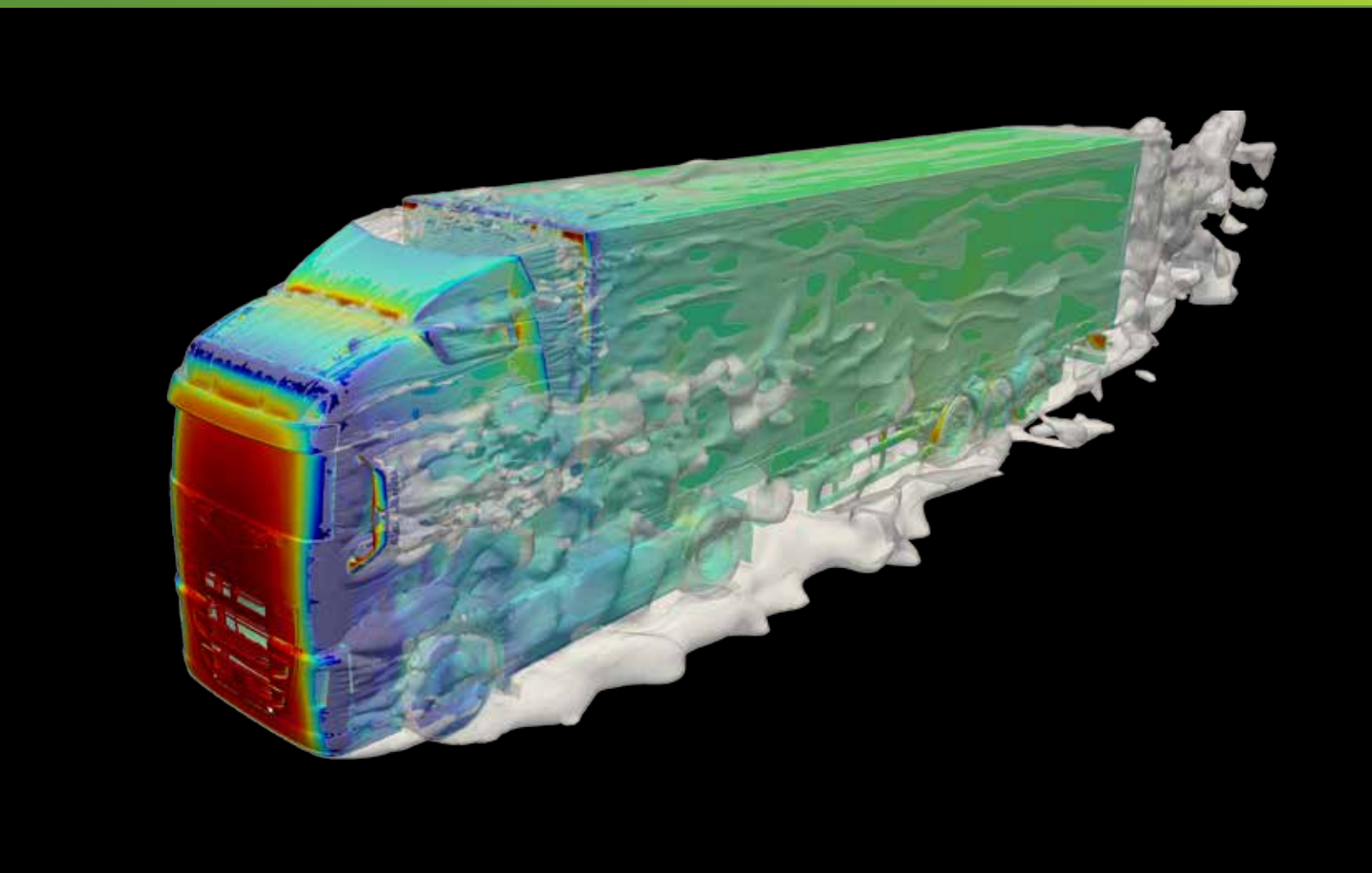
no.1 2019

PDC Center for High Performance Computing

PDC Newsletter



The PDC Newsletter is published by PDC at EECS, KTH.

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

Editor: Erwin Laure
Editorial Staff: Genet Edmondson
Layout: Genet Edmondson
Graphic Design: Maria Malmqvist
E-mail: support@pdc.kth.se

ISSN 1401-9671

Cover

Results from a Computational Fluid Dynamics simulation (performed by Rumblestrip using Beskow) which shows the surface pressure and flow structures around an air deflector on the roof of a truck that is optimally positioned to reduce air resistance. Image © Rumblestrip, 2019

How to Contact PDC

Visiting address:
Teknikringen 14, "Plan 4",
KTH, Stockholm
Mail: PDC, KTH,
SE-100 44 Stockholm, Sweden
E-mail: support@pdc.kth.se
www: http://www.pdc.kth.se
Phone: +46 8 790 7800

Editorial

2019 has started big for high performance computing (HPC) in Europe! The EuroHPC Joint Undertaking has become fully functional and is preparing for the first major investments — at least two pre-exascale systems and several petascale systems. We discuss more about the EuroHPC plans and Sweden's involvement in these developments in this newsletter. In addition, the existing European ecosystem within PRACE is developing, with a new implementation project (PRACE-6IP) starting and a new edition of the scientific case being published. I sincerely recommend reading this scientific case that includes a wealth of information on what great research is being performed using our HPC resources.

Another part of the European HPC ecosystem is HPC-Europa3 — their Transnational Access exchange programme has enabled many European researchers to visit their colleagues in other countries and use the local HPC resources for their work. As part of this programme, many researchers have visited Sweden and used our HPC resources. If you would be interested in taking advantage of the opportunities offered by this programme — either in terms of travelling elsewhere yourself or hosting a fellow colleague — get in touch with us.

The future organization of e-infrastructures is also a big topic in Sweden. The Swedish Research Council (VR) has just published a new study on "An outlook for the national roadmap for research e-infrastructures" that analyses the current status of Swedish e-infrastructures and gives recommendations for their further evolution. I am sure this report, as well as its findings and recommendations, will be subject to many discussions in the coming months.

