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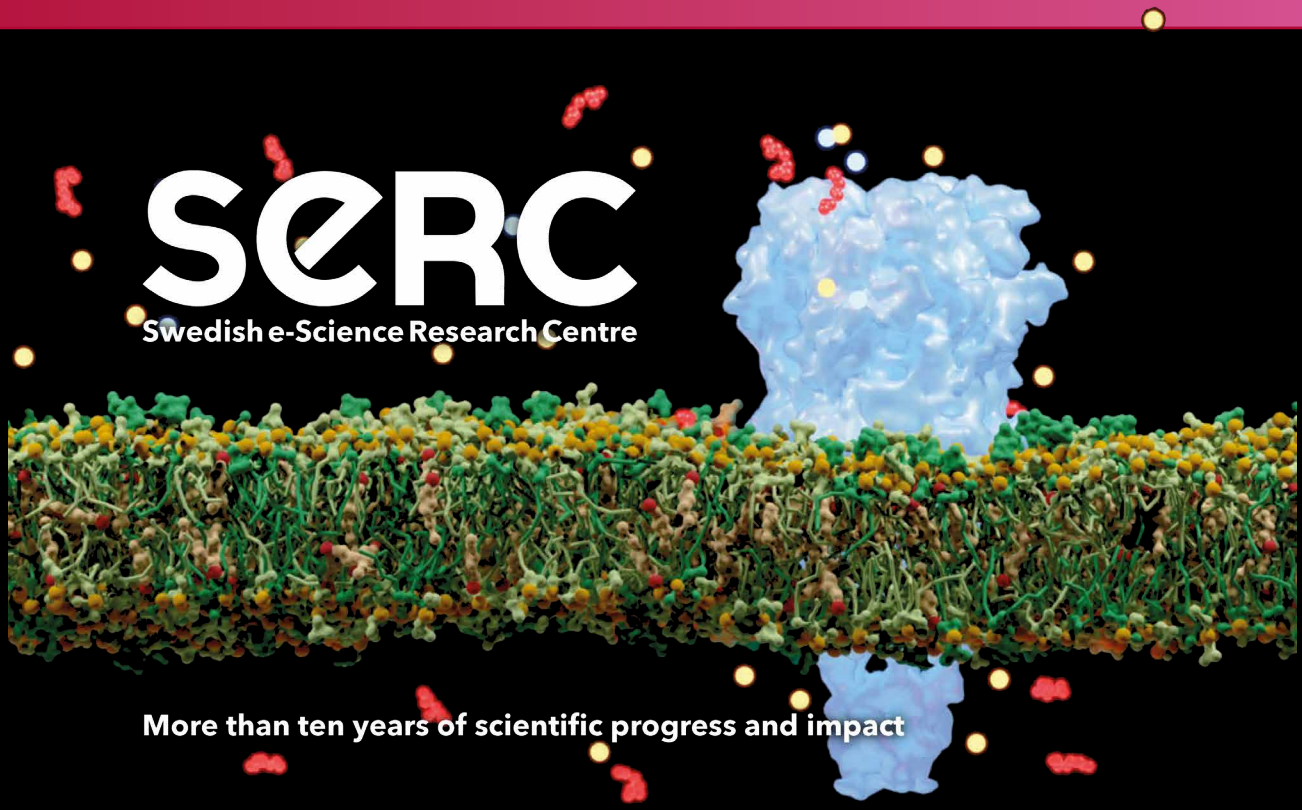
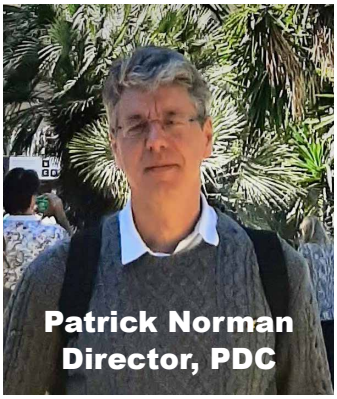
PDC Center for High Performance Computing

PDC Newsletter





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PDC operates leading-edge, high-performance computers as easily-accessible national resources. These resources are primarily available for Swedish academic research and education. PDC is hosted by EECS, KTH, and is a member of the National Academic Infrastructure for Supercomputing in Sweden (NAISS).

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Cover

The cover image is from the recently published SeRC brochure, which summarises more than a decade of SeRC's contributions to scientific progress and its impact on research and researchers in Sweden. The full brochure is available from the SeRC website at: https://e-science.se.

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Editorial

As we move towards the end of 2023, the transformation of Swedish high-performance computing (HPC) continues with the implementation of the National Academic Infrastructure for Supercomputing in Sweden (NAISS) and the different university branches within NAISS are finding their roles in this new landscape.

The establishment of NAISS has given a clear mandate to a single organisation and university to take full future control of Swedish hardware investments and operations. The previous model of tearing resources apart and spreading national investments between half a dozen different physical locations was not sustainable. Once the decision was made to change the approach, the NAISS proposal was widely embraced as is evidenced by the large number of universities that have declared themselves willing to pay NAISS membership fees. In this new NAISS era, it appears that the right balance has been found between localisation and delocalisation such that the new organisation embodies a national infrastructure with engaged universities. To implement centralisation for equipment but not application expertise may well turn out to be a potent recipe for HPC success.

Every Swedish national infrastructure, including that of HPC, is expected to be co-financed by the stakeholders to guarantee its necessity when gauged against other interests. The important decision made by NAISS here was to also take a step back from centralisation and let the lion's share of the universities' co-funding reside within the control of each of the universities. This is a bold and highly constructive move by NAISS that gives up organisational control of funding in favour of university participation in building an infrastructure that best meets the needs of its users. An adversary might say that was foolish because there is, in principle, no guarantee that the universities will continue funding Swedish HPC at the same levels as before. But I would argue that it is a risk worth taking since we need the universities to be invested and engaged in the question of how their co-funding is spent. Freedom is now given to each university to strategically link its e-science investments to those being made in other research areas at that university and not least in the experimental sciences

KTH is leading the way by expressing its full support for NAISS and continuing its strong financial commitment to the field of HPC. While the investments that are made will (in a sense "selfishly") reflect the priorities of other research activities at KTH, they will also, for the most part, benefit the national HPC infrastructure. Notably, KTH will promote the notion of the NAISS ecosystem being

an entity that, in addition to incorporating hardware and servers, also recognises knowledge, competencies, and software applications as being decisive factors for the advancement of natural sciences and engineering. Scientific software is in itself to be seen as part of the infrastructure, including the development and implementation of novel methods and algorithms. This view represents a paradigm change in Swedish HPC by blurring the boundary between research and infrastructure, and it can be implemented because the funding comes directly from KTH. This enables PDC and other research groups at KTH to participate in long-term efforts in the development of internationally leading scientific domain software that is anchored in strong research environments existing at KTH. It also promotes good software engineering practices and balances the work of Ph.D. students and postdocs, who typically have more short-term goals.

In return, for KTH, the development activities at PDC bring international recognition, industry contacts, and successful research environments that are able to compete for external funding in both the national and international arenas. KTH holds the leading position in the Swedish e-Science Research Centre (SeRC, https://e-science.se), which also gathers together the Karolinska Institute, Stockholm University, and Linköping University. SeRC is highlighting the importance of the Research Software Engineers who are the backbone of these types of long-term scientific software development activities (see *Research Software Engineer Teams: Organising the Most Advanced Level of User Support at the SeRC Universities*) and it is not a distant thought to use SeRC as an advisory body for the scientific software developments at PDC in the future. On the European level, PDC leads three of the EuroHPC centres of excellence (CoEs) and is a member of a fourth. Such an achievement is not only a token of success for KTH but also brings an international dimension into NAISS.

