



No.2 2015

PDC Center for High Performance Computing

Business Unit Newsflash

Welcome to the second PDC Business Newsflash!

The newsflashes are issued in the [PDC newsletters](#) or via the [PDC business email list](#) in accordance with the frequency of [PDC business events](#). Here you will find short articles about industrial collaborations with PDC and about business events relevant for high performance computing (HPC), along with overviews of important developments and trends in relation to HPC for small to medium-enterprises (SMEs) and large industries all around the world.

SMEs Can SHAPE-up for HPC

The [PRACE Partnership for Advanced Computing in Europe](#) Infrastructure provides world class high performance computing (HPC) and data management resources and services to further European research and development. In Sweden, the [Swedish National Infrastructure for Computing \(SNIC\)](#) is the organisation responsible for helping Swedish researchers to access the PRACE resources and PDC is the SNIC centre that coordinates this, which means that **PDC plays a very active role in PRACE projects – both representing the interests of Swedish HPC users within the infrastructure and promoting Swedish HPC research.**

While many people are aware of the PRACE programmes that provide resources for academic research, you may not be aware that PRACE also runs a program to help European small to medium-sized enterprises (SMEs) take advantage of the innovation possibilities opened up by HPC techniques and technology. **This SME HPC Adoption Programme in Europe is known as**

SHAPE. The second SHAPE Call for Proposals was held earlier this year and supported eleven projects from European SMEs. These companies will receive support from PRACE and its partners to assess how the use of HPC can increase their competitiveness.

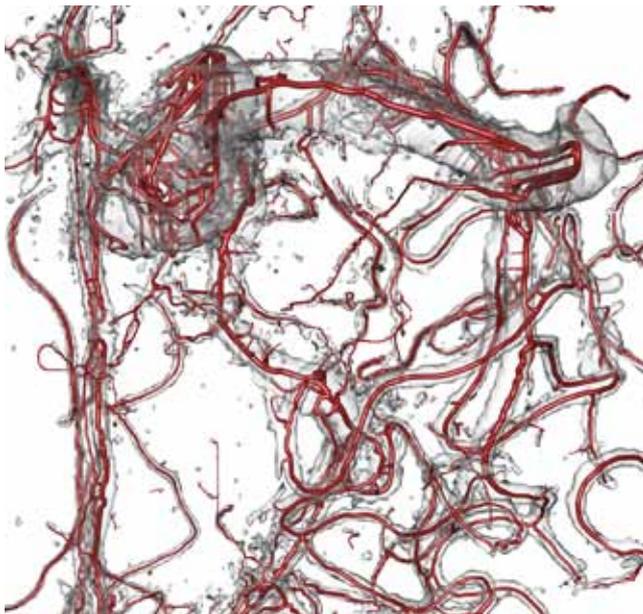
The next SHAPE call is expected to be opened in November 2015 and thus the PDC Business Unit is inviting interested SMEs to contact us now in order to prepare to engage in the upcoming SHAPE call. We can help you with the application process if you are thinking of applying to the next SHAPE call.

This is a great opportunity for Swedish SMEs to get access to the **most powerful European academic systems and excellent HPC software experts** in scalability and optimization techniques – and all free of charge! For further information, please contact us via email: business-unit@pdc.kth.se.



New Professor of Visualization at KTH

If you think about how the temperature or the values of stocks change over a day or a week, we all know it is easier to “see the bigger picture” of what is happening when we look at a graph, rather than a (boring) table of numbers. When it comes to the kinds of calculations that are being performed on supercomputers – for example, to simulate changes in the climate or the way that molecules in our bodies respond to new chemicals – these produce huge amounts of data that effectively consist of many different tables of numbers. It can be almost impossible to grasp what is going on just by looking at the numerical data that is churned out... and that is why we need computer-generated images that represent these vast amounts of complex information in easy-to-understand ways. **Producing such images is known as “scientific visualisation” and generating these types of images is not easy.** You cannot just draw a line the way you can to create a simple graph – visualisations often need to show multi-dimensional information, and hence there is often a lot of complex mathematics going on in the background to produce images with perspective.