With our current main system, Beskow, PDC is an important part of the Swedish e-infrastructure and, although the lifetime of the system has been extended until the end of 2020, preparations for the next system at PDC are already well underway. This includes working with the Swedish National Infrastructure for Computing (SNIC) to ensure the availability of an adequate budget, considering market and technology studies, and most importantly understanding the future needs of researchers using our systems. To assist with the latter, we organized an "extreme usage workshop" with the main user groups in January, which helped us to better understand their requirements and potential future usage models. If you have input or considerations on the design of PDC's future system — drop by or send us a note!

Training and education is a cornerstone of our activities and, with the growing importance of Artificial Intelligence (AI), we have partnered with PRACE to organize one of the first Deep Learning workshops within SNIC. Further activities along these lines will follow in the autumn and we are already preparing for our flagship event, the PDC Summer School, towards the end of August.

Finally, I would like to point you again to our blog (https://www.kth.se/blogs/pdc) where a lot of interesting HPC topics are being discussed. With this newsletter, we are making a start on publishing some of these interesting blog articles in our newsletter format too (for those of you who have not yet checked the online blog site). We hope that our blog and newsletter provide you with some interesting reading over the summer!

Erwin Laure, Director PDC

PDC Video by KTH

KTH recently made a short video about PDC – you can view it here: https://www.youtube.com/watch?v=662YYyOo12Q.

In This Issue

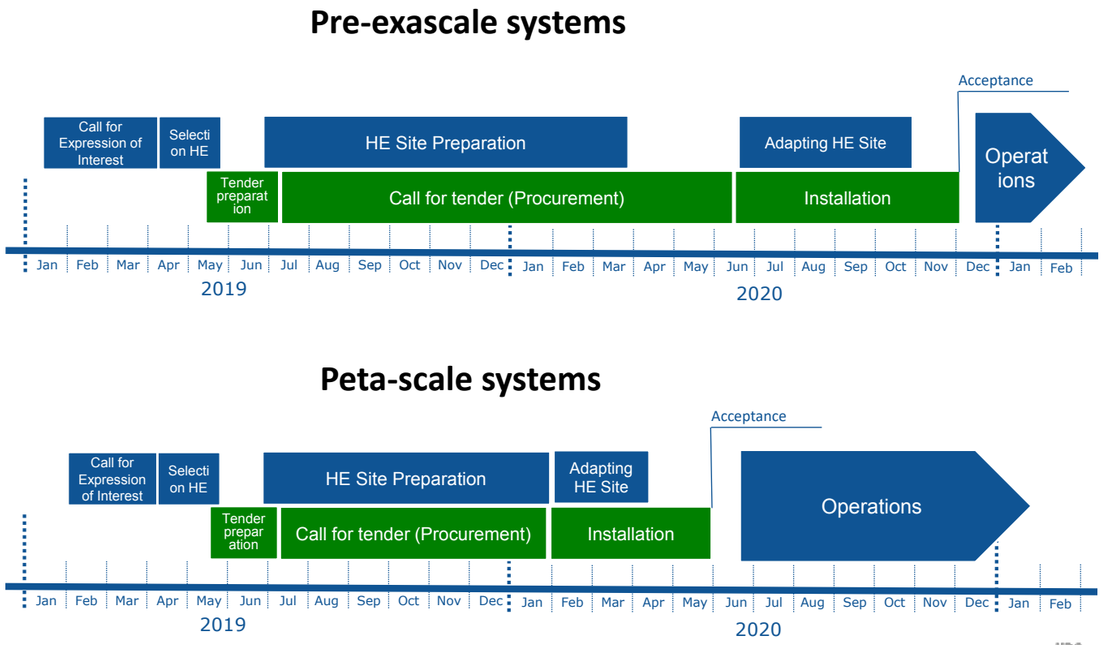
Above: PDC-SeRC Seminar, 8 May 2019

EuroHPC – Europe's Path to Exascale

Erwin Laure

The race towards Exascale (that is, achieving 10^{18} floating point operations per second) is accelerating and concrete plans are underway in the US, Japan, and China. For some time, Europe was lagging behind and did not have an overarching strategy backed by all the countries in the EU. This changed in November 2018 with the establishment of the EuroHPC Joint Undertaking (https://eurohpc-ju.europa.eu/index.html). EuroHPC is a joint initiative between the EU and European countries to develop a World Class Supercomputing Ecosystem in Europe. Today, 28 member and associate countries of the EU are part of this initiative and Sweden officially joined on the 5th of February 2019, represented by the Swedish Research Council (VR). EuroHPC, which will initially be operational until 2026, has already defined its first phase (covering 2019 and 2020) with a budget of close to 1 billion EUR, of which 486 million come from the actions already planned by the European Commission in the Horizon 2020 and Connecting Europe Facility (CEF) programmes. Two main aims have been defined for this first phase.

- The first is acquiring and providing a world-class petascale and pre-exascale supercomputing and data infrastructure for Europe's academic, industrial and public users, matching their demanding application requirements by 2020. This would be widely available to users from both the public and private sectors, to be used primarily for research purposes.
- The second aim involves supporting an ambitious research and innovation agenda to develop and maintain a world-class high performance computing (HPC) ecosystem in the EU, both exascale and beyond, which would cover all academic and industrial value chain segments, including low-power processor and middleware technologies, algorithms and code design, applications and systems, services and engineering, interconnections, know-how and skills for the next generation supercomputing era.



Above: Timelines indicating the planned acquisition processes for EuroHPC pre-exascale and petascale systems

Further funds in the next multiannual financial framework (MFF), together with support from member states, are expected to cover the 2021-2028 period, with already agreed strategic objectives, including

- the acquisition in 2022-2023 of two exascale systems, at least one of them with European technology,
- one post-exascale system,
- networking and coordination of HPC Competence Centres,
- support for the first hybrid HPC/Quantum computing infrastructure in Europe, and
- coordination with the other digital priorities like artificial intelligence, cybersecurity and digital skills.