PDC has three flagship programs: GROMACS, VeloxChem, and Neko in the fields of molecular dynamics, quantum chemistry, and computational fluid dynamics, respectively. The uncompromisable goal for each of these software projects is to develop an open-source program that delivers an HPC performance beyond the state-of-the-art in the respective scientific domains. This exemplifies the national benefit of KTH's strategic investment in HPC that also formed a cornerstone in the recent Swedish application to become a hosting nation within the EuroHPC JU. This application has been granted approval and, under the lead of Gert Svensson, preparations are being made for the procurement of a system (which will be named after Carl Axel Arrhenius) that will be far more powerful than anything presented before in Swedish HPC.

Patrick Norman, Director PDC

In This Issue

Staff Focus

Mathieu Linares

Mathieu Linares recently joined PDC as an application expert. Mathieu earned his Ph.D. in theoretical chemistry from the Paul Cézanne University, Marseilles, France, in 2005, under the supervision of Prof. S. Humbel. After five years as a postdoc, in 2011, Mathieu obtained an assistant professor position in the theoretical chemistry group at Linköping University and then became an associate professor there in 2015.

For the last five years, Mathieu has been working in the scientific visualisation group at Linköping University, Campus Norrköping, focusing on the development of visualisation tools for computational chemistry and in particular leading the development of the VIAMD software for visual interactive analysis of molecular dynamics. At PDC, Mathieu will be working on the interoperability between GROMACS and VeloxChem. He will also continue his work on advancing visualisation tools for computational chemistry, aiming to enhance PDC's user experience and accessibility.

In his leisure time, Mathieu likes to be in nature, trail and mountain running, or forest foraging. He also has a passion for music; he is an eclectic listener, plays several instruments and sings.

SeRC
Swedish e-Science Research Centre

Research Software Engineer Teams: Organising the Most Advanced Level of User Support at the SeRC Universities

Dan Henningson, SeRC Director, & Erik Lindahl, SeRC Co-Director

This short article describes how researchers in the Swedish e-Science Research Centre (SeRC) have successfully developed and improved simulation software that utilises the fastest computers in the world. As the organisation of the computational infrastructure in Sweden is changing rapidly, we believe that the lessons that have been learned by SeRC researchers may provide inspiration for Swedish e-science researchers, e-infrastructure providers and university leaders as they tackle the vitally important task of organising the most advanced forms of supercomputer user support in the future.

In connection with the national computer infrastructure moving from the Swedish National Infrastructure for Computing (SNIC) to the National Academic Infrastructure for Supercomputing in Sweden (NAISS), there are also extensive changes in funding and responsibility for the organisation of user support. User support can be broadly divided into three levels where responsibility for simpler user support (such as creating accounts) will lie entirely with NAISS, according to the NAISS contract with the Swedish Research Council (VR). The intermediate level of support will, for most Swedish universities, be organised through NAISS by means of co-funding from the universities. In contrast, the most advanced level of user support will be the direct responsibility of the universities themselves, both in terms of organisation and providing funding. This is a large change compared to how user support was managed before. Previously, all levels of support were organised through SNIC, and the universities only contributed funding. One advantage of the new approach is that, when it comes to advanced user support, the universities have the strategic freedom to invest in "strong" areas where the research has significant impact. This approach should also result in a stronger correlation between investments and benefits to local researchers. For this new approach to work well, there is a need for a broader discussion about how intermediate-

level user support should be distinguished from advanced user support and how advanced user support should be handled by the universities and computer centres. SeRC has helped build several strong environments comprising both outstanding research and infrastructure since 2010 at the KTH Royal Institute of Technology (KTH), Linköping University (LiU), Stockholm University (SU) and the Karolinska Institute (KI). To kick-start the next stage of the process, we have had a strategy meeting discussing advanced user support with SeRC principal investigators (PIs), Swedish e-infrastructure leaders and research software engineers at PDC. This short article summarises some of the lessons learned and invites others to start thinking about this important topic. It should not be seen as a final product but as an initiative to start a process where these matters are discussed among e-science researchers in Sweden.

Different Levels of User Support Need Different Staff and Organisations

Historically, Sweden has had no clear division between basic routine support, more specialised requests, and long-term software development. This has led to an emphasis on general expertise for handling matters of moderate complexity, but compared to other infrastructures, it has been very rare for Swedish infrastructure experts to develop specific expertise to a level where they define international infrastructure frontiers. With the new funding streams in Sweden, it will be more straightforward to define support responsibilities according to the IT Information Library (ITIL) framework standard levels.

- **Tier-1 support is the traditional helpdesk** handling routine matters, troubleshooting minor difficulties, and being the first source of assistance that occasionally escalates an issue to the next level. This work is funded entirely by the NAISS grant from VR and corresponds both to staff working on specific computing resources and to staff with broader national responsibility.
- **Tier-2 support covers intermediate-level services** performed by staff with extensive experience, including solving unknown errors that have been escalated by Tier-1, training, providing assistance with installing and benchmarking, and undertaking general programming, such as helping with workflows or data management, perhaps up to several weeks of assistance for an area with an important need. This level of support covers most of the application experts previously funded by SNIC. As the amount of time per case is limited – but there are many cases – this type of support needs to be managed and prioritised by infrastructure staff using a national ticketing system. NAISS is finalising agreements whereby the universities that will fund this level of support will contribute 1-4 million SEK each to provide nationally available application experts whose work will be steered and prioritised entirely by NAISS. Defining these scientific areas and how researchers will collaborate with these application experts is an important topic for the first NAISS User Forum in December this year.
- **Tier-3 support consists of highly advanced tasks** where staff whose profiles are dedicated to specific research areas will spend months or years

What is SeRC?

The Swedish e-Science Research Centre (SeRC) has been funded by the government's Strategic Research Area (SRA) initiative since 2010. The universities that are involved in SeRC are the KTH Royal Institute of Technology, Linköping University, Stockholm University and the Karolinska Institute, and some of SeRC's most important achievements have been summarised in a brochure that is readily available on the SeRC website: https://e-science.se. The centre funds about 40 principal investigators (PIs) through its Multidisciplinary Collaboration Programs (MCPs) in several areas. In each MCP, there are a number of collaborating projects, where each of the more application-oriented projects must clearly define how collaboration with a more method-development-oriented project is achieved, and vice versa. An important aspect within each MCP is the involvement of key e-science experts, often designated as RSEs (Research Software Engineers). This way, substantial collaboration has been achieved between method-development researchers and researchers from application areas, directly contributing to the success of SeRC.

writing new software, developing methodology, co-designing activities, and taking extensive responsibility for evolving the infrastructure in close collaboration with researchers who use the software. This category of support staff is expected to achieve independent international recognition from the impact of their work, and, according to the NAISS agreement with VR, these staff are entirely the responsibility of the higher education institutions. This level of support will be organised and steered independently of NAISS, and the resources available to different researchers and research fields will depend on investments by them and their universities. Some educational institutions – in particular KTH – have declared that their previous substantial co-funding to SNIC will now be directed towards this advanced level of support. It is important that other institutions follow this lead, and the SeRC universities (KTH, LiU, SU and KI) are well on the way to establishing and coordinating such activities. In the discussions so far, it has become apparent that the confusion between the tier-2 and tier-3 levels of support needs to be avoided, and we thus use the international designation "Research Software Engineer" (RSE) for the tier-3 most advanced level of expertise.

Organisation of RSEs and SeRC's Role

It is critical that the most advanced (RSE) user support is organised based on research areas and that RSE resources are prioritised long-term and controlled by the people whose research activities have a significant impact. However, this approach engenders an expectation that those researchers should take a share of the responsibility for funding the RSE organisation that provides the tier-3 support. SeRC has, in fact, built up such a support organisation over the last decade or so, and that organisation has contributed to creating research environments that have attracted several grants from the European Research Council (ERC) and the Knut and Alice Wallenberg Foundation (KAW), Centre of Excellence grants from VR, research grants from businesses, as well as co-funding from other infrastructure organisations and hardware vendors. These research environments encompass some of the SeRC universities' most internationally cited researchers.

