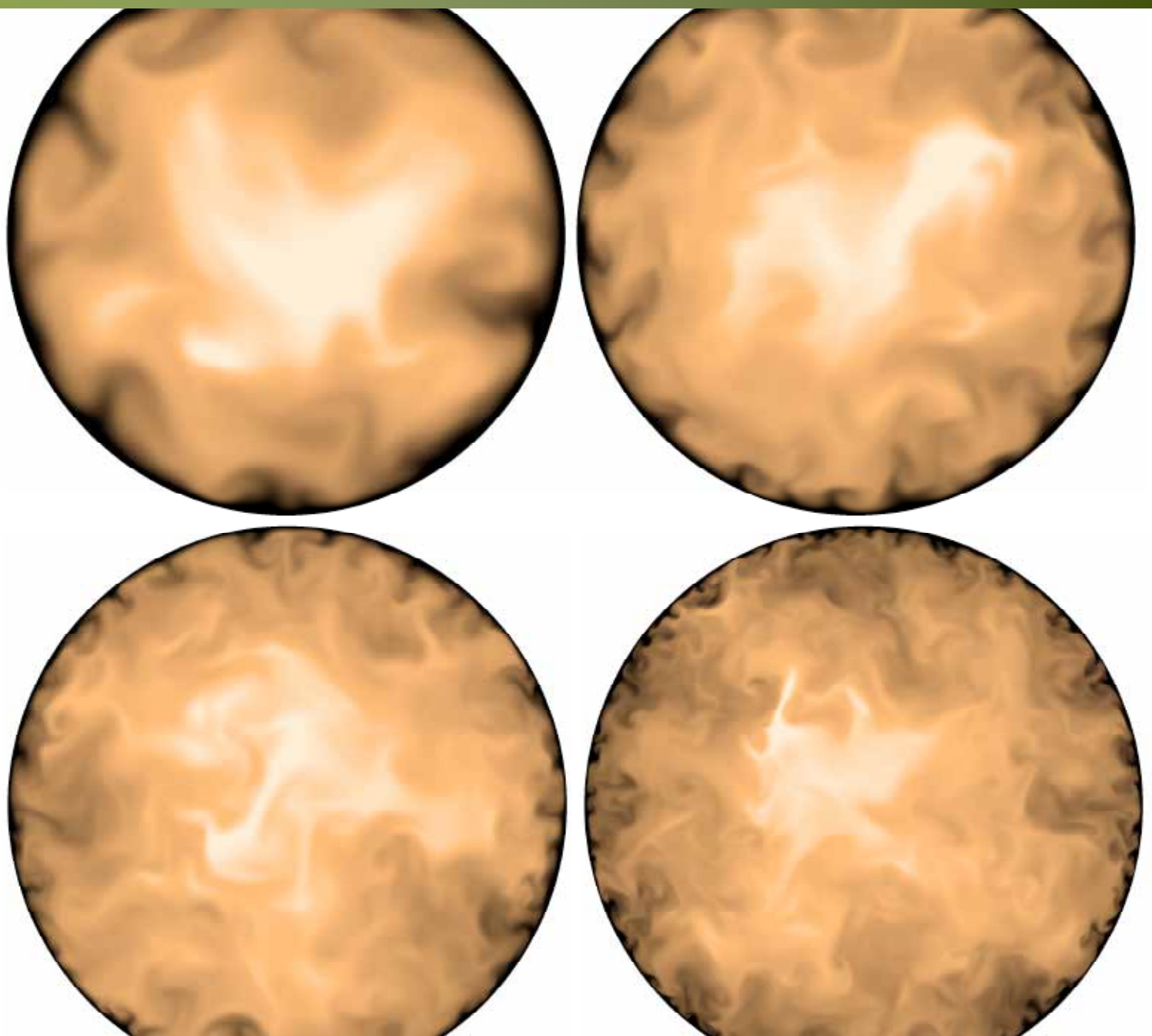

PDC Editorial

Erwin Laure
Director PDC-HPC

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

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On the cover:
Turbulent flow in pipes - see article on page 3.

So far 2012 has been a busy year for PDC and its users. Our flagship computer, Lindgren, has been busily serving a range of highly demanding Swedish research projects, as well as many European projects through PRACE's DECI programs. For a period in 2011, Lindgren provided more capacity than all the other SNIC systems put together, which meant that the system was under heavy stress. However, with new systems arriving at the other SNIC centers, particularly Abisko at HPC2N and Triolith at NSC, we now intend to put more focus on the main purpose of Lindgren, which is to serve the most demanding of the Swedish applications. As a consequence, we will successively reduce access to Lindgren for jobs with low core-counts after the summer.

Lindgren has not been the only thing keeping us busy at PDC; we have also invested in several pilot projects. In particular, we were able to expand the GPU cluster Zorn (originally owned by VIC-Stockholm) and can now offer a total of 40 GPUs to SNIC users who want to experiment with this new technology.

In the area of distributed computing, cloud computing has been gaining prominence amongst members of the scientific community, and PDC has been offering a cloud testbed to interested users. With the increasing focus on this area, particularly from the life science community, KTH has invested in a major upgrade of its cloud resources and we will soon be offering an academic cloud comprised of 384 cores.

To cope with the ever increasing electricity demands of modern computers, we started a project to reuse the heat produced by Lindgren more efficiently. As a result of this, KTH's chemistry building enjoyed "high performance heating" this winter, making PDC and KTH a greener environment.

Two major international projects were started in the fall of 2011: EUDAT which aims to build a European Data infrastructure, and CRESTA, which is one of the three EC exascale flagship projects. In EUDAT, PDC is representing SNIC and working towards an alignment of EUDAT's and SweStore's technology. The partnership with EUDAT is also helpful in fostering local collaborations, such as the storage projects being undertaken with SciLifeLab and INCF. Within CRESTA, PDC develops new adaptive runtime and performance analysis environments, and also works with important applications to improve their scaling towards exascale systems. The Swedish application contributions are the molecular dynamics package GROMACS, supported by Erik Lindahl's group at KTH's Theoretical Physics Department, and `nek5000`, supported by KTH's Mechanics Department in collaboration with the Argonne National Lab.

Finally, it's also time to say farewell to a good old friend in PDC's environment. Our foundation level resource "Ferlin" will retire as a national SNIC system on June 30. However, we will keep Ferlin accessible

for some users from the Stockholm region, and invite other users to seek time on other SNIC systems.

With this I'd like to wish you all a relaxing summer holiday as we look forward to the great results that will be produced on PDC's resources in the autumn.

Erwin Laure, Director PDC-HPC

Turbulent flow in pipes

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1 Introduction

Fluids are omnipresent in our daily life in the form of air in the atmosphere as a *gaseous* fluid or water in lakes and oceans as a *liquid* fluid. These fluids are usually in motion and the study of the various aspects of this motion is contained in the discipline "fluid dynamics". The flow of blood in the body, air flow patterns around buildings, or even – in an extended context – the flow of cars on highways and in traffic jams, or the formation of stars and galaxies can be considered as a part of fluid dynamics. Our main concern here is to study the flow in pipes, which is in some sense the most fundamental means of transporting fluids from one point to another. Despite the widespread use of pipes in engineering and biology, our understanding of the flow physics – in particular at higher speeds – is still incomplete. Numerous experiments have been and are being performed in large facilities around the world to unravel some of tthe mysteries (Cipra, 1996). Here we focus on a numerical approach to virtually study this flow case with supercomputers, and provide new physical insights.

