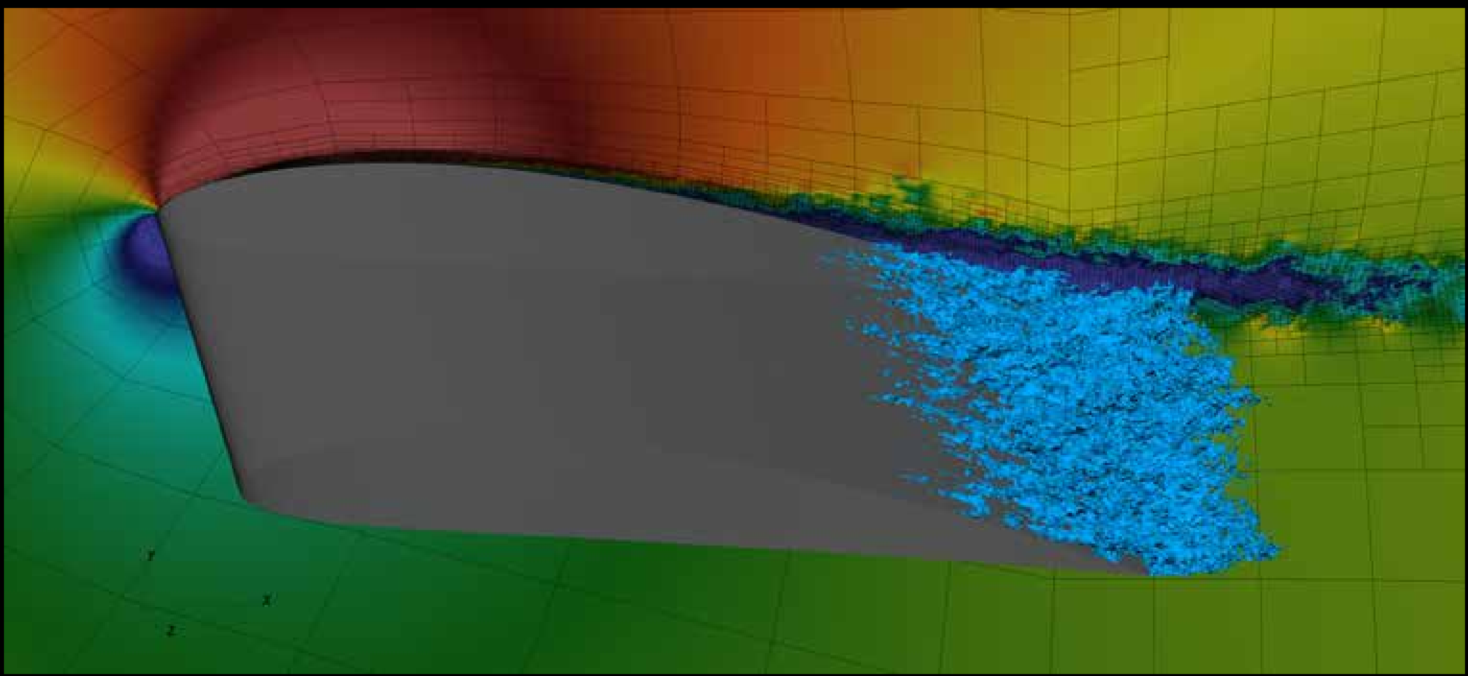
no.2 2021

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: Dirk Pleiter

Editorial staff: Genet Edmondson

Graphic Design: Maria Malmqvist

E-mail: support@pdc.kth.se

ISSN 1401-9671

Cover

During the final test phase of the new Dardel system at PDC, various research groups ran simulations on the system for a month. One of the pilot groups studied the air flow over aircraft wings and found excellent performance and stability with the new Dardel system.

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

At the end of a busy year that was overshadowed by restrictions related to the ongoing global pandemic, it is time to reflect on what has been achieved. In the last newsletter, we reported on the arrival of the first phase of the new Dardel supercomputer at PDC. Now we are proud that the system is available for researchers and is starting to fulfil its mission: to enable new and exciting research. To reach this point has involved overcoming more challenges than initially expected, but this is part of the risk when utilising brand new technology. It was right and important to make a forward-looking decision.

In his articles *Making Dardel Easy to Use* and *Dardel Update*, Gert Svensson highlights some of the changes PDC has introduced with Dardel, as well as various extensions to the system that are in the pipeline. The first users from different research teams in Sweden started to get access to the system in October as part of the final test phase. During this phase, both the supplier, HPE, and PDC tested the availability and stability of the system before final acceptance. Two of the teams present their first results in this newsletter. The team lead by Philipp Schlatter and Dan Henningson from KTH started to use Dardel for simulating wings (*Dardel-Pilots Simulate Wings Using NEK5000*), while Olle Eriksson's team from Uppsala University and their international colleagues show how to use the system for materials sciences (*Materials Theory Codes on Dardel at PDC*).

Together with our partners in Sweden, PDC continues to be involved in the evolution of the EuroHPC infrastructure. This opens up opportunities for Swedish researchers to leverage compute resources on upcoming pre-exascale systems like LUMI, for which access policies and mechanisms are now being established (*PRACE & EuroHPC JU Join Forces*).

For a research infrastructure provider like PDC, tight links to research are needed to ensure that it stays attuned to the needs of the researchers. In this newsletter, you will find two examples of PDC's engagement with research communities. Niclas Jansson and Jonathan Vincent describe how they and their colleagues are supporting the engineering community at a European level to get ready for exascale performance (*Towards Exascale in Engineering*). In the previous PDC newsletter, we briefly mentioned the exciting news that EBRAINS (the research infrastructure that emerged from the Human Brain Project) made it onto the ESFRI list of European research infrastructures. Mikael Djurfeldt provides an update on recent developments (*EBRAINS News*).

In the past, computing resources at PDC had mainly been used by computational scientists for numerical simulations. Meanwhile, data science methods have become ubiquitous and thus the use of PDC resources, as well as the research at PDC, is changing. Xavier Aguilar co-authored a recent publication where he explored how particle-in-cell simulations can be combined with deep-learning methods (*A Deep-Learning-Based Particle-in-Cell Method for Plasma Simulations*). Next year, Dardel will be augmented with several hundred AMD Instinct MI200 GPUs. These will be the most powerful GPUs available at the time of their deployment. These GPUs will not only accelerate simulations, but will also be useful for machine learning and artificial intelligence (AI) applications. We are therefore looking forward to teaming up with the AI Sweden initiative, which is described by Fredrik Viksten and Niclas Fock, who are driving the initiative (*AI Sweden Initiative*).

Using GPUs as compute accelerators is one example of how quickly technology is changing. Therefore, investing in training continues to be vital. This year the series of PDC summer schools continued (*PDC Summer School*), and fortunately the CodeRefinery project has been extended for a third phase (*CodeRefinery Enters Sustainability Phase*), so their valuable training will continue to be available to researchers seeking to improve coding skills. PDC looks for new opportunities to promote high-performance computing (HPC) education and hence is looking forward to becoming part of the EUMaster4HPC project, which aims to strengthen HPC education through joint- and double-degree master's in HPC programmes as well as coordinating curricula at a European level (*EUMaster4HPC*). And many of the established training efforts are continuing (*AI February at ENCCS* and *BioExcel CoE: Recent Activities*). EUMaster4HPC also aims to collaborate closely with industry, which aligns well with PDC's ambition to support private companies in using HPC for research and development, for example, in collaboration with ENCCS (*Swedish HPC Business Day 2021*).