SeRC's existing RSEs define the highest level of expertise in the infrastructure, and since they also have broad high-performance computing (HPC) experience, we have seen that they are often asked to help with general infrastructure tasks. However, the RSE role is separate from the tier-2 support tasks or administration. The RSE work should be organised in application domain teams with at least one scientifically responsible PI, and the practical RSE work is expected to take place equally divided between research groups and the common RSE environment at a centre. The long-term prioritisation between different scientific areas must be determined both by the likely scientific impact and demonstrated ability of the researchers to contribute funding to the common RSE environment. Together with the team lead, the scientifically responsible researchers should report annually how the support is used, for example, by giving details of how it defines the international infrastructure frontier, how the experts share their achievements through presentations and organising symposia at international HPC infrastructure venues such as PASC, ISC and SC, and how they build cross-disciplinary interactions with other RSE teams.

Lessons Learned from SeRC's Programs

Some of our ideas are based on experiences from SeRC's Multidisciplinary Collaboration Programs (MCPs), where research teams include researchers working on applications, method development, and core infrastructure. One of the most successful programs is the SeRC Efficient Simulation Software Initiative (SESSI), where researchers in the areas of Computational Fluid Dynamics (CFD) and Molecular Dynamics (MD) have been collaborating with computer scientists and programmers. The program has been going on for a decade and has had the main goal of further developing the GROMACS MD software and the derivatives of the Nek5000 CFD code to make them ready for exascale computer hardware, particularly making them run efficiently on graphics processing units

(GPUs) and other types of accelerators. While the work of these teams had already had an extensive scientific impact, there are broad shared sentiments that the work in SESSI required the RSEs to become much more professional and identify themselves internationally in the RSE role rather than only working in a research group. This, in turn, has led to dozens of new grants for infrastructure and has also been a key enabler for high-profile funding, for example, from ERC and KAW. The SESSI program has also resulted in significant cross-disciplinary information sharing that led to software being extensively rewritten, including a completely new code, Neko, that scales on the largest available GPU machines and that is a finalist for the 2023 Gordon Bell prize at the time of writing.

What are the success factors that we can identify in this program, and how can they be translated into requirements for the organisation of the RSE teams at the SeRC universities?

1. **The recruitment and identification of competent researchers** (from the professors and senior scientists leading the research to the researchers, postdocs and Ph.D. students performing much of the detailed work) is vital.
2. **Starting with concrete code and concrete science cases** is a key element, otherwise the different members of the team will not be able to work together efficiently but will tend to work on their own individual research problems instead of the complex multidisciplinary task of developing software that can actually solve an important scientific problem. There needs to be a critical path for advancing the science case, not just working on prototypes or general HPC activities, and the progress has to be measured by the progress being made towards this goal.
3. **Having a long-term strategic vision** is important as it takes time to achieve impact, and hence, it is imperative to focus on achievements that will have a major impact not just on science, but also within the international infrastructure landscape. This, in turn, requires a long-term commitment of resources, in particular resources that act as bridging funding when, for example, external EU project funding fluctuates. The new approach (whereby universities directly provide funding for RSEs) should strive to have a similar long-term nature, and the long-term focus must be maintained by a continued focus on concrete science cases and what is needed by the advanced research groups. There needs to be an organisation at the computer centres for the RSEs that the domain scientists can work with in the long term.
4. **Shorter-term complementary funding is needed for the RSE teams.** In order to keep focusing the work on concrete science cases, there needs to be shorter-term complementary funding. This is primarily done by writing and executing successful applications for additional funding. The shorter project funding is also very important to ensure that the researchers and the RSE teams have sufficient excellence and produce scientific results of sufficient quality. All of the MCPs initiated and funded within SeRC have had the requirement that SeRC cannot be the sole funder of the research, and this has been important for the scientific excellence of the work that has been performed.
5. **The focus needs to be on internationally leading software.** As mentioned, it is necessary to engage internationally excellent researchers in the software development processes, but the software itself also has to be internationally leading, meaning that it has to be top quality, have a large userbase, or feature some other high-impact aspects that mean that the people working on the software (in contrast to the scientific applications) will participate in international research and infrastructure collaborations. An excellent example is the GROMACS software, which clearly excels in both aspects. This means that one focus of the RSE team is the impact of the software itself as a success factor within academic research and education or in industry.

We believe that these success factors for the development of the codes for MD and CFD are generally applicable but may need to be developed further to also include the needs of additional areas within e-science.

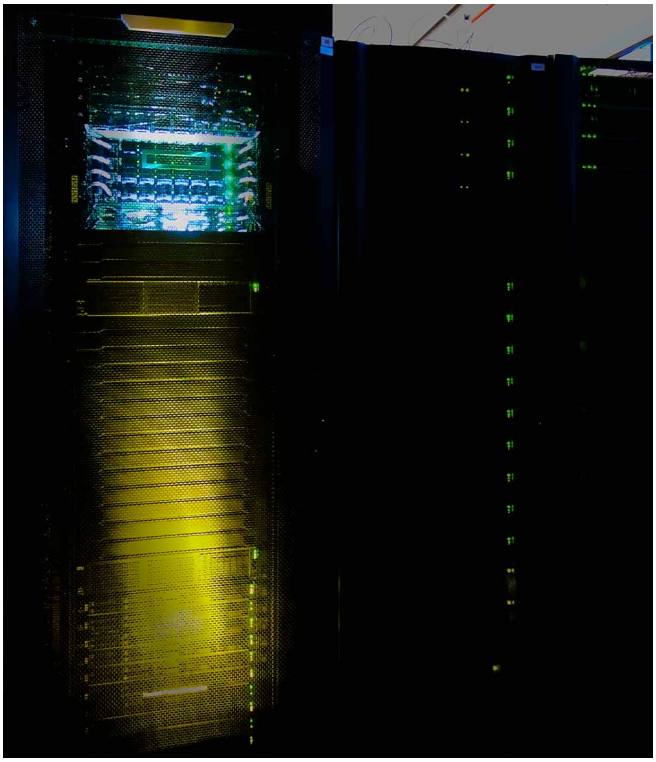
Dardel Status

Gert Svensson, PDC

As reported in the Dardel Inauguration article in this newsletter, Dardel was officially inaugurated on the 23rd of August to celebrate the fact that all the hardware for the system was in place. There is still work being done to get the system functioning optimally – much of the complexity is arising from the current cluster manager software, a relatively new product called CSM. Dardel is also still in the process of being updated to a more recent version of the software stack (known as "Raspberry").

Proposal to Replace CSM

Hewlett Packard Enterprise (HPE), the company that delivered the Dardel system, has suggested changing the current cluster manager, CSM, to another cluster manager called HPCM. HPCM is a less complex cluster manager that has worked well on other cluster installations for many years. HPE has recently provided PDC with a test rack for HPCM (at no additional cost), and the first tests with this manager are being performed as this article is being written. This test rack makes it possible to test HPCM and any future versions of the entire software stack without affecting the stability of the production system. If everything goes well, the aim is to switch all of Dardel over to HPCM and the latest software stack before the summer of 2024. We hope this will lead to a system that is considerably easier to manage and more stable.



Above: HPCM test rack on the left in the photo

Status of Dardel

A new software stack, Raspberry, is now installed on Dardel in parallel with the previous software stack, which is known as Strawberry. Raspberry is now configured and is undergoing an internal test (by PDC) to determine whether recompilation of all or only some applications is needed. Information for user testing will be sent out when the internal testing has been completed. We are promised that the annoying Lustre bug (resulting in SIGBUS crashes) has been corrected in Raspberry.

Compensation for Delays

The Dardel project has been considerably delayed by the vendor, and, in accordance with the contract, PDC is entitled to compensation for that. The compensation can be used to improve and extend the system. For example, it could be used to purchase more GPUs or some newer GPUs for testing purposes, or to adapt the storage system for other types of workloads. Researchers who are using Dardel are invited to contact PDC at support@pdc.kth.se and give input and suggestions about how the compensation could be used to upgrade, improve or extend the system: what would be most useful for your research? A minor lack of performance in the GPU benchmarks has already resulted in six more GPU nodes that will be installed during the spring of next year.