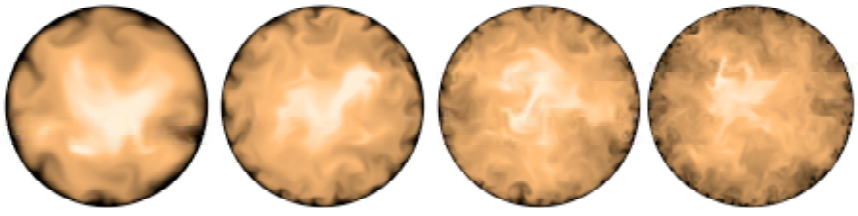

Figure 1:
Instantaneous cross-sectional views of axial velocity giving a quick idea of the effect of the Reynolds number Re on the characteristics of a flow. The chaotic motion of the fluid as well as the wall-normal mixing increases with higher Re. This can be seen by the more frequent occurrence of small structures close to the walls. An increase in Re can be viewed as a pipe flow with a higher flow rate. From left to right, top to bottom: $Re_D = 5300$, $Re_D = 11700$, $Re_D = 19000$ *and* $Re_D = 37700$.

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There are two basic states of fluid motion: *laminar* and *turbulent*. A laminar flow is characterised by a very regular sheet-like motion (lamina is from Latin meaning thin sheet or plate). In contrast, a turbulent flow is chaotic, irregular and is dominated by various eddies of different sizes. (The word turbulent also originates from Latin where turbulentus essentially means chaotic or riotous.) The first sketches, or visualisations as they would be referred to nowadays, of turbulent flows date back to Leonardo da Vinci in the fourteenth century. It is well known that most fluid flows observed in nature, for instance in the atmosphere, or encountered in engineering applications, are indeed turbulent.

The presence of turbulence is usually connected with negative associations. Either the airplane is shaking, or the frictional drag is increased considerably over the laminar value. Indeed, a rough estimate says that about 10 % of the total energy consumed in the world is used to overcome turbulent friction in one way or another. On the other hand, there are certainly positive aspects of turbulence. For instance, mixing is increased in a turbulent flow, allowing us to cool a cup of coffee quickly with a little cold milk, or letting combustion engines burn fuel and oxidiser efficiently.

The spatial and temporal evolution of a viscous fluid can be described by the Navier –Stokes equations. These equations are derived by applying Newton's second law to a continuum. The exact formulation of these equations was developed over a few centuries until the mid-1800s with contributions of people as famous as Isaac Newton, Daniel Bernoulli, Leonhard Euler, Claude-Louis Navier and George Stokes. This lead to a comparably simple set of differential equations, consisting of the conservation of mass and the conservation of momentum. The presence of strong non-linearity in the Navier –Stokes equations makes it literally impossible to find exact analytical solutions to these equations, except for a few simple non-turbulent cases. This highlights the necessary and important role of supercomputing within the field.

One of the most profound developments in modern fluid dynamics came from Osborne Reynolds in a paper dated 1883, in which he studied experimentally the flow in a thin glass pipe. He discovered that a non-dimensional number, nowadays called the Reynolds number, is crucial for deciding whether the flow is laminar or turbulent. The Reynolds number is defined as $Re = UL/\nu$ with a characteristic length L (for instance the wing cord length), a velocity U (the speed of the airplane), and the fluid properties described by the kinematic viscosity ν. The Reynolds number can be interpreted as a measure of the inertial forces divided by the viscous forces, and is by far the most important non-dimensional number in fluid mechanics. Laminar flows exist at relatively low Reynolds numbers and, in this case, the motion of the fluid particles can be predictable and along observable paths. However, as mentioned previously, most fluid flows encountered in real situations are turbulent. This is because many gases and liquids have low viscosity combined with sufficiently large moving objects which means that most practical flows are characterised by large values of the Reynolds number.

Turbulent flow with its chaotic nature consists of swirling flow structures (vortices or eddies) with characteristic length, velocity and time scales which are spread over broad spectral ranges. The size of the largest eddies in a turbulent flow is determined by the characteristic length scale of the mean flow (for instance, the diameter of the pipe or the size of an immersed object) whereas for the smallest eddies, their size depends on the Reynolds number. At high Reynolds numbers, there is a wide range of eddy sizes. The largest eddies, which are generated directly by shear in the mean flow, contain most of the turbulent kinetic energy and are largely unaffected by viscous stresses. However, due to inertial effects, these large eddies break down and transfer energy to smaller eddies that in turn spread the energy to yet smaller structures. This process continues until a scale is reached at which the inertial forces become com-

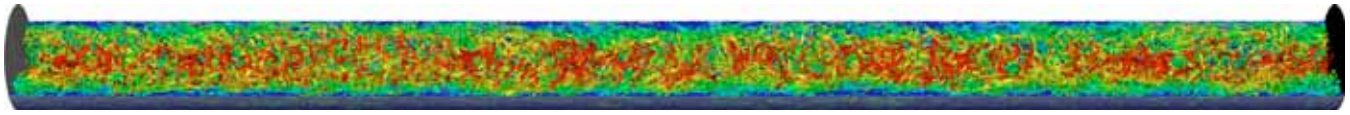


Figure 2:
Isosurfaces of negative λ_2 (Jeong & Hussain, 1995) coloured by axial velocity u_z/U_b for $Re_D = U_b D/\nu = 19000$ (U_b denotes the average axial velocity, D the pipe diameter and ν the viscosity). For the sake of visualisation, the pipe has been cut open, and only the lower half is shown.

parable to the viscous stresses and the kinetic energy is dissipated by the latter into heat. This particular feature is usually termed the *turbulence cascade* and is one of the cornerstones of turbulence research; even poems have been written about it.[1]

The understanding of the flow close to solid walls has been profoundly increased by the German physicist Ludwig Prandtl, who introduced the concept of the *boundary layer* in 1904 (see a very interesting historical description in the book edited by Davidson *et al.*, 2011). According to his conjecture, it is only a thin region of the flow adjacent to the wall that feels the influence of viscosity, whereas the free-stream further away can be treated inviscidly. Subsequent studies by researchers as prominent as Theodore von Kármán helped unravel the now classical picture of near-wall turbulence, including a description of the mean-velocity profile (the "law of the wall" and the log layer). Given the immense technological implications of drag and turbulent friction, a profound understanding of such turbulent boundary layers is needed, be it for deriving accurate turbulence models or understanding the physical processes in a better way. In particular, computational studies are a means to increase our understanding of the dominant dynamical processes near walls.

2 Computer simulations

There are various aspects of fluid flows that are not yet fully understood and complex geometrical configurations yield even more complex flow phenomena. To tackle such issues, flows were traditionally studied exclusively in either nature or laboratories and wind tunnels. Supercomputers can now be used more and more to simulate complex flows, and allow a scientist to conduct virtual experiments. The computational cost, however, is excruciating if a full model of reality is wanted. Accordingly, scientists try to simplify the problems at hand as much as possible by considering generic geometrical configurations. Typical examples of canonical flow configurations are pipes, plane channels and boundary layers.