The Commission has proposed supporting EuroHPC in the next MFF with 2.7 billion EUR from the Digital Europe Programme (DEP) and with additional funds from Horizon Europe. These funds are expected to be matched by the member states resulting in an overall budget of over 5 billion EUR.

In a first step, EuroHPC is planning the acquisition of two pre-exascale systems, reaching a performance of 150 petaflops with a total cost of ownership of up to 250 million EUR. A call for hosting entities (HEs) has recently closed and three consortia are competing: a Spanish-led consortium proposing the Barcelona Supercomputing Center (BSC) as the host, an Italian-led consortium putting CINECA (which is the Italian interuniversity high performance computing consortium) forward as the host, and a Finnish-led consortium supporting a data centre in Kajaani run by CSC (which is the Finnish IT Center for Science) as the host. Sweden, together with other countries, has joined the Finnish bid. If that particular bid is successful, the equivalent share of the system will be made available to Swedish researchers via the Swedish National Infrastructure for Computing (SNIC). EuroHPC is expected to make a decision in June and then the procurement process for the systems will start, with the aim being to have them available for researchers in late 2020.

As far as the research programme, EuroHPC will launch the first calls for HPC technologies soon. A key focus of the research programme will be the continued development of European exascale technologies (including the European Processor Initiative), application support, and support for small to medium-sized enterprises (SMEs).

Staff Focus

Miguel Zavala-Aké

Miguel Zavala-Aké is a physicist who develops code to recreate nature. He has developed an analytical approach that makes it possible to address different kinds of problems ranging from star formation to the mechanics of the heart, from statistics to quantum mechanics, and from C++ to Python. Miguel has just started a postdoctoral position at PDC with a focus on the visualization and analysis of data in running time.

During his bachelor's degree in Engineering Physics, Miguel carried out a numerical study related to solid state physics. After that, he received a master's degree in Physics working on numerical studies simulating star formation. During that time, he was involved in developing a tool related to scientific visualization, and numerical simulations using CUDA (Compute Unified Device Architecture). Shortly before finishing his master's degree, Miguel started working for a petroleum company. Almost two years later, he started his Ph.D. in Aerospace Science and Technology at Barcelona Supercomputing Center (BSC), Spain. The studies that he is performing at this stage are related to the computational aspects involved in the physical interactions of multi-components of gas turbines.

During 2019 three more companies started collaborations with PDC; one of them is a start-up company called Rumblestrip. In case you are not familiar with the terminology, "rumble strips" are a road safety feature to alert inattentive drivers to the potential danger of diverging from a safe direction. They do this by causing a tactile vibration and audible rumbling transmitted through the wheels into the vehicle interior. This means that when a vehicle is driven onto a section of rumble strips on a road, the vehicle shakes and vibrates, making the driver aware of the danger. The company Rumblestrip bases their business on the fact that, by using sensors that enable you to listen carefully to the shakes and vibrations, you can gain deep insights about a vehicle's performance; the company listens to vehicles when they drive on the roads in order to develop software solutions that enhance vehicle performance.

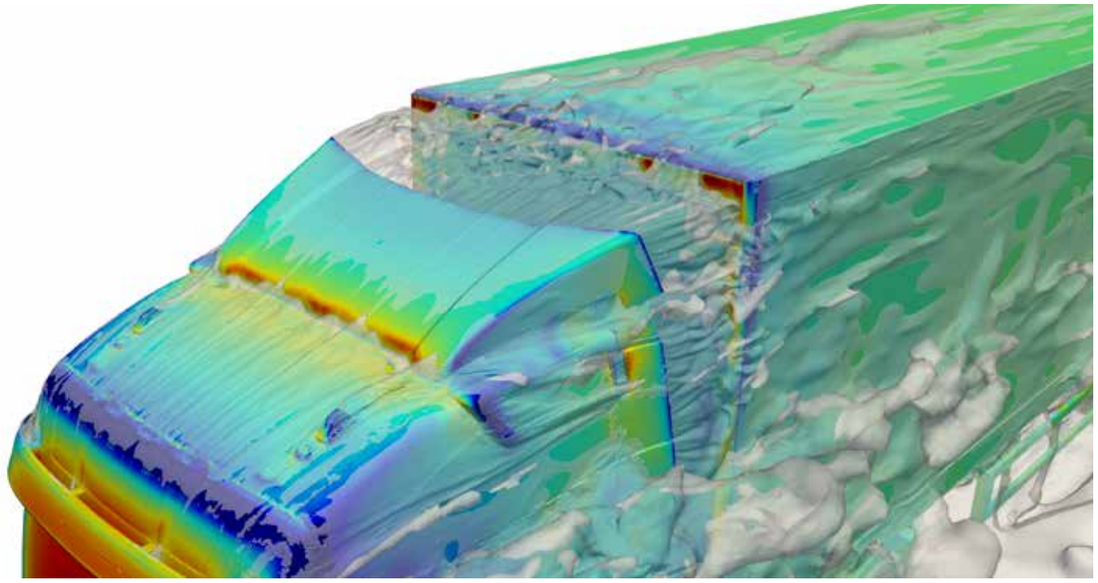
Here Andreas Persson, the Chief Technical Officer at Rumblestrip, discusses what Rumblestrip produces and how the company collaborates with PDC.

Rumblestrip Collaborates with PDC

Andreas Persson, Rumblestrip

With increasing fuel prices and environmental awareness, it is very clear that the heavy transport industry needs to continuously improve the fuel efficiency of its trucks. Aerodynamic drag is one of the biggest contributors to total fuel consumption, so manufacturers spend many millions each year on developing the aerodynamic properties of their vehicles, which must live up to ever tighter regulations regarding emissions.

The roof air deflector, which sits on top of the cab roof, is the single most important component for reducing air resistance – provided it is adjusted correctly with regard to the trailer height and gap. Sadly, many trucks, in reality, drive around with incorrectly adjusted roof deflectors. The result is that haulers on average unnecessarily waste several percent of their fuel. In the worst cases, the penalty can be in excess of 10 %. This is significant in an industry where every fraction of a percent in reduced fuel consumption is chased by the engineers!