Above: PDC will receive three of these GPU blades as compensation, which will provide a total of six nodes with four GPUs each.

Below: Trish Damkroger (a Senior Vice President at HPE) and Jay Kirkland (a Corporate Vice President at AMD) with Dardel during a tour of the PDC computer room that was part of the Dardel Inauguration on 23 August 2023

Sweden's Most Powerful Supercomputer Inaugurated at KTH

Gert Svensson, PDC

The fastest supercomputer in Sweden, an HPE Cray EX system called Dardel, was inaugurated at the KTH Royal Institute of Technology in Stockholm on the 23rd of August 2023.

Dardel is one of the flagship supercomputers of the recently established National Academic Infrastructure for Supercomputing in Sweden (NAISS) and is hosted by the PDC Center for High Performance Computing at KTH. About 150 people attended the inauguration in person, while others participated via Zoom. NAISS and PDC were glad to welcome HPE and AMD (the companies that supplied Dardel and processors for the system, respectively), as well as representatives from other high-performance computing (HPC) centres and organisations, including attendees who travelled from other European countries, the USA and further afield in Sweden. It was great for there to be such a turnout from the HPC research community in Sweden, including researchers from various companies and academic institutions.

The inauguration program was hosted by Patrick Norman (Director of PDC), and included speeches by Anders Söderholm (President of KTH), Gert Svensson (Deputy Director of PDC), Jan-Eric Sundgren (Chairman of the NAISS Steering Committee), Katarina Bjelke (Director General of the Swedish Research Council), Trish Damkroger (a Senior Vice President from HPE), Jay Kirkland (Corporate Vice President for Platform Solutions Engineering from AMD) and Niklas Melin (Head of Simulation Enablement at Scania). In addition, there were tours of the PDC computer hall, and three of the research codes

Above: (From left to right) Anders Söderholm, Katarina Bjelke, Erik Lindahl, Björn Nilsson, Damien Declat, Aldert Groenenberg, Gert Svensson, Jan-Eric Sundgren, Trish Damkroger, Jay Kirkland, and Patrick Norman in front of one of the rows of cabinets that house the Dardel system

that are developed at PDC – GROMACS, Neko and VeloxChem – were presented by Erik Lindahl, Niclas Jansson and Patrick Norman, respectively. The event concluded with Ingemar Lindahl and Teresa Wennberg giving presentations (including a fascinating video) about Nils and Thora Dardel, in honour of whom the Dardel system is named.

The Dardel system has two partitions: the GPU partition, which is housed in one of the cabinets just behind the speakers in the photos on the previous page, features AMD Instinct™ MI250X GPUs and was the 5th most energy-efficient supercomputing system in the whole world, as noted in the June 2023 Green500 list. The GPU partition was 77th globally in terms of speed (see the June 2023 TOP500 list), while the CPU partition was in 153rd place in the TOP500 list for June 2023. The CPU partition is based on AMD EPYC™ processors, which are also utilised in the nodes of the GPU partition.

Katarina Bjelke, Director General of the Swedish Research Council, was one of the speakers during the inauguration and highlighted the importance and benefits of Dardel being the foremost supercomputer in Sweden.

"Dardel will be Sweden's fastest and most energy-efficient supercomputer to date, and one of the most environmentally friendly also in the world when viewed from the point of climate impact per number of calculations.

Above: Katarina Bjelke speaking at Dardel Inauguration

Large number crunching machines have had an ever-increasing importance for research and innovation, and their importance will get only bigger and bigger. They are now critical in most areas like (as we heard today) climate research, energy transition but also drug discovery and security, just to mention a few. For example, supercomputers have been used for the benefit of society for fighting organised crime, mitigating the effects of the COVID-19 pandemic, and they are also routinely used in forecasting extreme weather events. Probably very useful this last summer also.

So, for Sweden, whose economy heavily relies on the export of world-leading technology across many sectors, it is extremely crucial to have access to international competitive facilities for data analysis, simulation and artificial intelligence, and Dardel takes Sweden in the right direction here."

You can hear Katarina's comment here: play.kth.se/media/Katarina+Bjelke+at+Dardel+Inauguration/0_n13z12pz.

Swedish high-performance computing research is certainly going in the right direction: **a group of researchers, led by Niclas Jansson at PDC, have been selected as finalists for the Gordon Bell Prize, which is regarded as the equivalent of the Nobel prize for computing**. As Patrick Norman, Director of PDC, said at the inauguration:

"Now (we] can proudly say that we, for the first time ever in the Swedish history, we have a finalist in the selection for the Gordon Bell prize. [...] (Someone is cheering for that, and that is certainly warranted!) So, we are one out of six finalists, and the winner will be announced in this year's supercomputing congress in Denver. And, well, cutting out the text from Wikipedia gives you an idea of how big this is.

"The **Gordon Bell Prize** is an award presented by the Association for Computing Machinery each year in conjunction with the SC Conference series (formerly known as the Supercomputing Conference). The prize recognises outstanding achievement in high-performance computing applications. The main purpose is to track the progress over time of parallel computing, by acknowledging and rewarding innovation in applying high-performance computing to applications in science, engineering, and large-scale data analytics." *Wikipedia*

Below: Niclas Jansson (left) being congratulated by the PDC director, Patrick Norman (right)

This is kind of mentioned as the Nobel Prize in supercomputing. And it goes to an outstanding achievement in the development of applications. And I would like to take the opportunity and invite the lead developer of this software program [Neko] to the floor and make him visible. That's Niclas Jansson."

You can hear Patrick congratulating Niclas here: play.kth.se/media/Patrick+Norman+at+Dardel+Inauguration/0_f2mqe000.

Trish Damkroger, a Senior Vice President from HPE, added her congratulations.

"I would like to also send my congratulations to Niclas for the Gordon Bell finalist award [...] that is quite an achievement to be a finalist in what is truly the Nobel prize for supercomputing."

You can hear Trish's congratulations here: play.kth.se/media/Trish+Dammkroger+at+Dardel+Inauguration/0_ubtp4hx3.

Jay Kirkland, Corporate Vice President for Platform Solutions Engineering from AMD, also commented on how impressive this achievement of the Neko development group is.

"Congratulations Niclas. You're going to hear that from everybody, I know. I mean, that award is an amazing award. Ever since I've been [...] really working on HPC, I've heard about this award being the Nobel Prize for this area, so to be in the finalist there is, you know, awesome."

Jay can be heard congratulating Niclas here: play.kth.se/media/Jay+Kirkland+at+Dardel+Inauguration/0_siatkm31.

The Neko software is used for computational fluid dynamics simulations, which are essential, for example, in the development of greener vehicles, aircraft and sea-faring vessels, as well as for arranging arrays of wind generators so as to be maximally efficient. Neko is designed to make it easy to run these types of simulations on today's massively parallel pre-exascale systems.

In addition to Neko, staff from PDC are involved in developing several other world-leading software applications for high-performance computing research, including GROMACS and VeloxChem. GROMACS supports simulations of biomolecular systems at varying levels and is one of the most widely used scientific software packages in the world, while VeloxChem is a quantum chemistry software application for calculating molecular properties and simulating spectroscopies. As Patrick Norman (Director of PDC) noted, KTH is "not only focusing on hardware and bare metal but also on companioning software for science and engineering applications", which is vitally important these days as "having a supercomputer without proper applications is a little bit like having a synchrotron without beam lines". The support KTH is providing so that PDC "can really do sustainable software development in the future" is therefore very important for future HPC research both in Sweden and globally, as the GROMACS, Neko and VeloxChem codes are all provided as open source.