Direct numerical simulation (DNS) is perhaps the most straightforward approach available to solve the Navier –Stokes equations numerically. It involves no turbulence modelling and directly[2] solves the equations of fluid motion thus attempting to capture all eddies in the flow field. In order to do so, the domain size needs to be at least as large as the largest structures in the flow, and also resolve the smallest turbulent eddies. Consequently, the computational cost of performing a DNS including all scales roughly grows by Re^3 . With such high computational costs, DNS is mainly used as a research tool to study flows with low to moderate Reynolds number. Only recently has computer power increased sufficiently to attempt fully resolved numerical solutions of truly turbulent flows. However, even if computers grow according to Moore's law, a realistic flow simulation of a commercial airplane is impossible in the near future. Rough estimates predict that to happen in about 50 years.

There are, of course, many possible strategies related to how to discretise and solve the Navier –Stokes equations, differing in accuracy, efficiency, flexibility, parallel scaling etc. Here, we are focusing on large-scale simulations with a very high level of (numerical) accuracy. Therefore we used the code `nek5000` (Fischer *et al*., 2008), which is a computational fluid dynamics solver based on the spectral element method (SEM, see Deville *et al*., 2004) that is well known for its (spectral) accuracy, favourable dispersion properties, and efficient parallelisation. In `nek5000`, the incompressible Navier –Stokes equations are solved using a Legendre polynomial based discretisation. The equations are cast into weak form and discretised in space by the Galerkin approximation where the test and trial spaces are restricted to certain (and different) velocity and pressure spaces respectively, using the $P_N - P_{N-2}$ SEM discretisation. The non-linear terms are treated explicitly by third-order extrapolation (EXT3), whereas the viscous terms are treated implicitly by a third-order backward differentiation scheme (BDF3).

One of the most important aspects in `nek5000` is its extraordinary capability for massively parallel runs, having demonstrated good scaling on up to 200000 cores. In Figure 3 we show measurements that we obtained for the simulation of turbulent flow in a three-dimensional diffuser (Ohlsson, 2010). The specific machines utilised for the comparison were the Cray XE6 Lindgren and the AMD Opteron cluster Ekman at PDC (Stockholm), and the Blue Gene/P at the Argonne National Laboratory (ANL). These computers have quite different architectures: the Cray XE6 has dual 12-core nodes, Ekman is a distributed memory cluster with two quad-cores processors and full bisectional bandwidth (FBB) interconnect, and the Blue Gene/P has comparably slow

quad-core PowerPC nodes with a balanced network. The curves in Figure 3 show strong scaling for exactly the case used for the production runs presented in Ohlsson *et al.*, 2010, where a total resolution of approximately 220 million grid points was used. On all machines, we observed a very efficient usage of the hardware. The scaling is essentially linear up to 16384 cores on the Cray XE6 and up to 32768 cores on the Blue Gene/P, with efficiencies of about 90 %. It should be pointed out that for such a large number of cores (32768) there are less than 4 elements (~6700 grid points) present on each core, which puts high requirements on the efficiency of the global communication. After this point, the curves depart from the linear scaling, and we measure a speedup of 70 % on the Cray on 32768 cores and 77 % on 65536 cores.

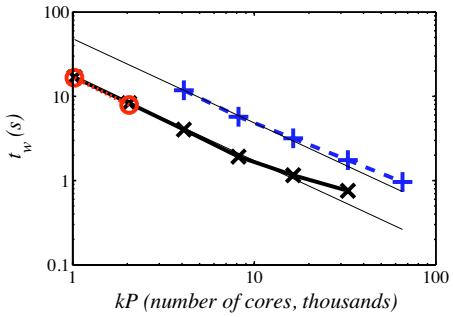


Figure 3: Wall time per time step for a fixed problem size (strong scaling) as a function of number of cores on Cray XE6, PDC (×), Blue Gene/P, ANL (+) and the AMD Opteron cluster Ekman, PDC (○). Ideal scaling is included for reference (solid line). Simulation performed by Ohlsson et al., 2010.

We maintain close collaboration with the main developer of `nek5000`, Dr. Paul Fischer at ANL, to maximise the performance of the code for our particular applications, and to contribute new features. Within the respective groups at KTH Mechanics, `nek5000` is used by about 15 graduate students in projects as diverse as the flow along real airplane wings, a jet in crossflow, Lagrangian particle motion in complex geometries, and the flow on a rotating disk; more details about some of these projects are given in Figure 6.

Using large-scale numerical simulations as a research tool can also be seen as an integral aspect of *e-Science*, in the sense that scientific progress is being promoted by computational infrastructure and tools. In particular, aspects such as algorithms, visualisation and parallelisation need to be continuously developed, and adapted to the latest computer architectures. Our research groups are therefore closely integrated into the Swedish e-Science Research Centre (SeRC). Furthermore, the code `nek5000` is also one of the applications that are part of the ongoing European project CRESTA[3]. This project, in which both PDC and Mechanics are actively involved, aims to make the whole process chain ready for exascale (exa = 10^{18}), including pre- and post-processing, software development/debugging, performance analysis etc. Also, we are engaged in pan-European activities related to supercomputer access. For instance, we have already been successful with the first Swedish PRACE (Tier-0) allocation[4] in 2011, and two DECI (Tier-1) allocations[5] were granted to researchers at KTH Mechanics.

3 Turbulent pipe flow

The flow of fluids in pipes with circular cross-sections is frequently encountered in a variety of environmental, technical and even biological applications. Typical examples of pipe flows can be found in urban drainage systems, transport of natural gas or oil in the energy sector (i.e. pipelines), or the flow of blood in veins and arteries. Accordingly, the understanding of flow physics in pipes has a direct and substantial impact on everyday life and an adequate knowledge of such flow problems will help in finding scientific methods to reduce drag and the like.

The study of turbulent pipe flows is closely related to finding the relation between the average flow velocity (i.e. the bulk flow) to the friction coefficient (or head loss), a relation of importance for all kinds of engineering calculations. Initially, Heinrich Blasius (a student of Prandtl) suggested a simple formula based on the so-called $1/7$ power-law approximation of the velocity profile, and more involved studies by Prandtl and Nikuradse finally lead to the famous *Moody diagram* (1944) which predicts the friction loss for both smooth and rough pipes.

As discussed above, the Reynolds number Re is the only non-dimensional parameter appearing in the Navier–Stokes equations. For pipe flow, two different measures of the Reynolds number are common: first, there is the *bulk Reynolds number* $Re_D = U_b D/\nu$, based on the pipe diameter, the mean (or bulk) velocity and the viscosity. Taking the characteristics of turbulence into account, another definition can be based on the ratio of the pipe radius and the smallest vortices close

to the wall, $Re_\tau = U_\tau R/\nu$. The latter *Re* is a convenient measure of the "intensity" of turbulence, as it establishes a connection between the integral scales (the pipe radius) and the size of the turbulent motions.