Above: CFD simulation showing surface pressure and flow structures around an optimally positioned roof air deflector.

Rumblestrip was founded in 2016 with a clear focus on developing more intelligent solutions, which make sure that the trucks on our roads achieve the lowest possible fuel consumption, while maintaining ease-of-use for the driver. Its first product - Ecosense Trailer Assist - is a fully automatic roof air deflector system that makes sure that the deflector is always set in the optimal position, without any user-input being necessary.

The core of the product is software that analyses the configuration of the truck as well as the aerodynamic flow field, and positions the deflector optimally at all times. To fully understand the behaviour of the flow field around different types of trucks and deflector settings, a large number of computational fluid dynamics (CFD) simulations are performed on the Beskow cluster at PDC.

A key goal of these simulations is to understand how the forces on the deflector vary with its angle, and how these relate to the drag value of the vehicle. Rumblestrip uses an almost fully-automated OpenFOAM process, from meshing on the computation nodes (snappyHexMesh) to postprocessing on Beskow or Tegner. A typical mesh size is in the region of 30-50 million cells, and a full Reynolds-averaged Navier-Stokes (RANS) simulation can be completed in only 4-5 hours on 128 cores.

Having access to the PDC supercomputers is a great asset for a young start-up company like Rumblestrip. Primarily, it makes virtually infinite scaling possible if there is a tight deadline. Compared to other high performance computing (HPC) solutions that Rumblestrip has tested, the main advantages of working with PDC are the raw performance, scalability, and excellent support, all of which make PDC a very compelling partner for Rumblestrip.

Staff Focus

Daniel del Castillo

Daniel del Castillo is a second-year master's student specialising in Machine Learning at KTH. He has taken courses such as Language Engineering, Neuroscience and Speech Technology, and is currently working on his master's thesis on singing-language identification from raw audio data. At the moment, Daniel is working part-time in first-line support at PDC, taking care of account management and addressing support requests. Daniel enjoys high-intensity training during his free time and likes playing ultimate frisbee and basketball. He also enjoys playing the piano and is a member of a second-hand store that tries to provide clothes and useful items for free to new tenants at his student accommodation.

Above: PDC-SeRC seminar, 8 May 2019

Above: PDC Pub, 8 May 2019

PRACE Deep Learning Workshop at PDC

Thor Wikfeldt, PDC

On the 20th and 21st of March, PDC organized a workshop on deep learning sponsored by PRACE. As could be expected, based on the current surge of enthusiasm surrounding deep learning methods, the workshop quickly filled up after registration was opened. The workshop was taught by two instructors from Finland, Markus Koskela and Mats Sjöberg, who both work at the CSC - IT Center for Science. Their extensive experience in developing, applying and teaching deep learning methods has enabled them to develop a comprehensive yet practical two-day introduction to deep learning - not an easy task considering the complexity of the subject! On the first day of the workshop, participants logged in to a CSC cloud service which provides access to Jupyter Notebooks with all the deep learning packages pre-installed, but no GPUs. On the second day, when more computationally demanding methods were explored, participants logged in to Tegner and ran their experiments on the K80 and K420 GPUs available on Tegner compute nodes. The lesson material mainly focused on convolutional neural networks (CNNs), recurrent neural networks (RNNs) and multi-layer perceptron (MLP) networks, along with important concepts such as supervised versus unsupervised learning, activation functions, backpropagation, automatic differentiation, pooling and dropout. Most of the exercises, analysing both image and text data, were based on using the Keras package with TensorFlow in the back end, but participants had the option to also try out the PyTorch package.

The course feedback we received showed that the participants were very happy with the workshop. PDC aims to deliver further workshops on machine learning and deep learning methods in the future, so keep an eye on the PDC website or subscribe to the pdc-announce mailing list if you are interested in attending!

Swedish Roadmap for Research e-Infrastructures Now Available

Erwin Laure, PDC

The Swedish Research Council (VR) has recently published "An outlook for the national roadmap for research e-infrastructures".

Many reports by the Swedish Research Council have identified a growing need for e-infrastructures for research. However, in Sweden, the current e-infrastructure landscape is relatively fragmented and many actors provide different kinds of services at different levels. At the same time, the global Open Science policy in research pushes the need for national alignment with international policies and good national coordination between infrastructures and e-infrastructures for research. The Swedish Research Council and the University reference group for research infrastructures (URFI) identified a need for a review to obtain independent advice from an international expert panel on how to deal with the growing demands for e-infrastructures for research. As a collaborative effort, VR and URFI initiated this review in October 2017.

During the work, the expert panel observed that a re-occurring theme is the fragmentation of e-infrastructures and differences in ownership and funding mechanisms and the problems this causes. If you would like to read about the independent analysis of the situation for Swedish national e-infrastructures for research and the specific recommendations that were proposed for how Sweden can continue the work on developing a coherent national strategy and roadmap for e-infrastructures for research, you can download the whole report here: https://www.vr.se/download/18.50a36236168b14238b1dbb/1552381575539/Outlook-national-roadmap-e-infrastructures-for-research_VR_2019.pdf.

Infrastructure on High Performance Computing

Pan-European Research

HPC Europa 3

HPCE3: 18 Months of Achievements

Lilit Axner, PDC

On the 18th of January 2019, the HPC-Europa3 (HPCE3) project had its first review by the European Commission after 18 months of existence. The total achievements of the HPCE3 project were reported in the 18-month progress report for HPCE3 and are summarised here.