I hope this summary shows how much the PDC team has achieved throughout the year. This provides a good basis for facing new challenges in 2022. The new year will bring significant extensions to the Dardel system. By adding a GPU partition, the compute performance of the system will be significantly increased. Now there are only a few months left to finalize the porting of applications and to get them ready for exploiting this new hardware. Another challenge that is ahead of us is the reorganization of HPC in Sweden, where we are looking forward to finding new ways of serving research in Sweden through an advanced and continuously modernized research infrastructure.

Let me finish with a big "thank you" to the PDC team. Every member of the team has contributed in different roles to what has been achieved during this year. Finally, I wish all our readers a happy and peaceful Christmas holiday. May it be an opportunity for you to recharge your batteries and refresh your minds for a good start to the new year!

Dirk Pleiter, Director PDC

In This Issue

Staff Focus

Daniel Araújo de Medeiros

Daniel Araújo de Medeiros has recently joined PDC as a doctoral student in high-performance computing (HPC). He finished his master's degree in computer science from the Federal University of Bahia, Brazil, in 2020 and also has a bachelor's degree in geophysics from the Federal University of Rio Grande do Norte, Brazil. His previous research consisted of the analysis and scheduling of hot functions for cloud applications in heterogeneous architectures (that is, ARM's big.LITTLE). For several years, Daniel was a researcher at the Geological Survey of Brazil, where he mainly worked with data processing and its interpretation for geoscience purposes.

At PDC, Daniel is being supervised by Dirk Pleiter. As a doctoral student, Daniel's main research will be carried out under the auspices of the TREX CoE consortium and relates to the understanding and optimization of quantum chemistry applications for the yet-unbuilt exascale systems.

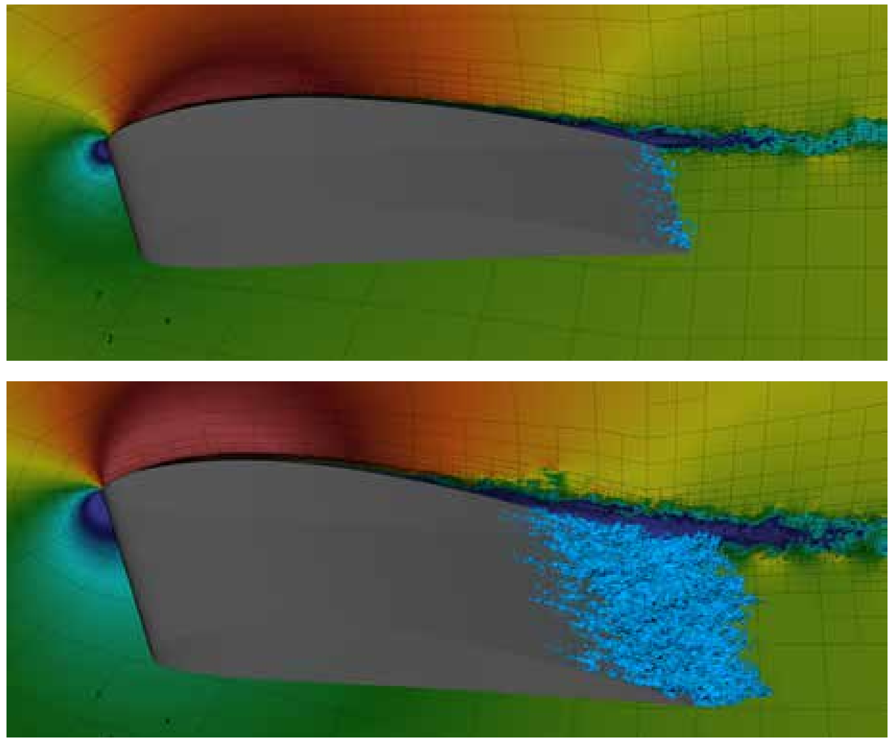
In his spare time, Daniel enjoys playing video games and reading. He also plays tennis and goes travelling to other countries whenever the opportunity arises.

Dardel-Pilots Simulate Wings Using NEK5000

Fermin Mallor, Kristina Durovic, Ardeshir Hanifi, Dan Henningson, Adam Peplinksi & Philipp Schlatter, KTH Engineering Mechanics, and Niclas Jansson, PDC

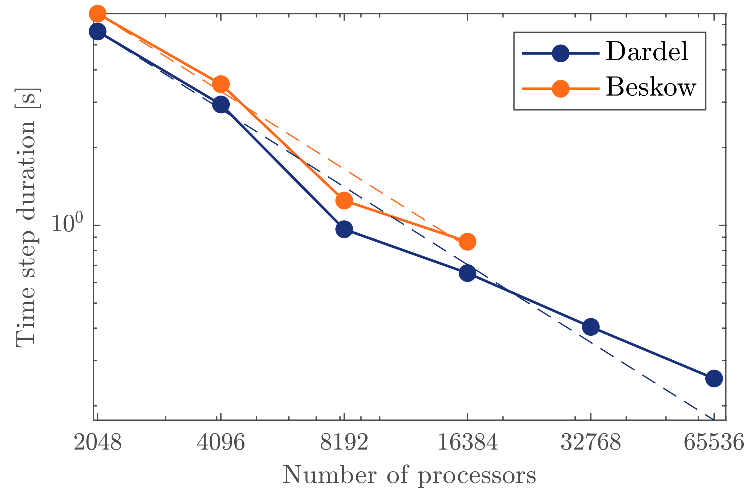
The pilot phase of the new high-performance computing system at PDC, Dardel, has been extensively used in the study of complex turbulent flow phenomena, mainly for two physical cases: the turbulent flow around an aerofoil at high angles of attack (AoA), and laminar-turbulent transition on a plate.

In our research, we study the behaviour of moving streamlined bodies submerged in a fluid; the prototype example is the motion of a wing in air, generating lift and drag. In the first case that was investigated during the pilot phase on Dardel, the turbulent flow around an infinite-span NACA 4412 wing profile at various Reynolds numbers (Re_c = 200,000; Re_c = 400,000 and Re_c = 1,000,000) and angles of attack (AoA = 5° and AoA = 11°) was studied through well-resolved large-eddy simulations (LES), which are also referred to as quasi direct numerical simulations (DNS). The NACA family of aerofoils was standardized by the National Advisory Committee for Aeronautics (NACA) about a hundred years ago in an effort to characterize the properties of wings in a systematic way. The complex simulations using these wing profiles are made possible by the introduction of adaptive mesh refinement (AMR) and non-conformal meshing into the spectral-element method code NEK5000, which makes it possible to increase the domain size while reducing the computational cost. The present work focuses on the appearance of backflow events under strong adverse pressure gradients (APGs) and high Reynolds numbers, which is relevant for understanding the initial stages of stall. The figures below show regions of backflow events for two different angles of attack, with the spectral element mesh generated by means of AMR in the background.