It is interesting to compute some Reynolds numbers of flows that we might be more familiar with. First of all, it is important to note that pipe flow below $Re_D = 2500$ is likely to be laminar, even though there is no hard threshold for turbulence transition. As an example, if you drink a can of soda through a straw you will reach $Re_D = 5000$. Blood in veins is about a factor of two below that, however pulsating creates additional complexity. In large pipelines systems for crude oil, such as the Trans-Alaska Pipeline System, the Reynolds number Re_D varies between 55000 and 340000 while the same parameter can reach values of the order of 10^7 for gas pipelines due to the low viscosity of gas in comparison to crude oil.

Of particular importance in flows delimited by solid walls is the near-wall region in which a large fraction of the drag stems from velocity fluctuations in a thin boundary layer adjacent to surfaces. Near-wall turbulence structures in wall-bounded shear flows primarily scale in terms of the so-called viscous length scale, which might be very small as Re is increased. However, according to recent experimental studies, very large-scale motions with lengths of $5R$ up to $20R$ are found in fully developed turbulent pipe flow (R being the radius). These structures, being strongest in the outer region, even extend throughout the layer and leave their footprint quite close to the wall. These large-scale structures are very energetic and active, and may at high *Re* dominate the flow altogether. Large-scale motions thus play an important role in the dynamics of turbulent pipe flows, indicating that a trustworthy experiment or simulation needs to include a rather long part of the pipe.

For physical experiments, pipe flow is the case which is easiest to realise as there are no artificial boundaries to be imposed except for the inflow and the outflow of the pipe. Therefore, pipe flow has been the prime canonical case for reaching high *Re*. As discussed previously, high *Re* can be obtained by either large diameter and high speed, or alternatively by low viscosity. These strategies are followed by two particular laboratory experiments worth mentioning here: the so-called SuperPipe at Princeton and the CICLoPE[6] project in which KTH Mechanics is a partner. In the SuperPipe, the highest $Re_D = 3.5 \times 10^7$ ($Re_\tau = 5.3 \times 10^5$) is reached by pressurising air in a comparably small pipe ($D = 13$ cm and a length of 26 m) to 180 bar, at the expense of very small (and hard to measure) turbulent structures. On the other hand, the ongoing CICLoPE project aims at building a 115 m long pipe with a diameter of 0.9m in a tunnel near Bologna (Italy), thereby reaching $Re_D = 2.3 \times 10^6$ ($Re_\tau = 40000$).

For fully resolved simulations it will not be possible to match numbers like these within the next decades. However, with the help of large computers, DNS is also increasing its *Re* into regions of practical relevance. For instance, our recent large-scale boundary-layer simulations performed on the Ekman cluster at PDC have become a widely used database (Schlatter *et al*., 2009, Schlatter & Örlü, 2010). Moreover, we could compare one-to-one simulations and experiments from the KTH wind tunnel (Örlü & Schlatter, 2012), and conclude that we have been able to replicate in the computer the exact same conditions down to the smallest scales. Such results can also be seen in the context of "numerical experiments", i.e. conducting experiments in a virtual wind tunnel (simulation). This simulation-based framework has some advantages compared to real experiments, and will certainly be an emerging area in the future.

Having mentioned that pipe flow is the most accessible canonical flow experimentally, it is quite the

Table 1: Details of the numerical simulations performed for the present project. To conclude all the simulations at the four Reynolds numbers a total of about 10 million CPU hours is needed, of which the simulation at the highest $Re_\tau = 1000$ takes up more than 80 %.

Re_D	# of elements	# of grid points	Re_τ	# of cores	Time/ time-step
37700	1264032	2.184×10^9	998.6	8192	8.7 sec.
19000	853632	437.0×10^6	548.1	4096	2.0 sec.
11700	237120	121.4×10^6	360.5	2048	1.1 sec.
5300	36480	18.67×10^6	182.2	1024	0.55 sec.

opposite situation for simulations. Due to numerical difficulties related to the cylindrical coordinates and the corresponding numerical singularity arising along the symmetry line, it is the only canonical flow case that has not yet been thoroughly studied using DNS, as opposed to plane channels and boundary layers. Starting with a classical paper about 15 years ago by Eggels *et al.*, 1994 at low Reynolds number, and a recent study by Wu & Moin, 2008, focusing only on mean-flow quantities, there are now a few ongoing projects numerically studying pipe flow with sufficient Reynolds number (in Australia, Korea, Italy, USA and Sweden); one of these is the present project. Table 1 gives an overview of our ongoing simulations at PDC (Lindgren). The goal of this series of simulations is to set up a database with well validated runs covering the range of $Re_\tau = 180$ to1000, all obtained in a long pipe ($L = 25R$) employing the same high resolution to capture the finest turbulent motions. Such data will be valuable not only to increase our knowledge of generic wall turbulence, but will also allow for the development of better models of turbulence for industrial applications. Furthermore, the current work is a complement to the previously mentioned KTH simulations of high-Reynolds number turbulent boundary layers and channels, and is also relevant in conjunction with the experimental studies within the CICLoPE project.

Figure 1 shows the evolution of the flow with Reynolds number: clearly the chaotic vortices get smaller, and move towards the wall where the turbulence intensity peaks. It immediately becomes clear why direct simulations of turbulence are very expensive in terms of grid resolution: even the finest motion needs to be resolved in order to obtain a correct picture of wall turbulence. This is further evidenced by Figure 2, which puts the turbulent vortices in relation to the pipe length. At this moderate Reynolds number, we can already distinguish at least two ranges of scales: smaller vortices making up the bulk of the turbulence, and also larger scales which feature a coherent length of about 4-8 radii. It is in particular the origin and mutual interaction of these scales that still awaits conclusive explanation. Other questions arise related to the shape of the turbulent vortices: is there a generic alignment of eddies with certain shapes, for instance hairpin-like structures, or is there more or less chaotic organisation of all the swirling motion? We expect that with the present set of simulations at least partial answers will be found.

Further insight into the vortical structures in the flow can be gained from Figure 4 which shows a cross-cut of the axial vorticity ω_z. Again, the very active near-wall region is apparent, dominated by intense counter-rotating vortices. These vortices are connected to the famous near-wall streaks with a spacing of 100 viscous units, that are ubiquitous in any wall-bounded flow. Furthermore, plots of the vorticity can be used to establish the adequacy of the numerical mesh, as wiggles would contaminate the vorticity field in case of insufficient resolution.