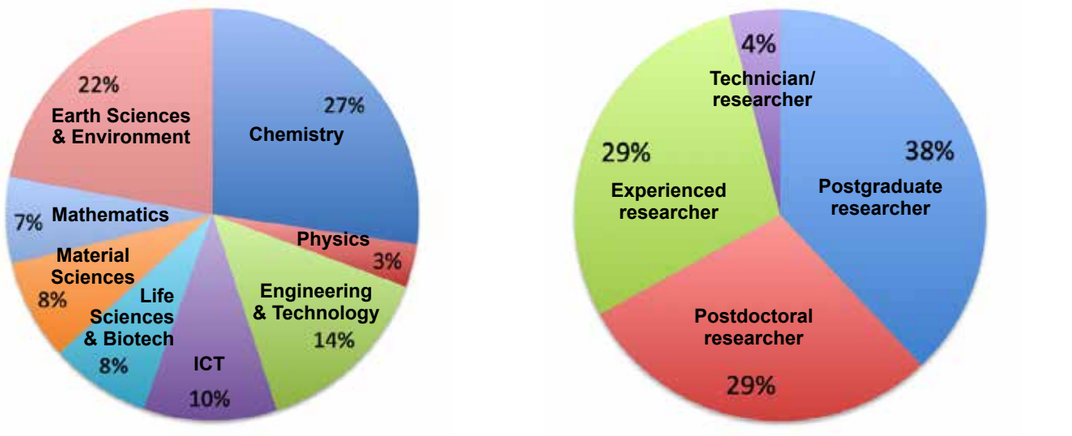
Transnational visits

A total of 266 applications for research visits were received, of which 204 were accepted (which equates to 77%). During the initial 18 months, a total of 143 user projects have been supported – including visits (which were either completed during the period or were still ongoing at the end of the 18 months). Of these, in 4 cases, a majority of the researchers were not working in the EU or an Associate State (1 from Belarus, 2 from Iran, and 1 from the USA). Of the remaining 61 applications that have been approved, 6 visits have been cancelled, and the rest are either underway or will take place during 2019.

The research visitors have come from 27 countries in total, including 19 EU countries, 5 Associated States and 3 other countries. The countries from which the biggest number of researchers have come are Spain, Italy and the UK — all countries with well-established high performance computing (HPC) research groups and with the longest history of running Transnational Access programmes — and therefore likely to be the countries where the research communities have the greatest awareness of the HPCE3 programme.

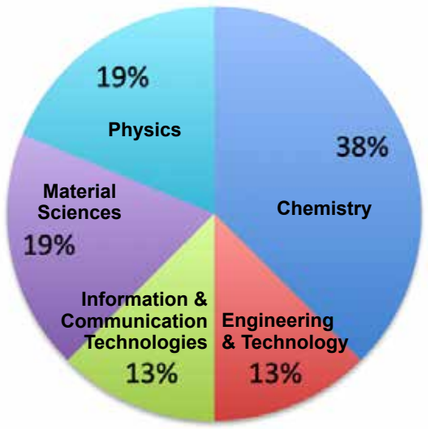
It is interesting to see the results comparing the users' scientific backgrounds and their research categories (see pie charts below).

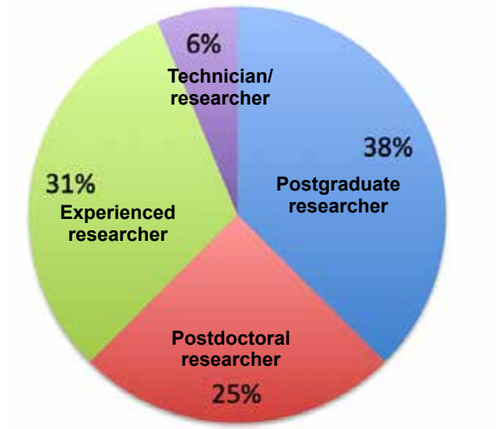
The results of the KTH partner (that is, PDC) in the review were excellent as we have managed to host more than half of the research visitors we had committed to host. It is interesting to compare the scientific backgrounds and the research categories of the visitors to Sweden with the overall picture (see pie charts on next page).



Above: These pie charts show the academic discipline and position of researchers who undertook HPCE3 visits during the first 18 months of the HPCE3 programme. The charts are based on figures from the HPCE3 First Transnational Access summary report, which is available at http://www.hpc-europa.eu/public-documents.

Below: These pie charts show the academic discipline and position of researchers who visited Sweden on an HPCE3 visit during the first 18 months of the HPCE3 programme.





Research

The HPCE3 project also has a dedicated work package to conduct research in the area of visualization. The aim of this work package is the provision of a lightweight virtualisation technology infrastructure to make it easy to port end user applications to different HPC centres and a mechanism to package single steps of a pipeline in the form of application containers while orchestrating their execution to compose an expected workflow. The team involved in this work package were able to evaluate different container technologies (e.g. Singularity, Docker and Shifter) to improve the portability of applications in order to orchestrate applications packaged as containers (for workload collocation and for benchmarking). They also conducted deeper analyses of not only container technologies but also the tools related to them so as to finish the study – this was done with the objective of proposing an architecture suitable to be deployed in different infrastructures. The results of this work are documented in the Deliverable D12.1 of HPCE3 and can be read at http://www.hpc-europa.eu/public-documents.

Events

1. HPCE3 committed to also foster the HPC culture for small to medium-sized enterprises (SMEs). The network of host centres extends to labs with strong technical-engineering characterizations and expertise. Consequently, the project committed to organizing three SME workshops. The 1st SME workshop, called "Simulation for Automotive Technologies with High Performance Computers (HPC)", took place on the 26th and 27th of November 2018 in Stuttgart, Germany. The goals of the workshop were to provide a face-to-face communication platform for SMEs to share their experiences of HPC usage for early prototyping and developing and to foster the industrial promotion of automotive applications, services and solutions, as well as to boost direct communication with representatives of European academia and industry. The workshop was a great success with about 30 participants attending from a wide range of different companies and organizations from around Europe. Participants were given the opportunity to learn about cutting-edge innovations for automotive technologies, such as Big Data and Machine Learning.
2. The HPC-Europa3 user group meeting, TAM — the Transnational Access Meeting, is an opportunity for the research visitors from each of the HPC centres to come together to present the results of the work they have done during their visits. The first HPC-Europa3 TAM was hosted by EPCC in Edinburgh on Tuesday 23rd October 2018, just at the end of the 18-month reporting period. In total, 40 HPC-Europa3 visitors were registered for TAM 2018. Of these, 25 were registered to give a talk, and 12 presented posters.