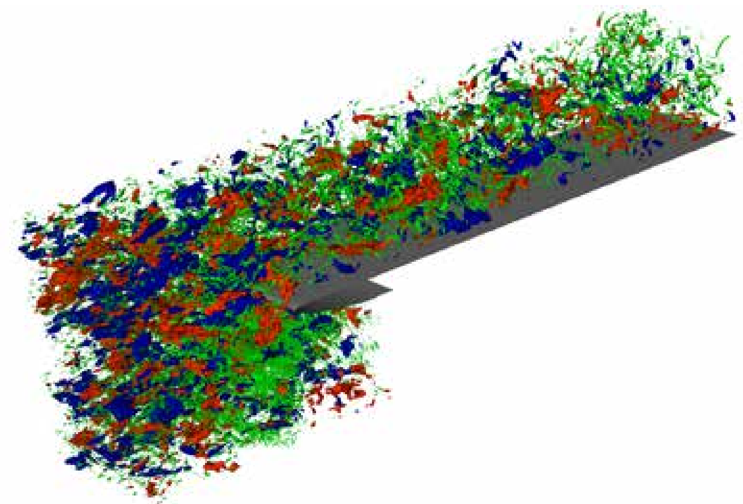
Above: Iso-contours of the regions with negative streamwise velocity for the 5° (top) and 11° (bottom) angle of attack cases at a Reynolds number of 400,000.

Below: Strong scaling of a one-million element wing simulation on Beskow and Dardel: dashed lines indicate ideal speed-up



Strong scalability tests were performed on Dardel with a periodic wing case with close to one million elements and polynomial order 7 (around half a billion grid-points). The results are shown in the figure above, along with a comparison with results from the same case run on PDC's previous flagship system, Beskow. A clear performance increase (equivalent to around a 20% speed-up for the same number of CPU cores) is found for the new system as compared to Beskow.

As part of the pilot test phase for Dardel, laminar-turbulent transition on a flat plate caused by ambient free-stream turbulence (as happens, for example, in turbomachinery) has also been studied. Recently, an unexpected variation of transition location with the length scale of the free-stream turbulence (FST) was observed in the experiments performed in the KTH wind tunnel. These new simulations, which confirm some of those findings, will help with understanding the interaction of the FST with the boundary layer (especially in the region close to the leading edge), and which properties of FST really determine the transition location. This will help to clarify which effects really determine the transition location, and eventually allow for better models to be used in design processes.



Above: Freestream turbulence around a flat plate with leading edge; our simulations resolve all steps from the generation of the turbulence up to their receptivity into the boundary layer and subsequent transition

Materials Theory Codes on Dardel at PDC

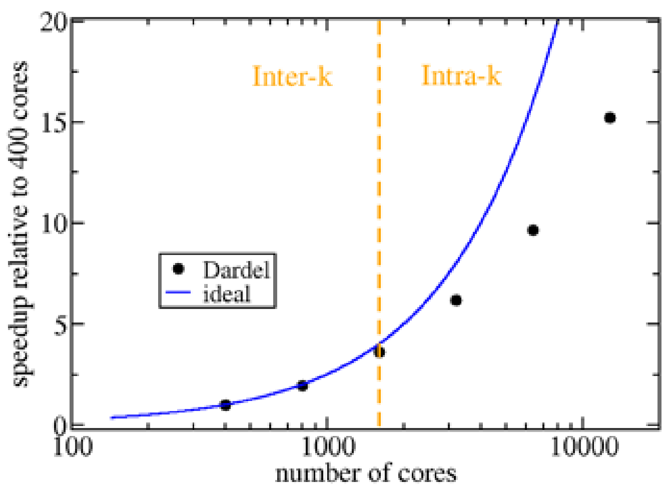
Johan Hellsvik, PDC, Olle Eriksson, Department of Physics and Astronomy, Uppsala University, & Igor Di Marco, Asia Pacific Center for Theoretical Physics

Quantum mechanical modelling based on density functional theory (DFT) has evolved to be a cornerstone of computational materials science, which is applicable to a wide range of functional materials, quantum materials, and materials relevant to green technologies. DFT provides a tractable means to model the complex interactions of a quantum mechanical many-body system.

Within a pre-production project that has been running on the new Dardel HPE Cray EX supercomputer at PDC (with Olle Eriksson as the principal investigator), codes developed at the Materials Theory Division at Uppsala University have been installed and tested on the CPU-partition of Dardel. The codes are being developed in close collaboration with groups at Örebro University, the KTH Royal Institute of Technology, the Federal University of Pará in Belém, Brazil, the University of Sao Paulo, Brazil, and the Asia Pacific Center for Theoretical Physics (APCTP), South Korea. These codes include the full-potential all-electron DFT programs RSPt and Elk, and the atomistic spin-dynamics program UppASD. These codes also involve the augmentation of electronic structure theory to include effects of many-body physics – in the form of dynamical mean field theory – which is an effort that involves in-house and externally developed quantum many-body solvers.

Whereas the atomistic spin-dynamics approach – which implements a lattice model for particles (spins) interacting with short-range interactions – is naturally suited for partitioning the problem volume over distributed computer memory (with parallel sampling and time evolution of the system on the nodes of a supercomputer), the DFT programs implement models with interactions on both shorter and longer length scales. With regard to the effective scaling of program performance towards exascale computing, the DFT programs and algorithms therefore pose a challenge, as performance is dependent on – and in part limited by – the need for individual execution threads and ranks of a program to access state variables that are global to the physical model.

The focus for the present project is to tune the performance on the Dardel CPU nodes, while keeping an eye out for chances to explore possible opportunities to adopt kernels of the materials theory codes to the Dardel GPU nodes in the future. Solving the Schrödinger equation in reciprocal space, a DFT program can be parallelized over a finite set of wave vectors (k points) within the Brillouin zone of the material. As an example from using the Dardel CPU nodes, for the full-potential linearized muffin-tins orbitals code RSPt, the strong scaling performance for algorithmically and memory demanding intra k-point parallelization – as well as the more tractable inter k-point parallelization – are under investigation, with preliminary findings indicating good performance as well as opportunities for further improvement. Nevertheless, the tests have also shown that the optimal number of processes per node for maximizing performance is half the number of available cores, which points to some delay in the MPI communication. Work to minimize these delays will proceed by exploring additional combinations of compilers and libraries, and further tuning of the code.



Above: Speed-up for DFT+U modelling of a 64-atom heterostructure with RSPt – close to ideal scaling is obtained for inter k-point parallelization

BioExcel Centre of Excellence: Recent Activities

Alessandra Villa and Rossen Apostolov, PDC

This autumn the BioExcel team at PDC have been continuing with our initiatives that support the computational biomolecular research community. The BioExcel webinar series hosted the core developers of MDAnalysis (a library for performing interoperable analyses of biomolecular simulations in Python) and the developer of 3dRS (a web-based tool for sharing interactive representations of 3D biomolecular structures and molecular dynamics trajectories). In addition, Charlotte Deane (from the University of Oxford) gave a stimulating webinar on computationally designing therapeutic antibodies. These webinars (and many more!) can be viewed at BioExcel's YouTube channel (https://www.youtube.com/c/BioExcelCoE) or on the BioExcel website at https://www.bioexcel.eu/webinars. As well as hosting webinars, BioExcel has been busy organizing the second winter BioExcel School on Biomolecular Simulations, which will be held as an online course in March 2022. If you would like to join us to learn more about a wide range of topics relating to biomolecular modelling and simulations, please register at https://bioexcel.eu/events/bioexcel-school-on-biomolecular-simulations.