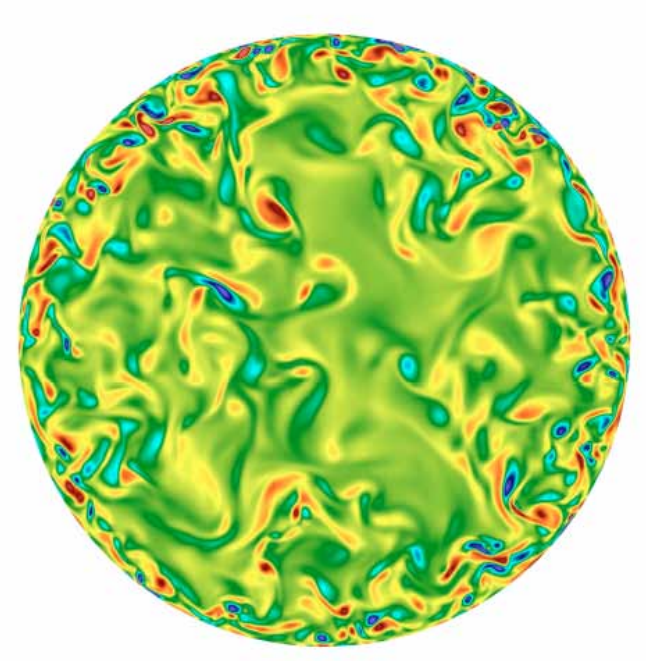


Figure 4: The instantaneous axial vorticity ω_z is displayed for $Re_D = 19000$ ($Re_\tau = 550$). The local rotation rate of a fluid element is given by the vorticity which is twice the angular velocity of that element. As such, the vorticity is a measure of the local "spin" of the fluid element. Here, the flow is clearly dominated by strong vortical motion close to the walls where small but intense counter-rotating vortices are observed. These vortices transport fluid to and from the wall-region and substantially affect the flow field. In the regions further away from the wall mainly larger-scale motions persist. Note that the resolution of the smallest vortices is crucial for faithful DNS. In particular, for high-order methods the appearance of wiggles is a sign of insufficient resolution, which is avoided in the present setup.

Finally, we present quantitative results from our simulations, namely the mean velocity profiles U_z for the various

simulation, see Figure 5. It is amazing to realise that the axial mean velocity of the turbulent flow, instantaneously being the chaotic and intertwined ensemble of vortices as shown in Figure 2, follows the comparably simple law of the wall, namely $U_z^+ = (1-r)^+$ close to the wall and $U_z^+ = \kappa^{-1}\ln(1-r)^+ + B$ further away. Even though an approximate derivation of these laws going back to von Kármán (1930) is quite straightforward and part of any turbulence course, a conclusive theoretical justification is missing; in particular the values for the coefficients κ (the so-called Kármán constant) and B are the subject of ongoing discussion.

The present simulations will of course produce a lot of data, both in terms of flow statistics but also instantaneous velocity fields for subsequent analysis. For instance, at the highest *Re*, each individual velocity field is about 100 GB, and we are storing about 200 fields, which totals to about 20 TB. Such capacity is available in Sweden through the Swestore project which we are using for these simulations. Furthermore, we are collaborating within SeRC in order to extend visualisation techniques for such large data sets, using various techniques such as interactive visualisation, volume rendering, stereo (3D) effects etc.

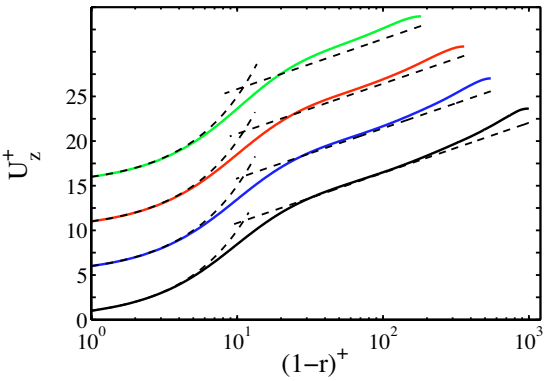
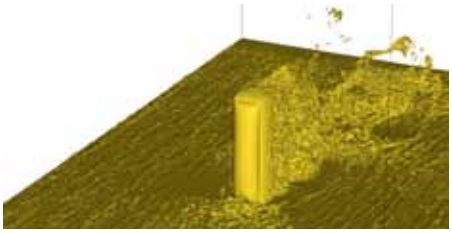


Figure 5: Profiles of the mean axial velocity component U_z^+ taken from the present simulations together with the so-called law of the wall (dashed lines); increasing Re from top to bottom, shifted by $\Delta U_z^+ = 5$ In the viscous sublayer for $y^+ = (1-r)^+ < 5$, the profiles naturally coincide with the linear relation $U_z^+ = y^+$, while at larger distances from the wall for $y^+ > 30$, it is readily observed that the mean velocity profiles more and more approach a logarithmic behaviour $U_z^+ = \kappa^{-1}\ln(1-r)^+ + B$ (here $\kappa = 0.41$ and $B = 5.2$). The robustness of the log-law in a variety of wall-bounded flows can be considered one of the most remarkable results in turbulence theory.

(a)

(b)



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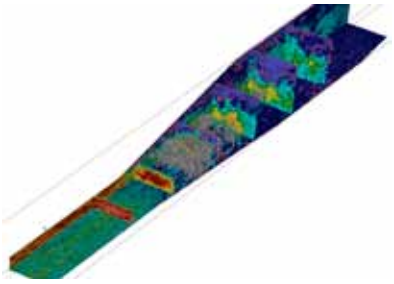
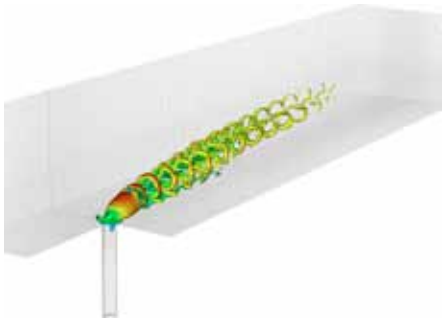


Figure 6: Other flow cases studied with `nek5000`*:*
(a) Transition to turbulence on an air foil in order to investigate the effect of free-stream turbulence on the boundary layer (receptivity). Understanding the transition process on wings is essential for future development of energy efficient aircrafts (Figure by Mohammad Hosseini).
(b) As a part of the Canadian CFD-challenge in 2012, the flow around an obstacle mounted vertically on a flat plate has been studied by Malm et al., 2012. The obstacle has a quadratic cross-section of diameter d and a height of 4d which yields a length-to-diameter ratio of 4. Such a configuration can be considered as a simplified model of a skyscraper. The figure shows isosurfaces of instantaneous streamwise velocity.
(c) The effect of pressure induced separation on the flow field inside a 3D diffuser is studied via well-resolved DNS by Ohlsson et al., 2010. The figure shows instantaneous streamwise velocity. This flow problem is selected due to its widespread engineering applications and the presence of reliable experimental data for comparison, and the problems of turbulence models to correctly predict this separated flows.

(d)



(d) Vortical structures in a jet-in-crossflow with a mesh including a flush-mounted pipe. This case consists of a jet of fluid exiting a nozzle and interacting with the surrounding fluid. It is a flow of high practical relevance with a number of applications like smoke and pollutant plumes, fuel injection and mixing or film cooling (Figure by Adam Peplinski).

References

• Cipra, B. 1996 A new theory of turbulence causes stir among experts. Science 272, 951.

• Eggels, J. G. M., Unger, F., Weiss, M. H., Westerweel, J., Adrian, R. J., Friedrich, R. & Nieuwstadt, F. T. M. 1994 Fully developed turbulent pipe flow: a comparison between direct numerical simulation and experiment. J. Fluid Mech. 268, 175 –209.

• Davidson, P. A., Kaneda, Y., Moffatt, K. & Sreenivasan, K. R. (editors) 2011 A Voyage Through Turbulence. Cambridge University Press.