For many researchers, TAM represents an early opportunity to present their results, and, for junior researchers with little conference experience, it offers a chance to gain some experience of presenting their research in a relatively relaxed and friendly environment.

More information and statistics about the HPCE3 project can be found at http://www.hpc-europa.eu/public-documents as this article is only a short summary of the details in the report.

Recent PRACE Developments within the HPC Ecosystem

Lilit Axner, PDC

PRACE-6IP

On the 28th and 29th of May 2019 in Bratislava PRACE 6IP started with a kick-off. All 26 member countries gathered to discuss the work plan, opportunities and ambitions for the coming two years. As was mentioned in our previous newsletters, there are two major changes that will happen within 6IP.

1. The DECI optional program is being reorganized and merged even more closely within PRACE.
2. A new work package within PRACE-6IP is dedicated to so-called "Forward-looking Software Solutions Projects", where ten software projects will be selected to be worked on.

For this second change, PRACE launched an internal call for applications in order to select a list of software to work on. As a result of the first call, 34 letters of intent were received, for which 15 proposals were later submitted.

The submission and review process was conducted according to the timeline agreed on in the written consultation between the partners. In particular, the platform for proposal submissions opened on the 30th of May 2018 and closed on the 30th of August (with the first submission being received on the 28th of August), proposals were sent for review from the 13th of September onwards, and the review deadline was extended to the 1st of November. The Scientific Steering Committee (SSC) ranking meeting was held on the 15th of November, which was then followed by the management board meeting for the funding decision on the 11th of December 2018. After the deliberations, eight proposals were accepted to be developed as forward-looking software solutions.

Project Title: *Particle kinetic codes for Exascale plasma simulation*
Project Leader: Paul Gibbon, Jülich Supercomputing Centre

Project Title: *Modernisation of Plasma Physics Simulation Codes for Heterogeneous Exascale Architectures*
Project Leader: Martti Louhivuori, CSC

Project Title: *Linear Algebra, Krylov-subspace methods, and multi-grid solvers for the discovery of New Physics (LyNcs)*
Project Leader: Constantia Alexandrou, CaSToRC, The Cyprus Institute

Project Title: *Performance portable linear algebra*
Project Leader: ETH Zurich

Project Title: *Performance Portable Communication Layer for Grid Applications*
Project Leader: Mauro Bianco Swiss National Supercomputing Centre (CSCS)

Project Title: *LoSync - Synchronisation reducing programming techniques and runtime support*
Project Leader: Mark Bull, UEDIN

Project Title: *NB-LIB: Performance portable library for N-body force calculations at the Exascale*
Project Leader: Prof. Erwin Laure, KTH

Project Title: *FEM/BEM based domain decomposition solvers*
Project Leader: IT4Innovations

Currently, the second internal call for applications is open with the intention being to accept from two to four applications.

PRACE and EuroHPC

Another interesting activity involving PRACE has been the development of the European HPC Ecosystem that was initiated by PRACE and its 26 partners over the last ten years. As you know, PRACE is supported by the PRACE member states and through the EU by a series of implementation projects, and thus PRACE can weave a common European umbrella over national HPC ecosystems. PRACE has become a trusted liaison between HPC-infrastructures and European HPC users, involving highly rated advisory committees with members from the academic and industrial sectors.

PRACE and EuroHPC have missions that are almost complementary. While EuroHPC acts as a high-level financing agency and must essentially be a top-down activity, PRACE is a science-driven infrastructure developed as a bottom-up activity. Joining both of these together in a strong partnership will create the best possible synergies for the benefit of European research communities. More information about these developments can be found at http://www.prace-ri.eu/postitionpaper-eurohpc-prace-2019.

Third Edition of the PRACE Scientific Case for Computing in Europe 2018 – 2026

The third edition of the PRACE Scientific Case for Computing in Europe for 2018-2026 continues a tradition established by the HPC in Europe Taskforce (HET) at the beginning of the PRACE project and supports the vision that the PRACE infrastructure will enable high-impact scientific discovery and engineering research and development across all disciplines in Europe. It provides a clear overview of the achievements of computational science across various domains. While producing this document, the PRACE Council received recommendations from the PRACE SSC which were analysed and taken into account to further fulfil PRACE's mission. You can find a description of this and the scientific case in the complete document which is available at http://www.prace-ri.eu/third-scientific-case.

PDC Pub & Open House

Thor Wikfeldt, PDC

On the 8th of May, PDC held its annual Pub and Open House, where current and prospective PDC users are invited to visit PDC, take a guided tour of the computer rooms hosting Beskow and Tegner, and interact with PDC staff over drinks and snacks in a relaxed atmosphere. This year the Pub was preceded by an interesting PDC-SeRC seminar given by Prof. Stefano Markidis on current developments, challenges and future prospects for exascale computing — a topical subject given that China, USA, Japan and Europe all have ambitions to deliver an exascale computing system in the near future. The seminar was well attended and was followed by an opening and welcome to the Pub given by our director, Erwin Laure. Guided tours of the computer rooms were given by the deputy director, Gert Svensson, who has been around since the early days of PDC and has a wealth of interesting information to share. Although the number of people attending the Pub was not as large as we have sometimes seen in previous years, it was clear that those attending enjoyed the event. And it wasn't all just jovial small talk: some complicated usage issues that were brought up by researchers attending the Pub were discussed at length and solved during the Pub!

Above: PDC Pub & PDC-SeRC Seminar, 8 May 2019

The PDC Blog contains a variety of posts with useful information about high performance computing. Below is one article from the blog in case you missed it. You can read other blog posts here:
https://www.kth.se/blogs/pdc.