Are you (interested in) performing molecular simulation using GROMACS? If so, the following initiative may also be of interest to you. In collaboration with the EuroCC National Competence Centre Sweden (ENCCS), BioExcel has released a GROMACS tutorials web page where the tutorials that are regularly given in training workshops about GROMACS are provided as interactive Jupyter Notebooks. You can download the notebooks to run locally, or even run them in your browser using Binder (see https://mybinder.org). To try the notebooks, go to https://tutorials.gromacs.org.

About a year ago, BioExcel helped to change the format for GROMACS support from a mailing list to a forum. That has resulted in a very active forum with more than a thousand page views per day! So if you have any questions about GROMACS, do have a look at the GROMACS forum at https://gromacs.bioexcel.eu. And if you are using GROMACS at an advanced level, keep a watch on the BioExcel events page https://bioexcel.eu/news-and-events/events or the PDC news page https://www.pdc.kth.se/about/pdc-news, as BioExcel will soon hold a workshop at the CSC – IT Center for Science in Finland.

Dardel 1st Phase Inauguration 25 January 2022 16.00-17.30

It is time to celebrate: the first phase of the new Dardel system at PDC recently passed the final acceptance tests and the process of migrating researchers (and their data) from the earlier Beskow and Tegner systems to Dardel is underway!

Please join us in January for this online event which will feature presentations from researchers who have been using Dardel during the test phase.

For details and to register, see https://www.pdc.kth.se/about/events/general/dardel-phase-1-inauguration-1.1127765.

Above: Stefan Lundin, OHB Sweden, was one of the speakers at the Swedish HPC Business Day 2021.

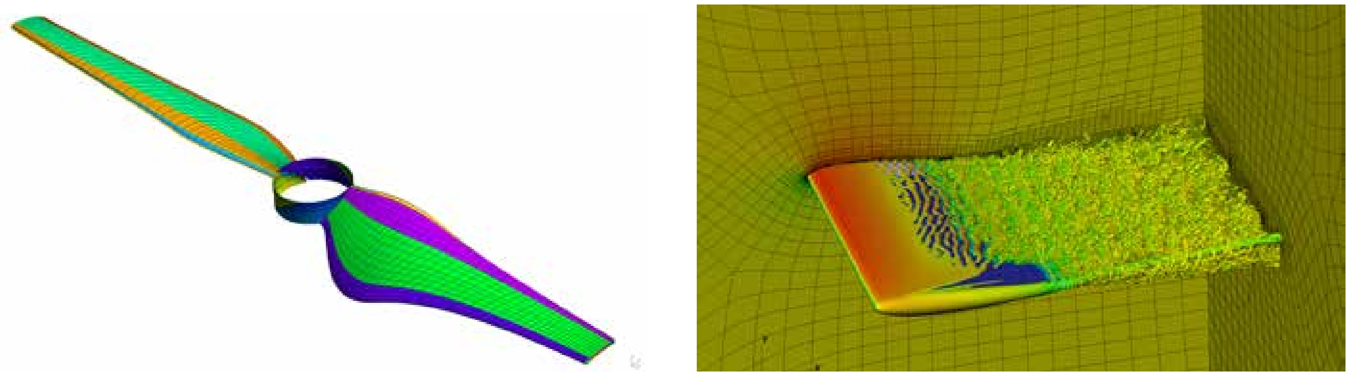
Towards Exascale in Engineering

Niclas Jansson & Jonathan Vincent, PDC, and Timofey Mukha, Adam Peplinski, Saleh Rezaeiravesh & Philipp Schlatter, KTH Engineering Mechanics

The European Centre of Excellence (CoE) for Engineering Applications, EXCELLERAT, is one of the European CoEs aiming at supporting key engineering industries in Europe and promoting interaction between academic research and code development with industrial workflows. EXCELLERAT thus focuses on complex computational fluid dynamics (CFD) simulations using high-performance computing (HPC) technologies and answers the engineering community's needs by providing expertise in various aspects of numerical modelling from application development to performing simulations and data analysis. It also provides a bridge between industrial partners, computer centres and the academic community.

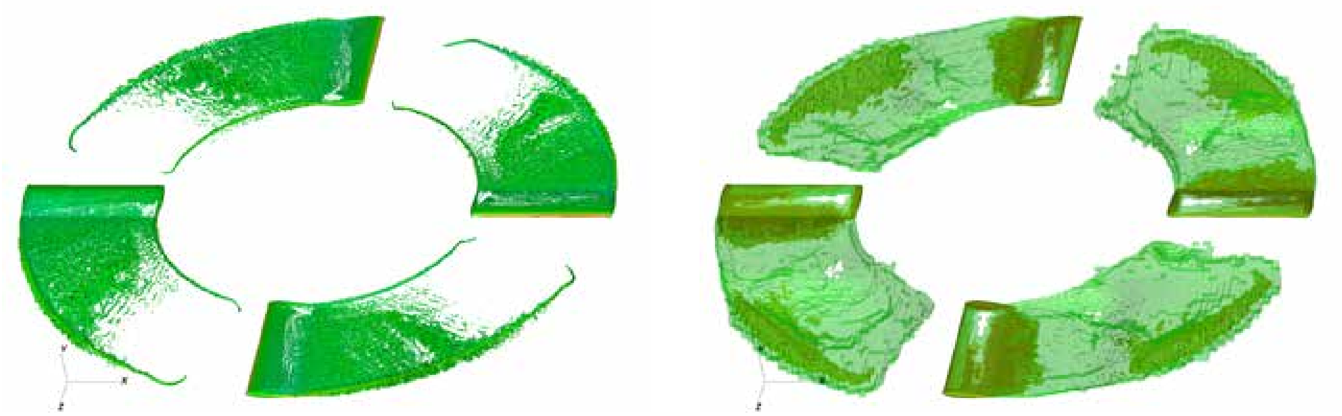
In the field of turbulence simulations, NEK5000 is one of the six reference codes selected for EXCELLERAT. It is a high-fidelity CFD solver based on a high-order Spectral Element Method (SEM) used for modelling a number of different flow cases, including industrially relevant applications, such as nuclear reactor thermal-hydraulics. An important method improvement in the code was the implementation of an Adaptive Mesh Refinement (AMR) algorithm that makes it possible to control the computational error during a simulation and reduce it at minimal cost by proper mesh adjustment. One of the set goals of EXCELLERAT was to extend this AMR method in NEK5000 to fully three-dimensional flows making it a robust solver capable of adaptively solving complex industrially relevant problems. A number of different aspects of numerical modelling were considered here starting from mesh generation and solver parallel performance, through solution reliability (Uncertainty Quantification) and ending with in-situ data analysis and visualization. After three years of work, EXCELLERAT can present its developments in the form of mature tools, and the results of the flow simulations performed with relatively complex and industrially relevant cases, such as the simulation of a flow around a three-dimensional wing tip. Although this flow case is relevant for a number of industrial areas, like aeronautics, automotive or bio-engineering, there is an apparent lack of high-fidelity numerical data for high-Reynolds-number turbulent flows. The second main case we considered was performed in cooperation with CINECA and involved the simulation of rotating parts, in particular, a drone rotor with an Eppler E64 wing profile.