• Deville, M. O., Fischer, P. F. & Mund, E. H. 2004 High-Order Methods for Incompressible Fluid Flow. Cambridge University Press.

• Fischer, P. F., Kruse, J., Mullen, J., Tufo, H., Lottes, J. & Kerkemeier, S. 2008 NEK5000: Open source spectral element CFD solver. https://nek5000.mcs.anl.gov/index.php/MainPage.

• Jeong, J. & Hussain, F. 1995 On the identification of a vortex. J. Fluid Mech. 285, 69 –94.

• Malm, J., Schlatter, P., Henningson, D. S., Schrader, L.-U. & Mavriplis, C. 2012 Spectral element simulation of flow around a surface-mounted square-section cylinder. in CFDCS 2012 Challenge, Canmore, May 9-11.

• Ohlsson, J., Schlatter, P., Fischer, P. F., & Henningson, D. S. 2010 Direct numerical simulation of separated flow in a three-dimensional diffuser. J. Fluid Mech. 650, 307 –318.

• Schlatter, P., Örlü, R., Li, Q., Fransson, J. H. M., Johansson, A. V., Alfredsson, P. H. & Henningson, D. S. 2009 Turbulent boundary layers up to Re_θ=2500 studied through simulation and experiment. Phys. Fluids 21, 051702.

• Schlatter, P. & Örlü, R. 2010 Assessment of direct numerical simulation data of turbulent boundary layers. J. Fluid Mech. 659, 116 –126.

• Wu, X. & Moin, P. 2008 A direct numerical simulation study on the mean velocity characteristics in turbulent pipe flow. J. Fluid Mech. 608, 81 –112.

• Örlü, R. & Schlatter, P. 2012 Comparison of experiments and simulations for zero-pressure gradient turbulent boundary layers at moderate Reynolds numbers. Submitted.

Acknowledgments

Dr. Paul Fischer (Argonne National Laboratories) is gratefully acknowledged for providing the `nek5000` code, and for assistance setting up the simulations. Development of the nek5000 algorithm is supported by the U.S. Department of Energy Applied Mathematics Research Program.

We would also like to thank Azad Noorani, Drs. Geert Brethouwer, Ramis Örlü and Adam Peplinski, and Profs. Arne Johansson and Dan Henningson for many discussions on DNS of turbulent flows. Financial support is provided by the Göran Gustafsson Foundation and the Swedish e-Science Research Centre. The computer time was made available by the Swedish National Infrastructure for Computing (SNIC) and by the upcoming DECI Project PIPETURB.

Footnotes

1 Lewis Fry Richardson's famous rhyme from 1922: Big whorls have little whorls, Which feed on their velocity; And little whorls have lesser whorls, And so on to viscosity (in the molecular sense).

2 The expression "direct numerical simulation" was introduced by Steven Orszag in 1970 to express the fact that the flow solution is obtained directly from the governing Navier–Stokes equations.

3 Collaborative Research into Exascale Systemware, Tools & Applications — http://cresta-project.eu

4 Partnership for Advanced Computing in Europe — www.prace-project.eu

5 Distributed European Computing Initiative

6 Center for International Cooperation in Long Pipe Experiments — www.ciclope.unibo.it

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Heating up Chemistry with a Cray

Gert Svensson, PDC and Johan Söderberg, Hifab, Stockholm

Have you ever burned your knees when using a laptop? Bearing in mind that a supercomputer at PDC can use around thirty thousand times as much power as an ordinary laptop, try to imagine the kind of heat that is produced in the computer room at PDC. Now, how could all that extra heat be put to good use?

That was what we were wondering some years ago when planning began at PDC to install a further supercomputer during 2010. The new supercomputer was to be a Cray XE6 with 16 cabinets – which would nearly double the power consumption at PDC from around 800 kW to 1 300 kW, and consequently produce a great deal of additional heat.

We wanted to find a way to make use of the extra heat from the new Cray in a manner that contributed positively to the environment. Ideally, we were looking for a method of using the heat that would also refund some of the cost of the additional power that would be needed to run the Cray.

At the time, the PDC computer room was cooled using two methods: low density equipment was cooled by ambient cooling from ordinary Computer Room Air Conditioner (CRAC) units, and high density equipment was cooled with hot aisle encapsulated cooling from APC. Both methods used cold water from the Stockholm area district cooling system. That system was already quite environmentally friendly: the company providing the water that was used for cooling actually produced local district heating by using heat pumps to extract the additional heat from the returned (and thus heated) cooling water. If the company needed to provide additional cooling, they used sea water.

Although using district cooling was environmentally friendly, it was not financially efficient. Instead of being reimbursed for any heat that was produced, KTH would have had to pay around 0.30 SEK/kWh (at today's prices) to get rid of the excess heat energy. Moreover, during the cold season in Stockholm, KTH would have had to pay for district heating from the same energy company (currently at a rate of 0.45 SEK/kWh).

Therefore we decided to try to use the excess heat from the new Cray to heat one of

Custom made ducts on top of the Cray lead the air through industrial heat exchangers.

Staff Focus

Stefano Markidis

Stefano is a Postdoctoral Fellow at PDC. He received an M.S. degree from Politecnico di Torino (Italy) and a Ph.D. degree from the University of Illinois at Urbana-Champaign (USA). Before joining PDC, he worked as a researcher at the Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, and as a Capita Selecta Professor at the Catholic University of Leuven. In 2005 Stefano received an R&D100 award as part of the team that developed the CartaBlanca multi-physics code at the Los Alamos National Laboratory. At PDC he is part of the CRESTA EC-FP7 project to investigate the suitability of new programming models for the next generation exascale supercomputers. His research interests include the investigation of novel programming models for HPC, and innovative algorithms for parallel computing.

Staff Focus

Zeeshan Ali Shah

Zeeshan started studying IT in 1997 - beginning with a Diploma and progressing to a Masters degree in Software Engineering from SZABIST, Pakistan. Zeeshan was awarded a Gold medal for attaining the first merit position in the Masters of Computer Science programme.

In 2005 Zeeshan was admitted to a Masters program in Information Security at KTH during which he worked with FOI for a year, and then moved to PDC under the Grid Computing Group. For the last two years he has been managing the Cloud Computing at PDC and doing research in Security. Outside work, Zeeshan contemplates the Quran and enjoys touring the countryside and mountains.

the KTH buildings close to PDC. We formed a project group comprised of PDC and Akademiska Hus (which owns the KTH buildings), along with the consulting companies Sweco, Incoord and Hifab. The project group then investigated different methods for heating other buildings using the heat from the new Cray.

A major problem was that the two methods of cooling that were being used by PDC at the time produced a coolant temperature of 18 °C which was too low to heat normal buildings. That temperature could have been increased using heat-pumps, however that would have involved a further increase in the use of electricity. Calculations showed this approach to be barely economical.

The air cooled version of the Cray system takes in cold air (at less than 16°C) from under a raised floor and passes that air through the racks of computer components. The air becomes heated to temperatures of 35 – 45 °C, and is then passed out at the top of the racks. Hence the air coming from such a Cray system is at a high enough temperature to provide heating of the incoming air for a building. The question was how to extract heat from the hot air above the Cray and transport it to another building. Since various steps in the process would each decrease the temperature somewhat, it was important that the air would still be hot enough for heating the building.