Furthermore, **KTH and PDC are making significant contributions to HPC research on a European level as PDC is leading three of the ten European Centres of Excellence (CoEs)** that were awarded funding by the European High Performance Computing Joint Undertaking (EuroHPC JU) at the start of 2023: CEEC, BioExcel and Plasma-PEPSC. **KTH and PDC**

are also partners in two other European CoEs: EXCELLERAT (which is another of the ten EuroHPC JU CoEs funded in 2023) and PerMedCoE (which is funded by the EU Horizon 2020 research and innovation programme).

Anders Söderholm, the president of KTH, noted that:

"KTH-PDC has also been successful in the European arena and leads four out of ten centres of excellence, right? They were launched in January this year by the European High Performance Computing Joint Undertaking to support research and innovation with the help of HPC and building even stronger and faster high-performing computer systems. And that is one of the key indicators, I would say, that there is a really successful team here. We can thank Dardel and our excellent resources for this."

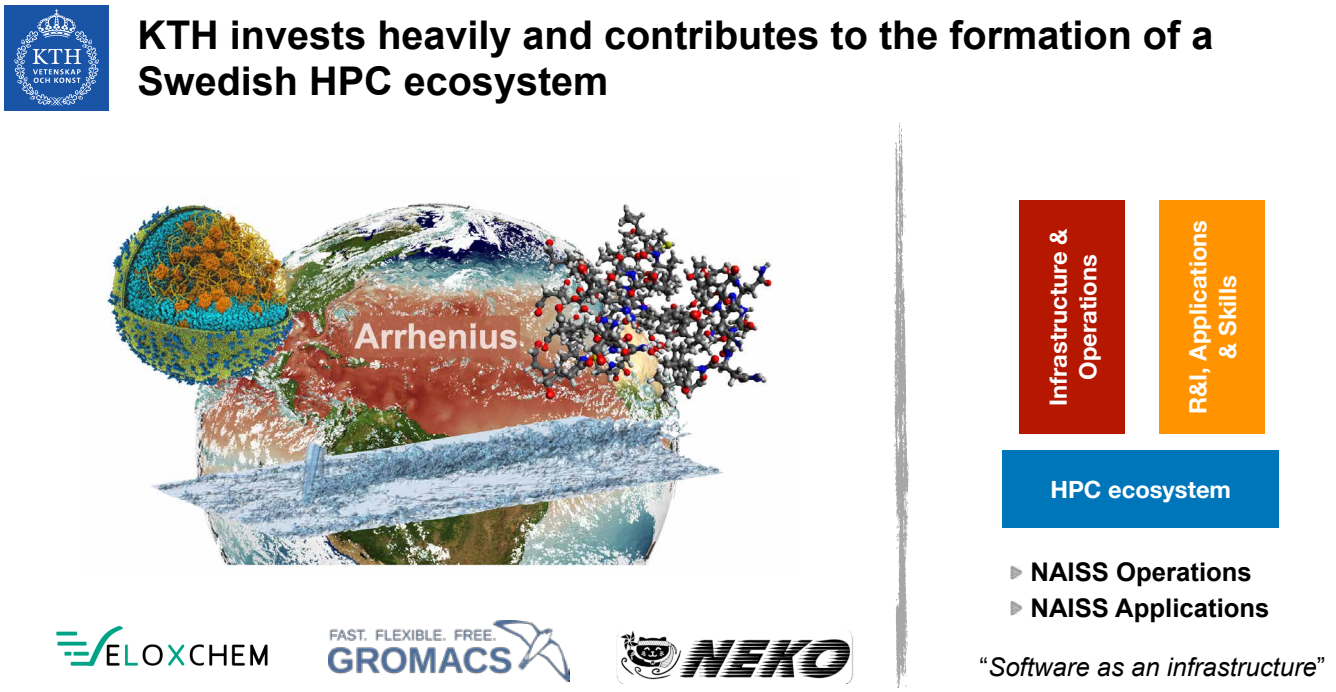
You can listen to Anders here: play.kth.se/media/Anders+S%C3%B6derholm+at+Dardel+Inauguration/0_6q3t9foo.

To support HPC research in Sweden and Europe, **PDC/KTH is also collaborating with NAISS on a project to establish a mid-range supercomputer system (called Arrhenius) in Sweden in the near future**. NAISS recently applied for a grant from EuroHPC to fund the system, and Patrick Norman, the Director of PDC, helped to author the application, which was approved very rapidly by EuroHPC. Jan-Eric Sundgren, Chairman of NAISS, explained about NAISS' ongoing process to establish Arrhenius.

"We have written a proposal to EuroHPC. I say we, I didn't really mean we: [...] three persons, [...] Patrick, Eric and Matts Karlsson [...], mainly did the job. And that [proposal] was submitted on the 14th of February this year and granted almost 250 million on the 15th of June. I have been working in my previous capacity at Volvo and at Chalmers with EU a lot, and by far, this is the fastest response I've ever heard of. And it also got extremely good grades. So, I think we are grateful to the writing team that did a fantastic job.

So, what is now in the pipeline? We are discussing with EuroHPC, we are discussing with VR [the Swedish Research Council] to secure the remaining resources that we lack from the Swedish government. And I'm very optimistic that this will be done during the course of this autumn such that we can start the procurement process in 2024 and have a system, sort of delivered, hopefully the first part of 2025."

You can hear Jan-Eric discussing progress on the Arrhenius project here: play.kth.se/media/Jan-Eric+Sundgren+at+Dardel+Inauguration/0_fu5682bb.



Above: Slide from Patrick Norman's introduction to the inauguration showing some of the major ways in which KTH and PDC are supporting HPC research

We are all looking forward to this new system, which will be beneficial for both academic and industrial research in Sweden by extending Sweden's computational capacity for research by an order of magnitude. Meanwhile, PDC will continue with the developmental work on a range of software applications to make sure they can easily be ported from running on Dardel to the even more massively parallel and faster Arrhenius system.

If you missed attending the Dardel Inauguration in person, you are welcome to catch up on the talks here.

- Inauguration speeches: play.kth.se/media/Dardel+inauguration+-+part+1/0_z6p009hb
- Presentations about GROMACS, VeloxChem and Neko: play.kth.se/media/Dardel+inauguration+-+part+II/0_m3dwssh4

However, please note that, for copyright reasons, the talks and film about the lives of Thora and Nils Dardel are not included. Those of you who speak Swedish can also read more about the inauguration of Dardel in the articles below.

- sverigesradio.se/artikel/har-ar-kths-nya-superdator-snabbast-i-sverige (in Swedish)
- www.nyteknik.se/tech/nya-svenska-superdatorerna-ska-gora-avancerad-forskning-mojlig/4188863 (in Swedish)
- www.teknikaliteter.se/2023/10/03/tolv-petaflops-som-i-en-liten-ask (in Swedish).

Lastly, if you are interested in using Dardel for your academic or industrial research, please get in touch with PDC Support (support@pdc.kth.se).

Left: Mentors and attendees at the Learn to Code GROMACS workshop, 7-8 September 2023, KTH, Stockholm Photo courtesy of Akash Deep Biswas

Workshop: Learn to Code in GROMACS

Alessandra Villa, PDC

The GROMACS team at PDC and SciLifeLab ran a workshop on learning to code in GROMACS (https://www.gromacs.org/workshop.html) on the 7th and 8th of September at PDC, which brought together six mentors and twelve attendees from different European countries and from both the academic and industrial worlds. There were two days of lectures and hands-on sessions. On the first day, Sebastian Wingbermühle (from the Department of Applied Physics at the KTH Royal Institute of Technology) introduced "GROMACS GitLab and version control" and, in the afternoon, Mark Abraham (former GROMACS development manager) spoke about "Software structure and interface". The following day, Andrey Alekseenko (from the Department of Applied Physics at KTH) gave a presentation on "Testing and testing infrastructure", and then Berk Hess (from the Department of Applied Physics at KTH) closed with "Everything around coding", a historical overview of GROMACS developments. During the hands-on sessions, the attendees worked closely together with mentors and addressed open issues with GROMACS and got directly involved in the review processes.