Scalability: Strong and Weak Scaling

Xin Li, PDC

High performance computing (HPC) clusters are able to solve big problems using a large number of processors. This is also known as parallel computing, where many processors work simultaneously to produce exceptional computational power and to significantly reduce the total computational time. In such scenarios, scalability or scaling is widely used to indicate the ability of hardware and software to deliver greater computational power when the amount of resources is increased. For HPC clusters, it is important that they are scalable, in other words that the capacity of the whole system can be proportionally increased by adding more hardware. For software, scalability is sometimes referred to as parallelization efficiency — the ratio between the actual speedup and the ideal speedup obtained when using a certain number of processors.

In this post we focus on software scalability and discuss two common types of scaling. The *speedup* in parallel computing can be straightforwardly defined as

$$speedup = t_1 / t_N$$

where t_1 is the computational time for running the software using one processor, and t_N is the computational time running the same software with N processors. Ideally, we would like software to have a linear speedup that is equal to the number of processors ($speedup = N$), as that would mean that every processor would be contributing 100% of its computational power. Unfortunately, this is a very challenging goal for real applications to attain.

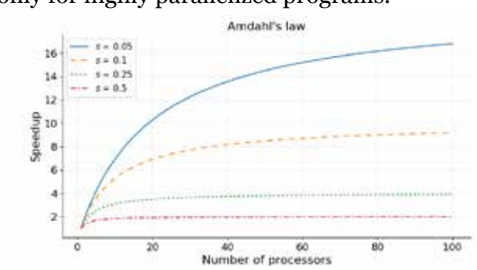
Amdahl's Law and Strong Scaling

In 1967, Amdahl pointed out that the speedup is limited by the fraction of the serial part of the software that is not amenable to parallelization [1]. **Amdahl's law** can be formulated as follows

$$speedup = 1 / (s + p / N)$$

where s is the proportion of execution time spent on the serial part, p is the proportion of execution time spent on the part that can be parallelized, and N is the number of processors. Amdahl's law states that, for a fixed problem, the upper limit of speedup is determined by the serial fraction of the code. This is called **strong scaling** and can be explained by the following example.

Consider a program that takes 20 hours to run using a single processor core. If a particular part of the program, which takes one hour to execute, cannot be parallelized ($s = 1/20 = 0.05$), and if the code that takes up the remaining 19 hours of execution time can be parallelized ($p = 1 - s = 0.95$), then regardless of how many processors are devoted to a parallelized execution of this program, the minimum execution time cannot be less than that critical one hour. Hence, the theoretical speedup is limited to at most 20 times (when $N = \infty$, $speedup = 1/s = 20$). As such, the parallelization efficiency decreases as the amount of resources increases. For this reason, parallel computing with many processors is useful only for highly parallelized programs.



Above: Speedup with increasing number of processors

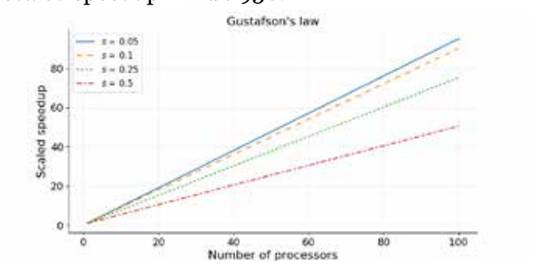
Gustafson's law and weak scaling

Amdahl's law gives the upper limit of speedup for a problem of fixed size. This seems to be a bottleneck for parallel computing; if one would like to gain a 500 times speedup on 1000 processors, Amdahl's law requires that the proportion of serial part cannot exceed 0.1%. However, as Gustafson pointed out [2], in practice the sizes of problems scale with the amount of available resources. If a problem only requires a small amount of resources, it is not beneficial to use a large amount of resources to carry out the computation. A more reasonable choice is to use small amounts of resources for small problems and larger quantities of resources for big problems.

Gustafson's law [2] was proposed in 1988 and is based on the approximations that the parallel part scales linearly with the amount of resources, and that the serial part does not increase with respect to the size of the problem. It provides the formula for *scaled speedup*

$$\textit{scaled speedup} = s + p \times N$$

where s, p and N have the same meaning as in Amdahl's law. With Gustafson's law the scaled speedup increases linearly with respect to the number of processors (with a slope smaller than one), and there is no upper limit for the scaled speedup. This is called **weak scaling**, where the scaled speedup is calculated based on the amount of work done for a scaled problem size (in contrast to Amdahl's law which focuses on fixed problem size). If we apply Gustafson's law to the previous example of s = 0.05 and p = 0.95, the scaled speedup will become infinity when infinitely many processors are used. Realistically, if we have N = 1000, the scaled speedup will be 950.

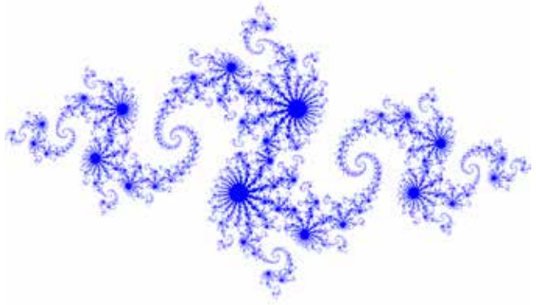


Above: Speedup with increasing number of processors under Gustafson's law

Measuring Parallel Scaling Performance

When using HPC clusters, it is almost always worthwhile to measure the parallel scaling of your jobs. The measurement of strong scaling is done by testing how the overall computational time of the job scales with the number of processing elements (being either threads or MPI processes), while the test for weak scaling is done by increasing both the job size and the number of processing elements. The results from the parallel scaling tests will provide a good indication of the amount of resources to request for the size of the particular job.

To illustrate the process of measuring parallel scaling, we use an example of OpenMP code, `julia_openmp.c`, which produces an image of a Julia set. A Julia set is associated with a complex function and can be converted to an image by mapping each pixel onto the complex plane. An example of an image for a Julia set is shown below.