Investigations of standard industry air-water heat exchangers showed that such units could be used, and would produce water temperatures suitable for use in a building. However the problem was where to place such units in the computer room as there was limited space. Placing the units about the computer racks would have solved the space issue, but could have had unfortunate consequences if there was an accident and water leaked out of the exchangers onto the computer racks.

Our final solution was therefore to hang the heat exchangers from the ceiling above the Cray, but slightly displaced so the exchangers were not directly above the computer racks. Although this did not completely eliminate the possibility of problems from leakages, it reduced the consequences of a small leakage considerably. Hot air from the top of the Cray was then fed to the suspended heat exchangers via chimney-like ducts.

The next question was to decide which building at KTH would be heated with the recycled heat. The project group investigated several alternatives and found that a nearby building which housed the Chemistry Laboratory at KTH was a good candidate. First of all the building was undergoing renovations at the time, so the changes needed for using the recycled heat could be incorporated into the renovation process. Secondly that particular building required large amounts of air to ventilate potentially dangerous fumes from the Chemistry laboratories without there being any recovery of heat to the fresh air in conventional ways.

The air-water heat exchangers hanging from the computer room ceiling would take the hot air from the Cray at 35 – 45 °C and cool it down to around 21 °C. That cooled air would then be expelled from the heat exchangers back into the computer room. Meanwhile, the water in the heat exchangers would have been heated up to around 30 – 35 °C. That heated water would

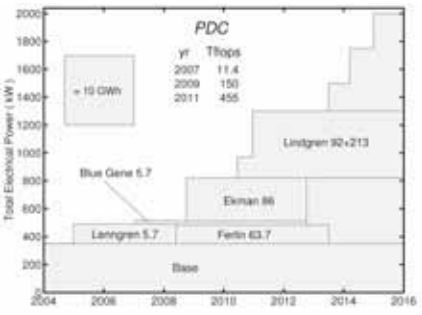
be circulated inside a closed circuit that could be cooled by three different heat exchangers that were placed in the basement outside the computer room. The water could be cooled by a combination of those three heat exchangers. One of the heat exchangers was dedicated for heat re-use with the Chemistry building, another used the Stockholm district cooling system, and the final heat exchanger could use ordinary cold tap water (as a back-up in case the other two heat exchangers failed to produce cold enough water).

Next we needed to find a suitable way to transfer the heat recovered from the Cray to the Chemistry building. One option for transferring the heated water to the Chemistry building was to lay new pipes between the buildings, however we assumed that would be too expensive to be viable. We therefore considered using the existing pipes in the KTH cooling network to transfer the recycled heat.

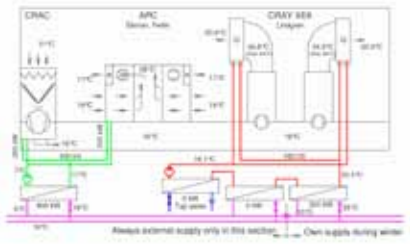
The KTH cooling grid is actually built as a network of loops and fortunately the PDC computer room is supplied from the same loop as the Chemistry building. It is possible to close valves in the network so a section of that particular loop is isolated with the PDC computer room upstream of the Chemistry building. Essentially this means that – with the addition of some components to the network - heated water can be sent from the PDC computer room to the Chemistry building via the existing cooling grid at KTH. Furthermore, cooled water (coming out of the Chemistry building) can be sent into the PDC computer room cooling system. However, just doing that is not enough as the amount of heat that the Chemistry building requires varies during the year, so under some conditions the Cray may need more cooling than can be provided by the Chemistry building.

When the outdoor temperature is over 10 °C this heat-recycling system cannot be used at all and the Stockholm district cooling system provides all the cooling for the Cray. From 0 - 10 °C the Chemistry building provides some cooling for the Cray with additional cooling coming from the Stockholm district cooling system through the second heat exchanger mentioned earlier. In sub-zero winter temperatures, the system really comes into its own and all cooling for the Cray is supplied by the Chemistry building.

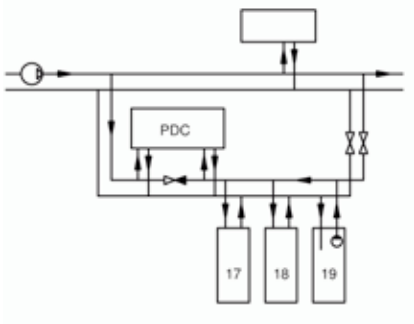
This system for heating the Chemistry building with waste heat from the Cray became fully operational during the winter of 2011-12. It has been effective in providing environmentally friendly cooling for the new Cray that also offsets part of its operational costs. However some optimizations are still required to reach the initially calculated target savings which showed that PDC should be able to send around 1 300 MWh of energy per year to the Chemistry building. This would reduce the PDC usage of district cooling by 1 300 MWh annually which corresponds to a savings of 390 000 SEK per year at current rates. Due to the fact that the Chemistry building already has an internal heat re-use system with around 50 % efficiency, their savings in district heating are 50 % of 1 300 MWh, or 650 MWh, which is equivalent to a saving of around 290 000 SEK at today's prices. However, as the rate is expected to rise dramatically in the near future, the savings from the heat re-use system should increase significantly.



Power consumption at PDC.



Layout of cooling in PDC: Ambient cooling via CRAC-units (left) and hot aisle APC connected via the pipe system KB104 to district cooling (with back-up). Pipe system KB105 serves the Cray racks with high temperature cooling downstream of the check valve backed up by conventional district cooling and tap water cooling.



Ring shaped cooling system at the campus. The check valve closes and a self-supplying section is formed once building 19 (the Chemistry building) is capable of taking care of all waste heat in the section. This happens at about 0 °C outdoor temperature. PDC uses coolant from both sides of the check valve.

Cloud Computing at PDC

Åke Edlund, PDC

The new PDC cloud computing cluster is currently hosting a number of Swedish and international users on a daily basis. Even if its 205 GigaFlops make it a dwarf in the PDC world, its easy-to-use flexible environment makes it an interesting experiment for the future. Through a number of cloud projects, and our involvement in the SNIC Cloud, PDC continues to gather knowledge in this area. From an earlier focus on infrastructure - how to get things in place, and how to make everything work properly - we are now also looking higher up the stack to the platform and service levels. In this new additional direction, the PDC cloud is currently focusing very much on how to help our bioinformatics users - something we have experience from previously (for example, SBC). One example of this work is the recently released Galaxy-as-a-Service. The cloud work is being performed in collaboration with a number of partners, especially through the SciLifeLab community.

Apply for Parallel Programming Support through SNIC

SNIC now has a number of application experts in Computational Science and Parallel Programming who are available to help with your code development projects. For example, these experts can help with debugging, profiling, and tracing, as well as with simpler optimization, parallelization or code porting tasks. Up to ten full workdays of assistance may be allocated to each request. The requests are handled in turn as the experts have time available.