The idea of a workshop to learn to code in GROMACS came from the challenge of on-boarding new developers. After brainstorming within Stockholm's GROMACS team, the discussion moved to the broader user community in order to understand their needs and interests. The workshop was the result of a collective effort and was a significant success. Overall, the feedback from the attendees was very positive; in particular, what they enjoyed most was the direct interaction with the mentors. Some people thought the workshop was too short, and others would have appreciated more time for the hands-on session, which shows how useful the workshop was. A big "thank you" to the mentors: Andrey, Berk, Magnus, Mark, Sebastian and Vedran!

ENCCS
EuroCC National Competence Centre Sweden

ENCCS Highlights 2023

Thor Wikfeldt & Apostolos Vasileiadis, ENCCS

The ENCCS team is excited to share some achievements from the first year of our second project phase (2023-2025). As a dynamic partnership between RISE and Linköping University, ENCCS has grown to a team of ten poised to tackle any industrial high-performance computing (HPC) project, organise and deliver interactive training events in multiple domains, and reach out to emerging HPC user communities across industry, academia, and the public sector.

We continue our dedicated efforts assisting companies and public authorities to utilise supercomputing systems to enhance their R&D productivity and competitiveness. Collaborations with small to medium-sized enterprises (SMEs) – such as Nilar, which automates battery inspection using AI vision, and Compular, which develops cutting-edge analysis tools for molecular dynamics simulations – as well as publicly funded authorities, like SLB-Analys and SMHI, have demonstrated the transformative power of HPC in multiple sectors. Success stories from our industry and public sector partners can be found at https://enccs.se/success-stories.

Training is another focus area for ENCCS. During 2023 we have organised 14 workshops and other events in collaboration with, among others, NVIDIA, AMD, NSC, RISE, TREX CoE and WACQT on topics including the effective usage of HPC software packages (like VASP and the CHAMP quantum Monte Carlo code), deep learning methods (like transformers, graph neural networks and scientific machine learning), GPU programming, HPC programming in Julia and Python, and quantum computing. Upcoming and past events can be found at https://enccs.se/events, while training material from past events can be found at https://enccs.se/lessons.

Above: The ENCCS team in Stockholm, June 2023

Below: ENCCS director Thor Wikfeldt at the National Supercomputer Centre (NSC) in Linköping with the rest of the team taking a tour of the machine room currently housing the Berzelius and Tetralith systems and in coming years eventually Arrhenius

Beyond our individual endeavours as a national centre, ENCCS is also deeply committed to European collaboration through the EuroCC, CASTIEL and Centre of Excellence (CoE) networks, where we contribute to a shared pool of expertise and useful resources. This interconnectedness fosters a thriving ecosystem of HPC excellence across Europe.

In an exciting recent development, the new EuroHPC supercomputer, Arrhenius, is set to be installed at the National Supercomputer Centre (NSC). ENCCS will play a pivotal role in enabling companies and the public sector to harness the immense potential of this cutting-edge resource.

ENCCS stands at the forefront of propelling businesses and institutions into a future powered by supercomputing. With collaboration, high expertise and effective education as guiding principles, we are committed to advancing the frontiers of HPC both nationally and across European borders.

If you want to stay up to date with our events and current work, be sure to subscribe to the ENCCS newsletter (https://enccs.se/newsletter) and follow us on LinkedIn (https://www.linkedin.com/company/enccs) and on X (https://twitter.com/EuroCC_Sweden).

EXCELLERAT P2

Adam Peplinski, Department of Engineering Mechanics, KTH

The European Centre of Excellence (CoE) for Engineering Applications, EXCELLERAT, has entered its second phase (known as EXCELLERAT P2) and is continuing its mission of supporting key engineering industries in Europe. This CoE is a conglomerate of business partners and high-performance computing (HPC) centres promoting interaction between academic research and code development with industrial partners.

PDC and the Department of Engineering Mechanics at the KTH Royal Institute of Technology were partners in EXCELLERAT P1 (the first phase of the project) and continue their involvement in this project working in the field of turbulence simulations. During EXCELLERAT P1, the main focus was on the development of a robust adaptive mesh refinement (AMR) workflow and uncertainty quantification (UQ) tools in a computational fluid dynamics (CFD) solver known as Nek5000 (which was originally developed by the Argonne National Laboratory, US).

In the second phase of the project, PDC introduced a new CFD solver, Neko, which is entirely developed at PDC. Both solvers, Nek5000 and Neko, are based on a high-order spectral element method (SEM) and are capable of performing high-fidelity simulations of advection-diffusion problems. They share multiple features and Nek5000 can be seen as Neko's predecessor. However, unlike Nek5000, Neko is a modern piece of software, which is written mostly in object-oriented Fortran 2008. It supports multiple hardware backends by defining a device abstraction layer and then writing hardware-specific kernels in CUDA, HIP or OpenCL. Neko was tested on multiple systems showing very good strong scaling properties, achieving 80% parallel efficiency when using up to 80% of the GPU partition of the LUMI system based in Finland, which is equivalent to 16,384 AMD MI250X Graphics Compute Dies (GCDs) where each MI250X GPU consists of two GCDs.

In EXCELLERAT P2, KTH continues its previous work on high-order hex-based meshing, AMR workflows, UQ techniques, in situ visualisation and improving the parallel performance of the solver, but this time in the context of Neko. Although this already covers multiple aspects of simulation workflows, there are new features

Staff Focus

Juan de Gracia

Juan de Gracia recently joined PDC as an application expert.

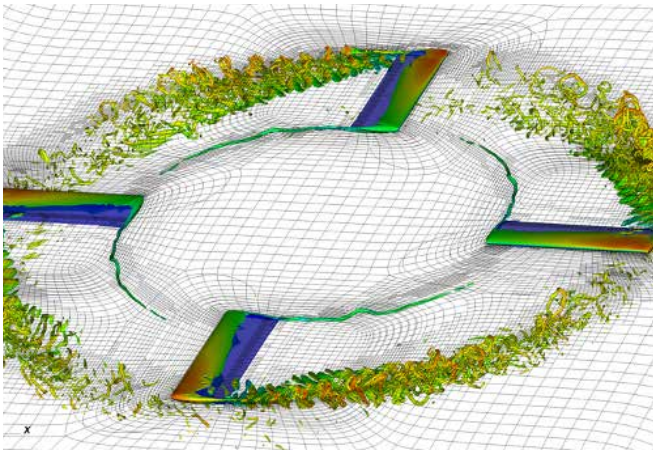
Juan earned his Ph.D. in Theoretical Chemistry from the KTH Royal Institute of Technology in 2022 under the guidance of Prof. Mårten Ahlquist. His doctoral research focused on catalysis using a multiscale modelling approach. During his Ph.D., Juan made contributions to the development of the VeloxChem software.

Following his Ph.D., Juan pursued a postdoctoral position at Chalmers University of Technology in Gothenburg, where he delved into quantum computing for quantum chemistry, specifically exploring the implementation of quantum chemistry algorithms on quantum computers.

At PDC, Juan's responsibilities include working on the interoperability between GROMACS and VeloxChem in collaboration with Mathieu Linares, conducting chemical reactivity modelling in VeloxChem, and exploring semi-empirical methods such as Empirical Valence Bond Theory.

In his leisure time, Juan enjoys bike rides, playing and listening to music, and, during the winter months, taking bracing cold dips in the lake.

Below: Vortical structures identified using lambda2 criterion for the "toy" rotor case simulated within EXCELLERAT P1



being considered in the second phase. These are in situ data analysis using streaming algorithms and noise prediction for incompressible CFD solvers. The first one is motivated by the wide use of data analysis algorithms – such as proper orthogonal decomposition (POD) or dynamic mode decomposition (DMD) – which rely on large amounts of data being saved to the disk and then analysis being performed at the post-processing step. However, this approach will not be feasible for exascale modelling due to the massive volumes of data and the cost of the I/O operations. That is why KTH is going to implement proper streaming algorithms for POD and DMD in Neko to avoid storing data on the disks and to extract the expected results on the fly during the simulation. In addition, the noise prediction will make it possible to utilise high-quality data and obtain good approximations for the far-field acoustics.