Filigree structures that have been segmented in a blood vessel data set

Tino Weinkauff, new professor at HPCViz

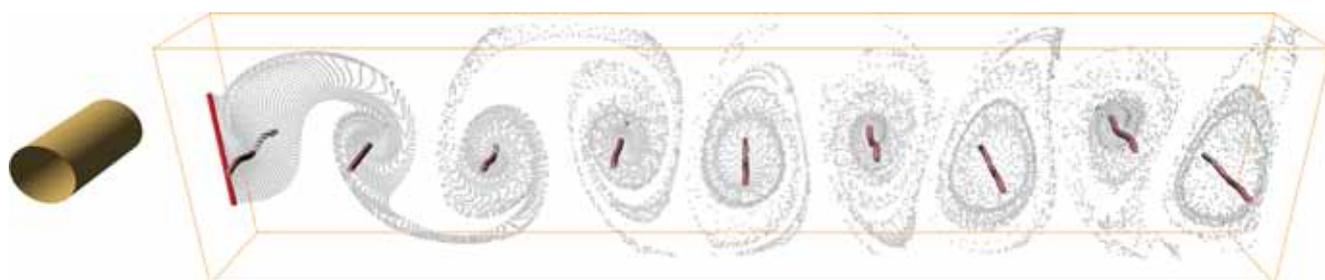


If you need to produce visualisation images to help with your research and development, Tino Weinkauff may be the man you need. Tino recently joined the School of Computer Science and Communication at the KTH Royal Institute of Technology as the Head of the Visualization group, which is part of the [Department of High Performance Computing and Visualisation \(HPCViz\)](#). Prior to coming to Sweden, Tino was a Senior Researcher and the Head of the independent research group on “Feature-Based Data Analysis for Computer Graphics and Visualization” at the Max Planck Institute for Informatics in Saarbrücken, Germany. In addition Tino has worked at the Courant Institute of Mathematical Sciences, New York University, USA and the Zuse Institute in Berlin, Germany, which is an interdisciplinary research institute for applied mathematics and data-intensive high performance computing. His doctorate on the “Extraction of Topological Structures in 2D and 3D Vector Fields” was undertaken at the Otto von Guericke University in Magdeburg, Germany.

Tino explained that, in his new position at KTH, “We do state-of-the-art research in visualization and feature-based data analysis. We target data from domains such as fluid dynamics and life sciences with methods ranging from offline feature extraction to interactive data analysis. Examples are vortex extraction and tracking in flows, or segmentation of filigree structures in volume data sets. Our visualizations

can be presented on a huge screen which provides great insights into intricate data.”

If you are interested in using the facilities at HPCViz or need help generating visualisations, please let the PDC Business Unit (business-unit@pdc.kth.se) know what you need to do and we will work with you to put you in touch with people who can help with visualisation in your research area.



A visualisation showing tracked vortices in an unsteady flow behind a cylinder

CFD with STAR-CCM+ Now Scales Brilliantly on PDC's Cray Supercomputer

Two of PDC's collaborative partners, CD-adapco and the National Center for Supercomputing Applications (NCSA) at the University of Illinois, recently proved that industrial use of computational fluid dynamics (CFD) can benefit from today's most advanced supercomputers. Together they set a new world record by scaling CD-adapco's flagship simulation tool, STAR-CCM+[®], to 102,000 cores on the NCSA's Cray supercomputer.

STAR-CCM+ is a comprehensive multidisciplinary engineering simulation tool used across many industries to stimulate innovation and to lower product development costs. CD-adapco joined with the NCSA and the supercomputer manufacturer Cray to push the code to new heights and address the ever-increasing demands of larger models and fast turnaround time.