We started by creating a workflow for the pre-processing step including hex-based mesh generation with the widely used gmsh library, and then developed proper tools for the simulation initialization. The workflow was used to generate suitable NEK5000 meshes for both the NACA 0012 aerofoil with a rounded wing tip and the drone rotor. There were multiple issues we had to deal with such as the proper definition of relative element orientations, and the proper projection of the grid points located at the domain boundary onto the prescribed surface. However, the most challenging and time-consuming step was the generation of a hex-based mesh. On the one hand, our AMR capability simplifies the whole meshing process providing flexibility of non-conforming meshes, but at the same time it makes meshing more demanding, as efficient AMR requires a relatively coarse initial mesh that still properly represents the domain geometry. The resulting meshes are shown in the images on the previous page. The image on the left shows the mesh on the rotor blade, while the right-hand image presents a vortical structure of the transient flow around the NACA0012 aerofoil with a rounded tip for Re=105. Black lines mark the elements' boundaries; each element consists of (N+1)×(N+1)×(N+1) grid points, where N is a chosen polynomial order. In the right-hand image, we can clearly appreciate the regions with increased resolution, identified by our AMR procedure.



Above: (Left) Rotor with Eppler profile and (right) NACA0012 profile with rounded wing tip, with vortical structures of turbulence developing through natural transition

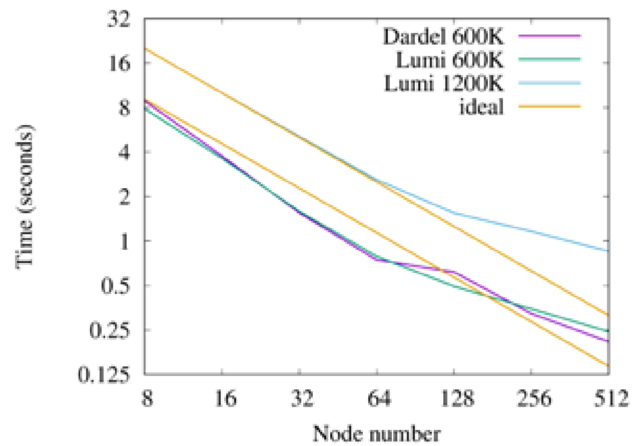
Below: "Toy" rotor – (left) vortical structures identified using the lambda2 criterion and (right) regions of higher refinement computed dynamically by ARM



We also worked on assessing the parallel performance of our AMR implementation in NEK5000 by looking into, for example, different mesh partitioners (ParMetis and ParRSB), and communication patterns in the pressure preconditioner. All the modifications that have been described enabled us to perform fully adaptive AMR simulations for the two use cases.

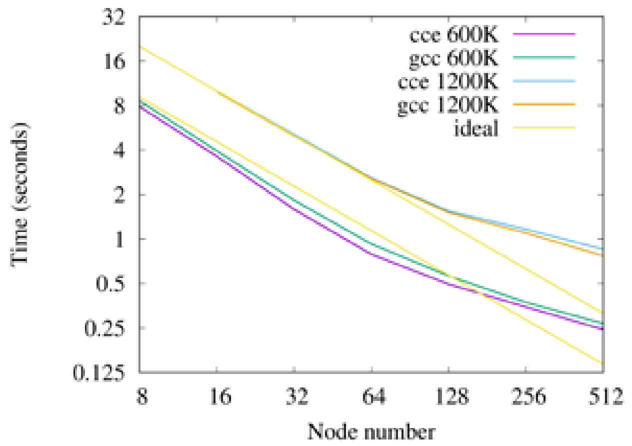
The figures at the top of this page show the results of a preliminary "toy" rotor simulation, at a Reynolds number Re=100,000 and with a rotor built out of four blades with NACA0012 aerofoils and rounded wing tips. These figures present the vortical structures of the transient flow and domain sections occupied by different refinement levels.

The toy rotor case was tested on the CPU partitions of the new supercomputers Dardel (at PDC) and LUMI (at CSC in Finland); we had access to both machines during their respective pilot phases. Two different setups were used: the smaller one with 631,712 elements and the larger with 1,262,258 elements, both with polynomial order 7. The data for strong scaling is presented in the following two graphs showing that our AMR branch of NEK5000 preserves the good scaling properties of its conformal version. On Dardel we achieved parallel efficiency of 0.7 on 512 nodes (out of 554 available nodes) with only 10 elements (5,120 grid points) per MPI rank. The graph at the



Above: Strong scaling data for our AMR case on Dardel and LUMI with different sizes and the Cray compiler

Below: Strong scaling data for our AMR case on LUMI with different sizes and the Cray and GNU compilers



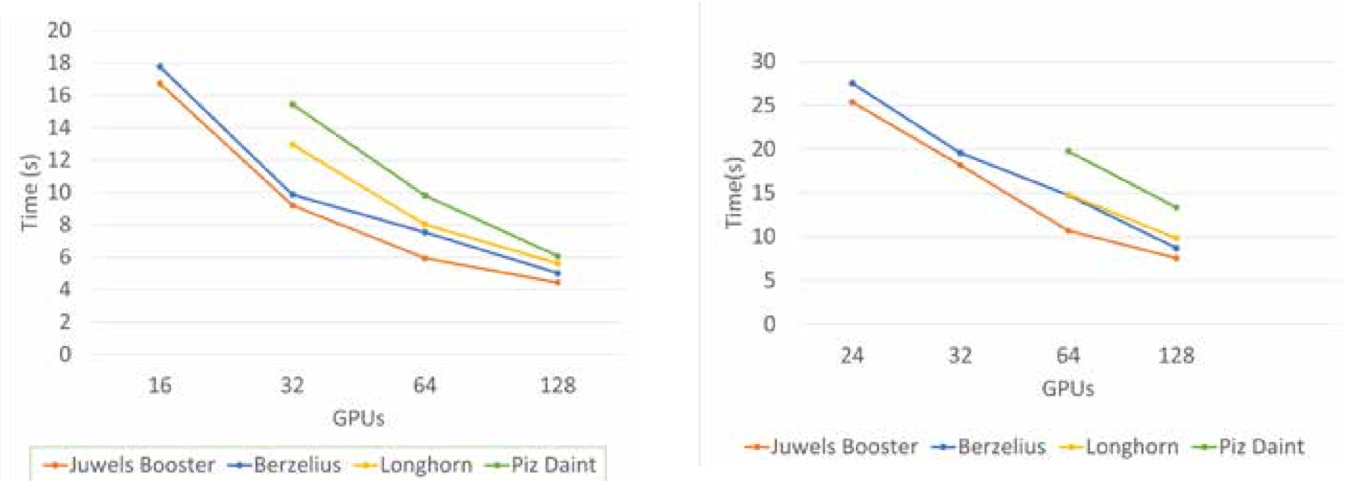
bottom of the previous page shows results for both Dardel and LUMI obtained using the native Cray compiler, while the graph above presents LUMI results obtained with Cray and GNU compilers. Both plots show the average execution time per time step and an ideal scaling curve.

Another important task for EXCELLERAT has been to improve NEK5000's exascale readiness, particularly with respect to accelerators. As a starting point, we used an OpenACC version of the proxy-app Nekbone, and used the experience gained from that to create an OpenACC + CUDA implementation of NEK5000. The graphs below show the results of the OpenACC NEK5000 implementation on several different GPU-based systems.

As further work we are looking at optimizing the kernels and moving more work to the GPUs to further improve performance. As part of the work to get NEK5000 working on the GPU partition of Dardel, we are also in the process of creating a version of NEK5000 that uses OpenMP for GPU offloading. This is important as this is more suitable for running on the AMD GPUs that will be installed on the Dardel system.