The `julia_openmp.c` code contains two OpenMP directives that start with "`#pragma omp`" (read more about OpenMP syntax from the OpenMP quick reference card). In practice, these two "`#pragma omp`" lines can be merged into one, as shown below. Note that we have added the `schedule(dynamic)` option, which provides better workload distribution at the cost of some extra overhead. This option also mimics the parallelization overhead in real applications (e.g. communication and load-balancing in MPI-parallelized programs).

```
# pragma omp parallel for schedule(dynamic) \
  shared ( h, w, xl, xr, yb, yt ) \
  private ( i, j, k, juliaValue )
  for ( j = 0; j < h; j++ )
  {
    ...
  }
```


The main function of `julia_openmp.c` is also modified to accept a height and a width as integer arguments from the command line.

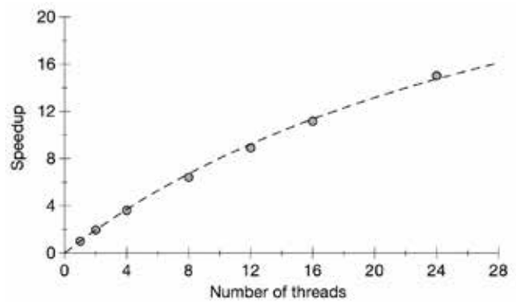
```
int main ( int argc, char* argv[] )
{
  if ( argc < 3 )
  {
    printf ( "Usage: ./julia_openmp height
width\n" );
    return 0;
  }
  int h = atoi(argv[1]);
  int w = atoi(argv[2]);
  ...
}
```

The strong scaling is tested by running the code with different numbers of threads, while keeping the height and width constant. The computational time for generating the Julia set is monitored for each calculation. The results are shown in Table 1 and the figure on the left below (which also shows the fitted curve based on Amdahl's law).

The weak scaling is measured by running the code with different numbers of threads and with a correspondingly scaled height. The width was kept constant. The results of the weak scaling test are shown in Table 2 and the figure on the right below, which also shows the fitted curve based on Gustafson's law.

Table 1: Strong scaling for Julia set generator code

Height	Width	Threads	Time
10,000	2,000	1	3.932 s
10,000	2,000	2	2.006 s
10,000	2,000	4	1.088 s
10,000	2,000	8	0.613 s
10,000	2,000	12	0.441 s
10,000	2,000	16	0.352 s
10,000	2,000	24	0.262 s



Above: Plot of strong scaling for Julia set generator code
The dashed line shows the fitted curve based on Amdahl's law.

Table 2: Weak scaling for Julia set generator code

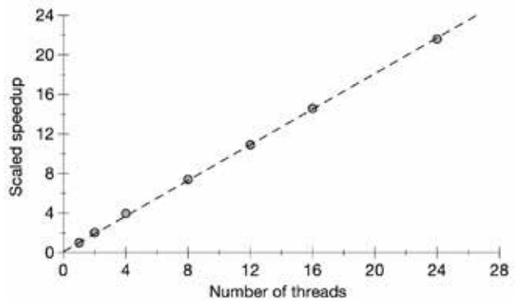
Height	Width	Threads	Time
10,000	2,000	1	3.940 s
20,000	2,000	2	3.874 s
40,000	2,000	4	3.977 s
80,000	2,000	8	4.258 s
120,000	2,000	12	4.335 s
160,000	2,000	16	4.324 s
240,000	2,000	24	4.378 s

Based on the formulae for Amdahl's law and Gustafson's law, it is possible to fit the strong and weak scaling results and obtain the ratio of the serial part (s) and the parallel part (p). We have done the fitting in the figures below, and the fitted value for the serial fraction s is 0.03 for Amdahl's law and 0.1 for Gustafson's law. The discrepancy in s is attributed to the approximations in the laws — the serial fraction is assumed to remain constant, and the parallel part is assumed to be sped up in proportion to the number of processing elements (processes/threads). In real applications, the overhead of parallelization may also increase with the job size (for example, from the dynamic loop scheduling of OpenMP), and in this case it is understandable that the weak scaling test, which involves much larger jobs than those in the strong scaling test, gives a larger serial fraction s.

Summary

This post discusses two common types of scaling of software: strong scaling and weak scaling. Some key points are summarized below.

- Scalability is important for parallel computing to be efficient.



Above: Plot of weak scaling for Julia set generator code
The dashed line shows the fitted curve based on Gustafson's law.

- Strong scaling concerns the speedup for a fixed problem size with respect to the number of processors and is governed by Amdahl's law.
- Weak scaling concerns the speedup for a scaled problem size with respect to the number of processors and is governed by Gustafson's law.
- When using HPC clusters, it is almost always worthwhile to measure the scaling of your jobs.
- The results of strong and weak scaling tests provide good indications for the best match between job size and the amount of resources that should be requested for a particular job.

References

1. Amdahl, Gene M. (1967). AFIPS Conference Proceedings. (30): 483–485. doi: 10.1145/1465482.1465560
2. Gustafson, John L. (1988). Communications of the ACM. 31 (5): 532–533. doi: 10.1145/42411.42415

PDC-Related Events

PDC Summer School 2019

19-30 August 2019, KTH, Stockholm

https://agenda.albanova.se/conferenceDisplay.py?confId=6743

PDC Industry Day

19 September 2019, KTH, Stockholm

For further details about the Industry Day, check the PDC Events calendar.

NVIDIA GPU Boot Camp and Deep Learning Workshop

24-25 September 2019, KTH, Stockholm

https://www.pdc.kth.se/about/events/nvidia-gpu-boot-camp-and-deep-learning-workshop-1.907535

HPC Sources

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

BioExcel
http://bioexcel.eu/events

CERN
http://cerncourier.com/cws/events
https://home.cern/scientists/events/computing

EGI
https://www.egi.eu/category/events

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

HPCwire
http://www.hpcwire.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.se/news-events
http://docs.snic.se/wiki/Training

XSEDE
https://www.xsede.org

Above: "A Perspective on Exascale Computing" by Stefano Markidis, PDC-SeRC Seminar, 8 May 2019