Any researcher affiliated with a Swedish tertiary institution (including Ph.D. students) can submit a request for Parallel Programming support.
It may be possible to allocate help to projects that require more assistance. If you have a project that might require more than ten workdays of assistance, please submit a request, so an application expert can assess how much assistance would be required. We can then discuss the options for assigning an application expert to the project for a longer term.

Please submit requests to application-support@snic.se.
More information, see docs.snic.se/wiki/Support.

How SNIC-PDC fosters Swedish research through the PRACE Research Infrastructure

Lilit Axner, PDC

The Partnership for Advanced Computing in Europe (PRACE) was set up to support European global leadership in public and private research and development. To this end, PRACE makes it possible for researchers from all over Europe to request time on European High-Performance Computing resources for running research.

The process of requesting time is handled through calls for applications from researchers to access European HPC ecosystems. Researchers can request various types of access to PRACE resources:

- Programme Access is available to major European projects or infrastructures that can benefit from PRACE resources and for which Project Access is not appropriate.
- Project Access is intended for individual researchers and research groups (including multi-national research groups) and allows access to the resources for a period of one year. Calls for Proposals for Project Access are issued twice yearly.
- Preparatory Access allows researchers to have relatively short-term access to resources to prepare proposals for Project Access. Applications for Preparatory Access are accepted at any time (www.prace-ri.eu/Call-Announcements).

In addition to these PRACE calls, researchers can also request access to HPC resources via Distributed European Computing Initiative (DECI) calls. DECI was set up to enhance the impact of European science and technology at

the highest level. It enables European researchers to obtain access to the most powerful national (Tier-1) computing resources in Europe, regardless of their country of origin or work. If requested, DECI also provides up to six months expert help with scalability and code performance.

The first implementation phase of PRACE (PRACE-1IP) started in September 2010. Since then, there has only been one call open for Programme Access, while PRACE calls for Project Access and DECI calls have been open every six months. Preparatory Access calls have been open constantly since that time.

In Sweden, PDC has been active in PRACE since the early days of the project in 2007, and was involved even earlier when the concept of a pan-European ecosystem was initiated under a different name.

PDC has continued its extensive activities as an active EU partner within PRACE. One of the major roles of PDC is to provide 10% of the yearly computing capacity of the Lindgren system as a resource exchange within DECI, thus giving Swedish applicants an opportunity to compute on fare-share bases at the other EU centers' Tier-1 systems that have different architectures.

PDC has also taken an active role in promoting PRACE calls and disseminating information about PRACE calls. Since September 2010 there have been five PRACE calls open, including three DECI calls. Application experts at PDC contacted many scientists, and helped them to submit application forms for these calls. As a result of these efforts, seven DECI applications from the Royal Institute of Technology (KTH), Linköping University (LiU) and Stockholm University (SU) were granted computing hours in the first two DECI calls. These projects were run on Tier-1 supercomputers in the Netherlands, Finland, Scotland, Switzerland and France. (The results of the third DECI9 call will be known around September 2012.) Moreover, a Swedish application from KTH for Project Access to one of the six European Tier-0 systems has been successful - the researchers were granted 49 million CPU hours on the JUGENE, GAUSS/FZJ BG/P system in Germany.

There has also been a successful application for Preparatory Access from the KTH Department of Computational Biology, CSC. This very interesting project was about visualizing the output from large-scale brain simulations and involved:

1) creating visualizations using large-scale simulation output from existing neural simulation codes, and

2) making extensions to some of the existing codes to allow interactive runtime (in-situ) visualization.

Tight collaboration with experts from three PRACE partners: The Netherlands, Serbia and Bulgaria produced excellent results.

The successful Swedish applications to date are listed to the right. We hope to see more Swedish projects approved when the results of the PRACE 5th call (including DECI) are announced later this year.

Tier-0 Project Access

Project name: REFIT - Rotation effects on flow instabilities and turbulence
Project leader: Arne Johansson, KTH Department of Mechanics, Sweden
(www.prace-ri.eu/PRACE-2nd-Regular-Call)

Preparatory Access Type C

Project name: Visualization of output from Large-Scale Brain Simulations
Principal Investigators: Prof. Anders Lansner, Dr. Simon Benjaminsson and David Silverstein
Research field: Computational Biology

DECI7 Tier-1 Project Access

1. Project Name: DiSMuN (Diffusion and spectroscopical properties of multicomponent nitrides)
Principal Investigator: Prof. Igor Abrikosov
Research area: Materials Science
2. Project Name: SPIESM : Seasonal Prediction Improvement with an Earth System Model
Principal Investigators: Dr Colin Johns and Prof. Francisco Doblas-Reyes
Research field: Earth Sciences and Environment
3. Project Name: MUSIC
Principal Investigator: Dr. Mikael Djurfeldt
Research field: Computational Neuroscience
4. Project Name: SIVE-2
Principal Investigator: Prof. Erik Lindahl
Research area: Biosciences: molecular dynamics simulation of viral entry

DECI8 Tier-1 Project Access

1. Project Name: PIPETURB - Large scale simulation of turbulent pipe flow
Principal Investigator: Dr. Philipp Schlatter
Research area: Engineering, Fluid Dynamics
2. Project Name: CANONS - Comprehensive Ab initio studies of Nitride and Oxide fuels and Nuclear Structural materials
Principal Investigator: Dr. Pär Olsson
Research field: Materials Science
3. Project Name: MBIOMARK - Multifunctional biomarkers for electron paramagnetic resonance imaging
Principal Investigator: Dr. Zilvinas Rinkevicius
Research area: Materials Science

The next issue of this newsletter will feature an in-depth article elaborating on the PRACE project.

PDC Related Events (Sponsored/Associated)

PDC Summer School 2012:
Introduction to High Performance Computing

20-31 August 2012, KTH Main Campus

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

NordiCloud:
Nordic Symposium on Cloud Computing and Internet Technologies

August 20-21, 2012, Helsinki, Finland

Åke Edlund is one of the co-chairs.

www.nordicloud.net Co-located with WICSA/ECSA 2012 www.wicsa.net

CRESTA meeting

September 11-12, 2012, KTH main Campus, Stockholm

The main topic of the next CRESTA meeting will be software development for the next-generation exascale super-computers. Further information will be available soon on the CRESTA website.

cresta-project.eu/

CECAM ScalaLife Workshop: High Performance Computing in Computational Chemistry and Molecular Biology: Challenges and Solutions provided by ScalaLife project

October 3-5, 2012, CECAM-HQ-EPFL, Lausanne, Switzerland

ScalaLife has invited renowned life scientists from Europe and the USA to discuss recent advances in large scale simulations and showcase their latest results. The workshop will also present the newest developments in three life science software packages: GROMACS, DALTON and DISCRETE.

The workshop features multiple hands-on sessions, giving the participants the opportunity to practice the modelling capabilities of the three software packages. These sessions will also include user-clinics, a unique opportunity for users to bring in their own problems and discuss the challenges they face in modelling with the developers of these packages.

The number of participants is limited. There is no attendance fee. Deadline for registration is the 1st of September.

www.scalalife.eu/content/cecam

www.cecam.org/workshop-0-672.html

Sources

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

CERN 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 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 tinca.pdc.kth.se/communityevents/all

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

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

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

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