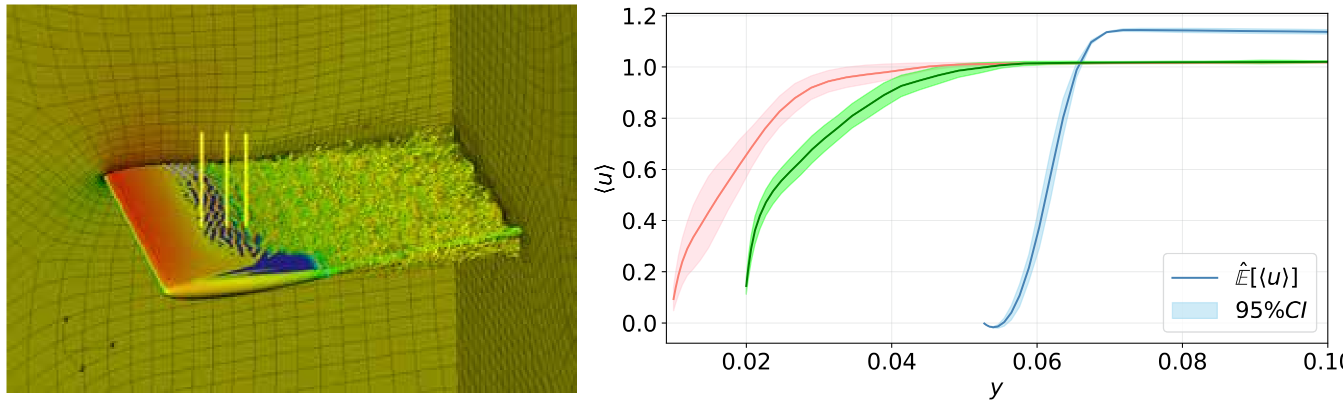
Even on exascale machines and with the algorithmic improvements in efficiency described above, simulations of wall-bounded flows at very high Reynolds numbers will remain prohibitively expensive if the whole boundary layer has to be resolved in space and time. To circumvent this, we have started to implement modern wall modelling in NEK5000. Wall models act as a substitute for resolving the smallest turbulent scales near the wall, thereby dramatically reducing the scaling of the grid size with the Reynolds number. Currently, we are testing our implementation on canonical wall-bounded flows, with the aim of applying wall models to the flow cases described earlier.

It is both important and interesting from the engineering design point of view to assess the sensitivity and robustness of scale-resolving simulations of fluid flows with respect to the variation of numerical, modelling, and physical parameters. There are also run-time factors that influence the reliability of the simulation results. An example is the uncertainty induced in the time-averaged quantities of turbulence simulations due to the finite number of samples included in the averaging – see, for example, the figure at the top of the next page. Since industrially relevant flows are computationally expensive and cannot be run for very long time-intervals, estimating confidence



Above: GPU performance of NEK5000 on various machines

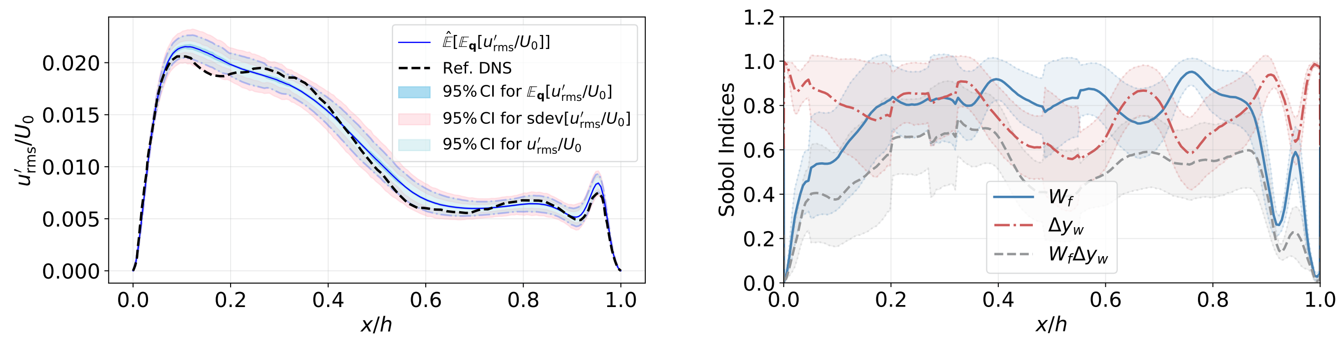
Below: Time-average uncertainty in the mean streamwise velocity profiles at the specified locations in the wing tip simulation



in the simulations is required to assess when a given simulation may be stopped when it reaches a specified confidence level. Another aspect, which makes the formal assessment of uncertainties and sensitivities in CFD even more important, is the emergence of data-driven methods such as Bayesian optimization where the algorithm is driven by the uncertainties. The progress in HPC makes it possible to apply such data-driven methods to large-scale flow simulations.

To achieve these goals of assessing uncertainty and robustness, relevant techniques in the fields of uncertainty quantification (UQ) and computer experiments can be employed. Implementing such techniques for CFD applications, in general, and the simulation of turbulent flows, in particular, has led to the development of UQit which is a Python package for uncertainty quantification. UQit has been developed and released in open-source under the aegis of EXCELLERAT so the wider research community can take advantage of it. Generally speaking, UQit can be non-intrusively linked to any CFD solver through appropriate interfaces for data transfer. The main features that are currently available in UQit are as follows: standard and probabilistic polynomial chaos expansion (PCE) with the possibility of using compressed sensing, analysis-of-variance-based (ANOVA-based) global sensitivity analysis, Gaussian process regression with observation-dependent noise structure, and batch-based and autoregressive models for the analysis of time-series. The flexible structure of UQit allows for combining different UQ methods and easily implementing new techniques. Therefore, UQit is planned to be continuously updated.

To demonstrate the importance of UQ in assessing accuracy, robustness and sensitivity of the flow's quantities of interest (QoIs) when the design parameters are allowed to vary, we have used UQit in different computer experiments using NEK5000. A novel aspect of the analysis is that we have been able to combine the uncertainty in the training data, for instance due to finite time-averaging, with the variation of numerical and modelling parameters. For instance, see the following figure which shows the combined propagation of uncertainty into a turbulent lid-



Above: (Left) Propagated uncertainty and (right) Sobol sensitivity indices for the u'_{rms} profile of a turbulent lid-driven cavity flow The numerical parameters are filter weight W_f and wall-adjacent grid spacing Δy_w. Note that the time-average uncertainties are included in the observed data.

driven cavity flow simulated by NEK5000. The analyses have been performed by probabilistic polynomial chaos expansion and Sobol sensitivity indices. The developed framework has also been applied to compare the performance of two widely-used open-source CFD solvers, NEK5000 and OpenFOAM, through the evaluation of different UQ-based metrics.

UQit has also been employed in collaboration with an EXCELLERAT partner to develop the workflow required for conducting online/in-situ UQ analyses relying on CFD simulations on HPC systems. The objectives can be diverse, including UQ and sensitivity analyses, constructing predictive surrogates and reduced-order models, developing data-driven models, and performing robust optimization. Currently, the collaboration has led to the successful development and implementation of novel algorithms for in-situ estimation of time-average uncertainties. Due to these streaming estimators, storing time-series data of flow simulations can be avoided.

We will continue our work within EXCELLERAT combining the presented tools and making use of them during the final simulation of our use case. As a first step, we will enable in-situ analysis for non-conforming meshes produced by AMR runs, together with a UQ analysis of the time averages.