The use case being studied during the second phase of EXCELLERAT is the continuation of one of the use cases from the first phase: "High-fidelity simulation of rotating parts". The code development enabled us to execute a simulation of a "toy" rotor with the AMR version of Nek5000 at the end of EXCELLERAT P1 (see figure above). Now we are going to extend it to the industrially relevant "Iowa" rotor, which is a double blade, twisted drone rotor with an Eppler E64 wing profile. We are going to demonstrate all of the EXCELLERAT P2 development with this particular use case, which will include performing AMR, UQ, acoustics and POD/DMD in situ.

BioExcel Activities 2023

Alessandra Villa & Rossen Apostolov, PDC

The BioExcel Centre of Excellence for Computational Biomolecular Research (BioExcel CoE, https://www.bioexcel.eu) has been actively involved in supporting the biomolecular simulation research community for many years now. As a result of BioExcel's successes in previous years, funding for the CoE was renewed for a further stage of the project, BioExcel-3, which began at the start of 2023. During 2023, the CoE has continued to provide support and training with activities such as the popular BioExcel summer schools and webinars and also introduced new initiatives, such as the Ambassador Programme.

Summer School

The BioExcel Summer School is one of the centre's most successful initiatives that targets early-stage researchers. This year's summer school was held in Sardinia and ran from 10-15 September 2023, where the trainers and attendees were very excited to meet each other. The 2023 summer school (https://bioexcel.eu/events/bioexcel-summer-school-on-biomolecular-simulations-2023) covered topics such as molecular dynamics simulations, biomolecular docking, free energy calculations, advanced sampling methods, and BioExcel Building Blocks (BioBB). The school also featured guest lectures

Above: BioExcel Summer School lecturers and participants, 10-15 September 2023

Below: BioExcel Summer School "sands-on exercises" during outings to nearby beaches at Pula and Nora, September 2023

on quantum mechanics/molecular mechanics and machine learning, plus a poster session and a career session. You can read more about the 2023 school at https://bioexcel.eu/bioexcel-summer-school-on-biomolecular-simulations-2023-helping-to-develop-the-next-generation-of-computational-biomolecular-researchers. As is usually the case, there was a lot of positive feedback from the people who attended the school. This is a typical example of what the attendees thought were the best aspects of the school.

> *"In conclusion, the quality of teaching, the ratio of breaks/lectures, and the overall vibes made this summer school a life experience that I would forever cherish and recommend anyone to participate in."*

> *"The willingness of organisers and trainers to help and discuss many kinds of subjects. Having close interaction with colleagues at different levels of expertise and different backgrounds. Having and promoting a nice and healthy way of community."*

Ambassador Program

One of BioExcel's strategies to achieve impact in the high-performance computing (HPC) life sciences community is through a newly launched Ambassador Program. The program aims to establish strong connections with the local communities in EuroHPC and to increase the uptake of HPC in general, as well as of BioExcel tools and expertise. One of the activities within the ambassador programme is the co-organisation of BioExcel workshops and training events tuned to the needs of the local communities. In principle, the BioExcel Summer School could be considered as one of the precursors of those activities as it provides a good general overview for researchers starting out in the biomolecular simulation area. In October this year, the first ambassador-driven workshop took place in Bratislava, where BioExcel co-organised a GROMACS-HADDOCK workshop (https://bioexcel.eu/events/bioexcel-eurocc-workshop-focused-on-gromacs) tuned to the needs of the Hungarian, Austrian, Slovakian and Czech Republic research community. The local community was in charge of the logistics, while BioExcel provided trainers and training materials. You can read more about the workshop here: https://bioexcel.eu/joint-bioexcel-eurocc-ambassador-program-workshop-in-bratislava-reaching-out-to-the-biomolecular-simulations-community-in-central-europe.

Other Activities

BioExcel is involved in a lot of initiatives to support the biomolecular simulation community and PDC has been a leading force, not only in the Summer School and Ambassador Program, but also in many other activities such as:

- the BioExcel webinars (https://bioexcel.eu/category/webinar) which feature notable developments in the field of computational biomolecular research,
- BioExcel forums (https://ask.bioexcel.eu and https://gromacs.bioexcel.eu) to support the community, and
- training materials (which are freely available at https://bioexcel.eu/training-and-events) and the competency hub (http://krc.bioexcel.eu) where researchers can browse competencies, career profiles and training resources to advance their careers.

Above: Participants at BioExcel Ambassador Programme workshop in Bratislava, Slovakia, 18-19 October 2023

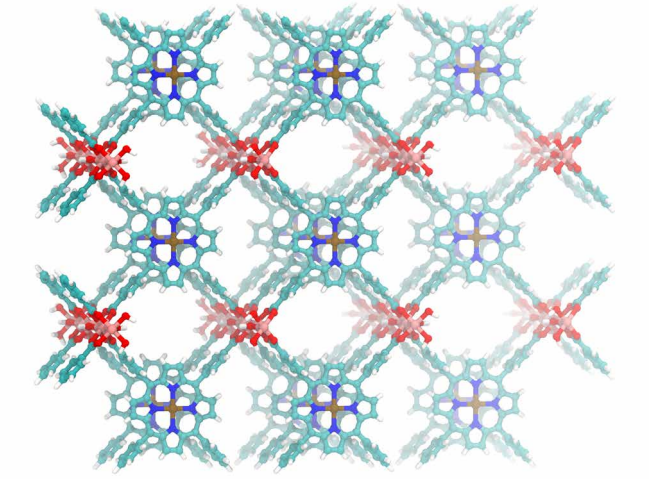
VeloxChem: Efficient Numerical Integration for Density Functional Theory

Xin Li, PDC, and Zilvinas Rinkevicius & Patrick Norman, Division of Theoretical Chemistry and Biology, KTH

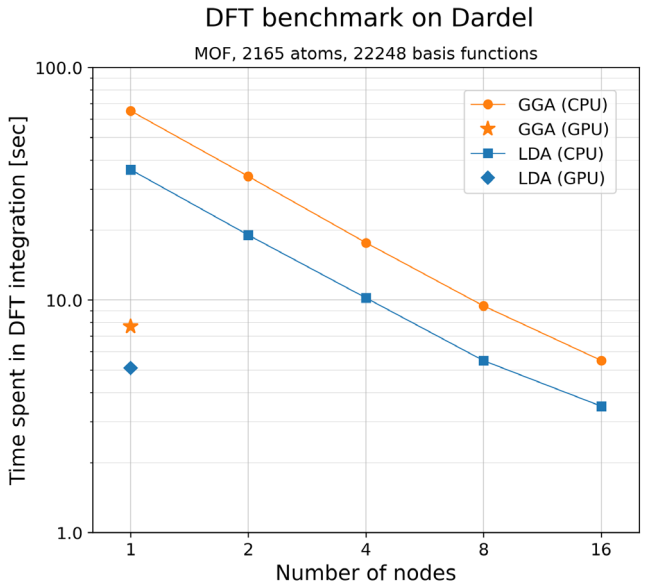
Density functional theory (DFT) is a widely used theoretical framework in the field of computational chemistry due to its versatility in the study of various systems and properties. It offers a favourable trade-off between accuracy and computational efficiency, which makes it particularly useful for investigating large and complex systems. DFT has, therefore, become an indispensable tool in scientific research and theoretical design of molecules and materials.