The result of this collaborative effort over the past eight months was a steady increase in scaling – from a 105 million cell model running

on 13,000 cores to a 1 billion cell model hitting the 102,000-core peak. The 1 billion cell model was 93% efficient on 60,000 cores, with 84% efficiency on 71,000 cores, 79% on 79,000 cores, and 75% on 102,000 cores. After the tests, the NCSA senior computational resource coordinator who led this extreme benchmarking project explained that these results show that even users who run on lower core counts can benefit from reduced runtimes – thus the code will scale well on the 53,632 Intel Haswell cores of PDC's Cray XC40, Beskow.

CD-adapco offers licenses that are completely uncoupled from the number of compute cores used in parallel to solve a problem. This is an important factor when planning to make industrial use of supercomputers – otherwise increasing license costs could become an obstacle. STAR-CCM+ can be run for industry use on Beskow at PDC, with on-demand licensing lowering the cost barrier for Swedish industrial research. For more information about running CFD simulations at PDC, please contact us: business-unit@pdc.kth.se.

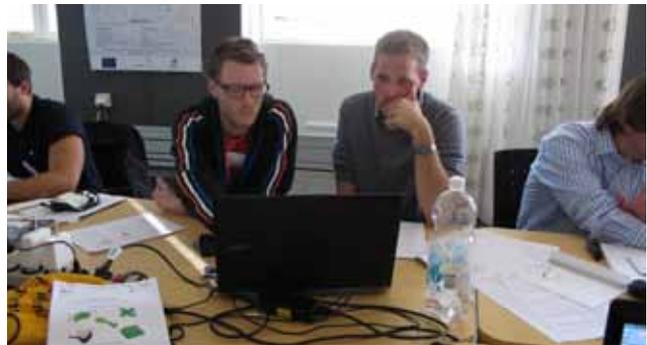
OpenFOAM and Comsol Workshop for Industry Research

Recently PDC, together with PRACE, organized a workshop on **OpenFOAM and Comsol MultiPhysics** that was specifically geared for researchers from industry. The workshop, which was held at PDC and ran from the 23rd to the 25th of September 2015, focused on HPC aspects of both pieces of software and on their parallelization techniques. The speakers were Anders Ekeröth and Mikael Fredenberg from COMSOL (which produces an interactive environment for modelling and simulating scientific and engineering problems) and Roger Almenar from the ESI Group (who are well-known experts in the area of virtual production engineering to support industrial innovation).

Anders has been with COMSOL since 1999, where he started out in the development department. He currently works with global technical support and product development in fluid mechanics at the Swedish office of the company, which is in Stockholm. Mikael has an M.Sc. in chemical engineering from the University of Lund. His specialty is in the areas of heat transfer and mass transfer. He works as a Sales and Support Engineer at COMSOL in the Stockholm office. Roger is currently Business Development and Project Manager for OpenFOAM. He has been

supporting customers in Computational Fluid Dynamics (CFD) since 1999, and with OpenFOAM since 2007.

The workshop had a large portion of hands-on sessions that focused on practical tips and tricks for improving scalability, load balancing and performance. During the workshop, participants were given access to the Beskow PRACE-Tier-1 system and the Tegner pre- and post-processing system, both of which are based at the PDC Center for High Performance Computing at the KTH Royal Institute of Technology in Stockholm. The workshop participants appreciated the opportunity to use Beskow, which is currently the fastest academic supercomputer in the Nordic countries. The workshop was well attended with around 20 participants from different countries.



OpenFOAM and Comsol workshop, 23-25 September 2015

Need Help with Your HPC Research?

PDC can help with scaling your industrial program codes and mathematical models for your company's benefit to make use of the latest technologies that are available today. If you do not have the most up-to-date computing facilities at hand, we also offer assistance and advice on gaining access to, and making effective use of, today's latest advancements in hardware and software, including our new compute infrastructure. Contact our Business Unit for more information!

Beskow, PDC's Cray XC40



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