References

1. N. Offermans, A. Peplinski, O. Marin, P. Schlatter, Adaptive mesh refinement for steady flows in NEK5000. Comp. Fluids,197, 104352, 2020.
2. S. Rezaeiravesh, R. Vinuesa, P. Schlatter, UQit: A Python package for uncertainty quantification (UQ) in computational fluid dynamics (CFD), Journal of Open Source Software 6 (60), 2871, 2021.
3. J. Vincent, et al.: Strong scaling of OpenACC enabled NEK5000 on several GPU based HPC systems.Inproc.InternationalConferenceonHigh Performance Computing in Asia-Pacific Region (HPC Asia 2022), Virtual Event, Japan, 2022. https://doi.org/10.1145/3492805.3492818.

CodeRefinery Enters Sustainability Phase

Johan Hellsvik, PDC, and Diana Iuşan, UPPMAX

Across all scientific disciplines, there is currently a great emphasis on reproducible research and Findable, Accessible, Interoperable, Reusable (FAIR) data so that research provides the greatest benefit to society. Custom-written research software and workflows are often a central part of research projects. This type of research software is the key to reproducibility and data management, but many researchers do not have training in software development beyond basic programming. Thus, it is difficult for the researchers producing such software to ensure that it is reusable by others, or even correct in the hands of the original author(s). The shift towards research enabled by software requires a profound and continuous transformation of research practices. A major challenge for the research community is the pressure to gain and maintain the necessary software skills in a very limited time while both technology and best practices evolve rapidly. These tools and practices are almost never part of a traditional academic curriculum, and learning foundational coding, data science skills, and associated best software practices in isolation without a support structure is inefficient and costly, both for the individual researcher and the research community as a whole.

The NeIC-funded CodeRefinery project https://coderefinery.org has been addressing these challenges for the past five years by teaching researchers about key tools and best practices. CodeRefinery is supporting students and researchers by advancing the FAIRness of software and development practices so that they can collaboratively develop, review, discuss, test, share, and reuse their codes. The standard workshop curriculum consists of lessons and exercises about basic and collaborative Git, code review, social coding and open software, reproducible research, Jupyter notebooks, code documentation, automated testing, and modular code development.

Up to now, more than 1,600 researchers from the Nordic countries have been trained and three instructor training events were held. In the past 18 months alone, four online workshops were held with an average number of 100 participants. The large-scale workshops were made possible with the additional support of the CodeRefinery community, which contributed 8 volunteer instructors and over 80 volunteer helpers for the hands-on sessions. The long-term impact of CodeRefinery workshops, measured through post-workshop surveys (3-6 months later) shows that, for example, about 60% of the learners have improved their usage of version control. Yet, the tools taught in CodeRefinery workshops are rarely part of academic curricula. Also, the need for training in research software engineering will only increase and become more diverse.

Acknowledging the remarkable contribution that CodeRefinery has made to FAIR practices and open science, NeIC will continue to fund the project for a third period. Thus, in 2022, CodeRefinery will enter a sustainability phase, the aim of which will be the help to ensure the long-lasting effects of the project, including maintaining the learning materials and further strengthening the community. Together with other organizations from Norway, Finland, and Denmark, the Swedish National Infrastructure for Computing (SNIC) will be contributing in-kind to the project, with staff working on CodeRefinery at both PDC and the Uppsala Multidisciplinary Center for Advanced Computational Science (UPPMAX). The collaboration between the project partners and the academic community in general will ensure that CodeRefinery continues to provide high-quality events in a variety of forms: online and in-person workshops, hackathons, and community meetups. In addition to the standard curriculum that has been offered up to now, there will be an increased focus on community-driven workshop delivery to facilitate on-demand workshops and to turn the Nordic network into a collaboration platform for other workshops.

For more information about the CodeRefinery project and upcoming workshops, please visit https://coderefinery.org. If you would like to get in touch with the CodeRefinery community, you may consider joining the chat https://coderefinery.zulipchat.com.

Making Dardel Easy to Use

Gert Svensson, PDC

PDC has been making changes so it will be easy to use Dardel, and further improvements are also in the pipeline. Here are some examples.

1. In addition to Kerberos login, **SSH login with secret/public key-pairs** is now available. There is a new login portal where public keys and allowed IP addresses can be uploaded, and the portal will soon be upgraded to use domain names. For more information, see https://www.pdc.kth.se/support/documents/login/ssh_login.html.
2. **SSH login to allocated compute nodes** is allowed (currently only from the login nodes, but the aim is to remove that restriction soon).
3. Dardel does not use AFS, so **home directories** are stored **in Lustre** and are backed up.
4. EasyBuild and SPACK are being used to install software packages in **easy-to-use modules**. Expert users can use recipes to install modified personal versions of already installed packages.
5. PDC, the University of Lund and the Swedish National Infrastructure for Computing (SNIC) have agreed to set up a project to install **ThinLinc on Dardel**. ThinLinc is a remote desktop solution, which makes it much easier for researchers who would prefer to use a graphical interface to work on Dardel. More information will be presented when ThinLinc is operational.
6. PDC has developed a **Quick Start Guide** for more experienced users who want to jump in and start using Dardel straight away (see: https://www.pdc.kth.se/support/documents/basics/quickstartdardel.html).
7. More **in-depth documentation** for using Dardel is also available (see https://www.pdc.kth.se/support). The documentation is continually being improved, so let us know (via email to support@pdc.kth.se) if you have ideas for improvements as you start working on Dardel.

A Deep-Learning-Based Particle-in-Cell Method for Plasma Simulations

Xavier Aguilar PDC

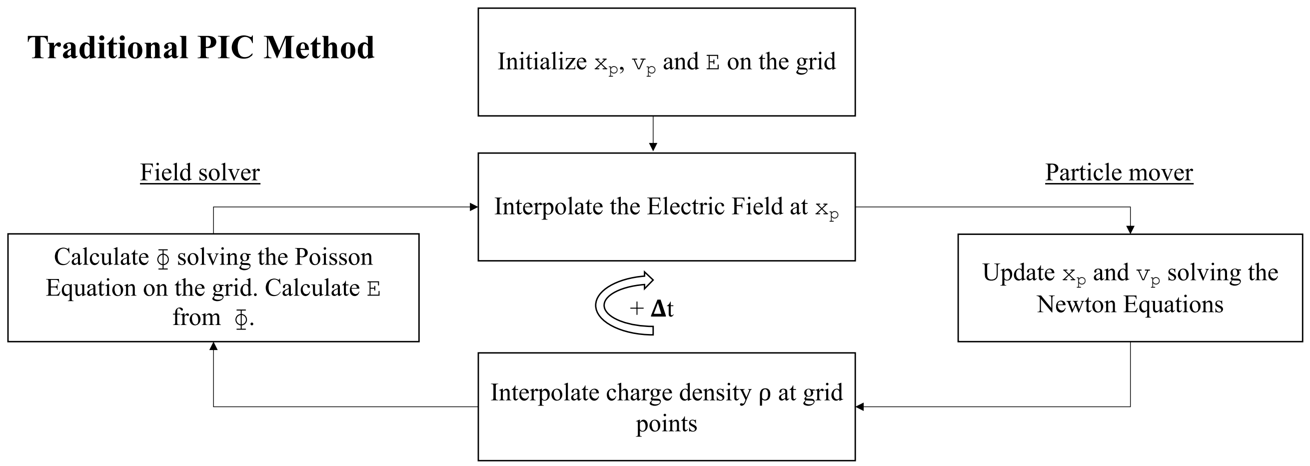
Particle-in-cell (PIC) methods are an important group of methods to help us understand the behaviour of plasma dynamics in complex phenomena and systems. Parallel PIC codes, such as VPIC [1], iPIC3D [2], and Warp-X [3], are run on the largest supercomputers in the world, and they are being applied in fields ranging from space physics and astrophysics to accelerators, fusion reactors or laser-plasma devices. However, simulating plasma phenomena is complex and requires a lot of computational power.