VeloxChem [1] is an open-source quantum chemistry software that was developed at the KTH Royal Institute of Technology for calculating molecular properties and simulating a variety of spectroscopies. VeloxChem offers DFT as one of its key features. In recent developmental work on the code, we have improved the efficiency of DFT numerical integration within VeloxChem, so now the exchange-correlation part can be run on computer systems featuring either CPUs or graphics processing units (GPUs). Conventionally, the computational cost of DFT is proportional to N^3 where N is the size of the system being studied; however, the numerical grid-based integration can, in practice, be done very efficiently by integrating over even-sized grid batches, such that the computational cost becomes asymptotically linear [2]. The key to such an efficient implementation is to make sure that the whole system is divided as evenly as possible into grid batches with almost constant computational cost on average. In VeloxChem this is done by repeated bisection of grid points into smaller and smaller boxes until the number of grid points in each box is below a given threshold. Due to efficient screening, the computational cost for processing each grid box will be almost constant on average, making it highly suitable for large-scale parallelisation.

Below: MOF structure used for testing DFT in VeloxChem



We tested the performance of DFT numerical integration in VeloxChem using a metal-organic framework (MOF) structure (illustrated above) that consists of more than 2,000 atoms. This is a very large system for quantum chemistry, and the number of basis functions exceeds 22,000, even for a moderate-sized basis set. Two flavours of DFT numerical integrations were tested on the Dardel compute nodes: the local density approximation (LDA), which is a rather crude approximation, and the generalised gradient approximation (GGA), which is more widely used in practice. Both LDA and GGA were tested by varying the number of Dardel CPU nodes that were used, and one can see from the solid lines in the graph below that the computational time decreases almost linearly



Above: Benchmark of DFT numerical integration on Dardel CPU and GPU compute nodes using MOF structure as a test case

in the logarithmic scale plot. We also tested the performance of LDA and GGA on a Dardel GPU node, as shown by the star and diamond markers on the graph. On a single GPU node, the time spent in LDA and GGA integration are 5.2 and 7.7 seconds, respectively. This is significant as it opens up the possibility of routine studies of large and complex chemical systems for scientific research in biochemistry, nanoscience and spectroscopy.

References

1. Z. Rinkevicius, X. Li, O. Vahtras, K. Ahmadzadeh, M. Brand, M. Ringholm, N. H. List, M. Scheurer, M. Scott, A. Dreuw, P. Norman. "VeloxChem: a Python-driven density-functional theory program for spectroscopy simulations in high-performance computing environments". WIREs Comput. Mol. Sci. 2020, 10:e1457. https://doi.org/10.1002/wcms.1457
2. J. Kussmann, H. Laqua, C. Ochsenfeld. "Highly Efficient Resolution-of-Identity Density Functional Theory Calculations on Central and Graphics Processing Units". J. Chem. Theory Comput. 2021, 17, 3, 1512–1521. https://doi.org/10.1021/acs.jctc.0c01252

Workshop on Quantum Scientific Applications

Stefano Markidis, PDC

In recent years, quantum computing has been making significant advancements. Tech giants like Google and IBM are racing towards the ambitious goal of reaching quantum systems with thousands of qubits by the end of this decade. While this quantum computing race develops, the big question remains: are we on the verge of realising practical and advantageous quantum computing scientific and engineering applications that can leverage this advanced quantum hardware?

In the history of computing, we have seen a pattern where hardware development outpaces the development of software and practical scientific and engineering applications. Like the early days of classical computing, quantum computing may soon be in a similar situation. To explore this issue, a workshop titled "Near-Term Scientific and Engineering Applications with NISQ Systems" was organised to critically examine the immediate potential of current quantum computer systems to solve scientific and engineering problems.

This workshop was supported by the KTH Digitalisation Platform and the Swedish e-Science Research Centre (SeRC) and hosted at KTH. Stefano Markidis and Ricardo Vinuesa organised the event and Digital Futures also contributed to the hosting. The workshop featured a diverse panel of internationally renowned speakers from various institutions such as MIT, Exeter University, Imperial College, the National Technical University of Athens, IQM, PASQAL, and Ericsson. Activities at the workshop included presentations, panel sessions on the prospects of scientific applications, and break-out group discussions.

A spectrum of important topics was addressed during the workshop discussions. Participants investigated quantum hardware co-design with scientific and engineering application development. Quantum scientific machine learning emerged as a significant point of interest, focusing on its potential to solve partial differential equations, which is a fundamental challenge in many scientific disciplines. Quantum lattice algorithms and quantum simulations were other key areas drawing significant attention.

The workshop outcomes shed light on the challenges and opportunities at the intersection of quantum computing and practical scientific and engineering applications. The result of the workshop will be shared with the broader community through a forthcoming position paper, offering a roadmap to quantum computing scientific and engineering applications.

Above: Panel session with (from left to right) Kevin Obenland (MIT), Panagiotis Barkoutsos (PASQAL), Muhammad Asad Ullah (Ericsson), and Stefano Markidis (KTH)

Introduction to GPUs Course

Johan Hellsvik & Jonathan Vincent, PDC

Supercomputers with both central processing unit (CPU) and graphics processing unit (GPU) nodes are heterogeneous systems which require programming models that can execute the calculations on the CPUs and GPUs in a stable and efficient manner. They are becoming the norm, compared to previously when many systems were solely based on CPUs. CPUs and GPUs are used for doing different types of calculation work. CPUs have large instruction sets and execute general code, whereas GPUs have smaller instruction sets that are tailored for running compute-intensive work in parallel on a large number of compute units (CU).

GPU computing is becoming increasingly important, and researchers are having to adapt older code to run on the newer GPU systems. To address this need, PDC staff members, together with experts from AMD, HPE and ENCCS, ran a course on GPU computing this autumn. The participants used the new Dardel system at PDC, which has 56 GPU nodes (each with four AMD MI250X GPUs) that are made available to Swedish researchers. Participants were given access to Dardel to run examples or their own code as part of the course. The course started with two online half-days in September followed by two days on-site at KTH in October.

During the course participants were introduced to writing code for GPUs using the programming models HIP, SYCL and OpenMP, as well as using tools such as AMD's Omnitools and the Cray Performance Tools to debug and optimise their GPU code. As exercise material, the participants were given serial code that was to be ported to GPU code in the respective frameworks. If you missed the course, the lesson material and exercises are hosted at the course's Git repository on GitHub: https://github.com/PDC-support/introduction-to-gpu.

PDC-Related Events

LUMI GROMACS Workshop

24-25 January 2024 (online)

Details will be available by early December at http://bioexcel.eu/events.

BioExcel Summer School

17-21 June 2024

Details will be available next year at http://bioexcel.eu/events.

PDC Summer School

last two weeks of August 2024, KTH main campus, Stockholm

Details will be available next year at https://www.pdc.kth.se/about/events.

BioExcel Conference

21-23 October 2024

Details will be available next year at http://bioexcel.eu/events.

HPC Sources

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

HPC in Sweden and Scandinavia

- ENCCS
  http://enccs.se
- NAISS
  https://naiss.se
- NeIC
  http://neic.no
- SeRC
  https://e-science.se
- SeSE
  http://sese.nu

European HPC ecosystem

- EOSC
  https://eosc-portal.eu
- ETP4HPC
  https://www.etp4hpc.eu
- EuroHPC
  https://eurohpc-ju.europa.eu
- HPC in Europe
  https://hpc-portal.eu
- LUMI
  https://www.lumi-supercomputer.eu
- PRACE
  https://www.prace-ri.eu

A selection of projects that PDC is involved with

- BioExcel CoE
  https://bioexcel.eu
- CEEC
  https://www.ceec-coe.eu
- EBRAINS
  https://ebrains.eu
- EUMaster4HPC
  https://eumaster4hpc.uni.lu
- EXCELLERAT
  https://www.excellerat.eu
- PerMedCoE
  https://permedcoe.eu
- Plasma-PEPSC CoE
  https://plasma-pepsc.eu

HPC news sources

- HPCwire
  http://www.hpcwire.com
- insideHPC
  https://insidehpc.com