Lately, Machine Learning (ML) and Deep Learning (DL) have emerged in high-performance computing (HPC) as a viable methodology to complement classical computational approaches. For example, DL methods are being used in computational fluid dynamics [4], weather forecasting [5], and with DL-based preconditioners and linear solvers [6,7].

This article presents some research work on the use of Deep Learning techniques applied to PIC methods. This work [8] was the result of a collaboration between one of PDC's application experts, Xavier Aguilar, and Stefano Markidis from the CST Division at KTH, and demonstrates that integrating DL techniques within PIC methods is a promising approach for developing new PIC methods beyond the current ones.

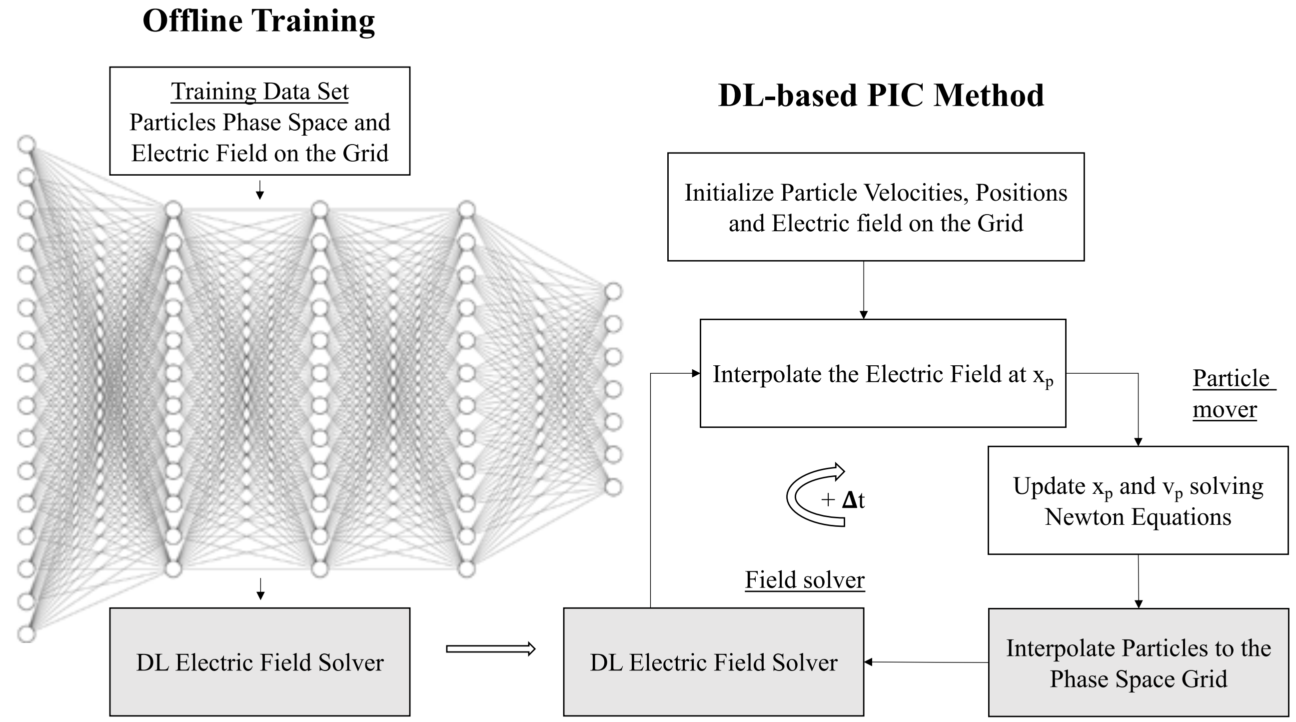
Traditional PIC methods use the algorithm depicted below. They start with an initialization phase, followed by a computational cycle which is repeated hundreds of thousands of times during the simulation. This computational cycle computes the electric and magnetic fields at particle positions, moves particles, computes charge densities on the grid, computes the electrostatic field using Maxwell's equations, and finally computes the electric field. We took this algorithm and modified it by introducing neural networks in its computational phase. In other words, we substituted some classical computations with DL as depicted at the top of the next page (in the grey boxes). The new DL-based PIC algorithm still retains the interpolation step to compute the electric field at the particle positions, as well as the particle mover, but uses an electric field solver that is the result of DL neural network training.

To train the neural network, we produced a data set of images representing a discretized particle phase-space together with its associated electric field for the two-stream instability, which is a well-known plasma benchmark. The figure at the bottom of the next page shows examples of several phase-space grids together with their electric fields. We generated thousands of these pairs using classical simulations and used them to teach a neural network to predict the electric field from a phase-space grid. More concretely, we generated 40,000 phase-space grids and 40,000 electric fields from classical simulations using different initial parameter configurations,



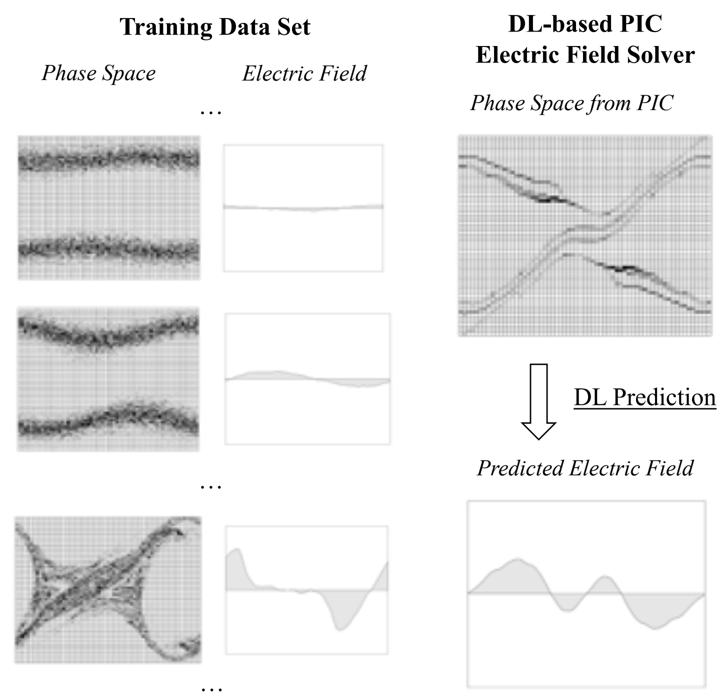
Above: Traditional PIC algorithm

Below: DL-based PIC method



that is, initial beam velocity and thermal speed. The total size of our initial data set was 5.2GB. We used this data to train two different network architectures, a Multilayer Perceptron (MLP) and a Convolution Neural Network (CNN). We ran our experiments on two 12-core Intel E5-2690V3 Haswell processors connected to an NVIDIA Tesla K80 GPU. For more details on the experiments and the setup, refer to the original paper [8].

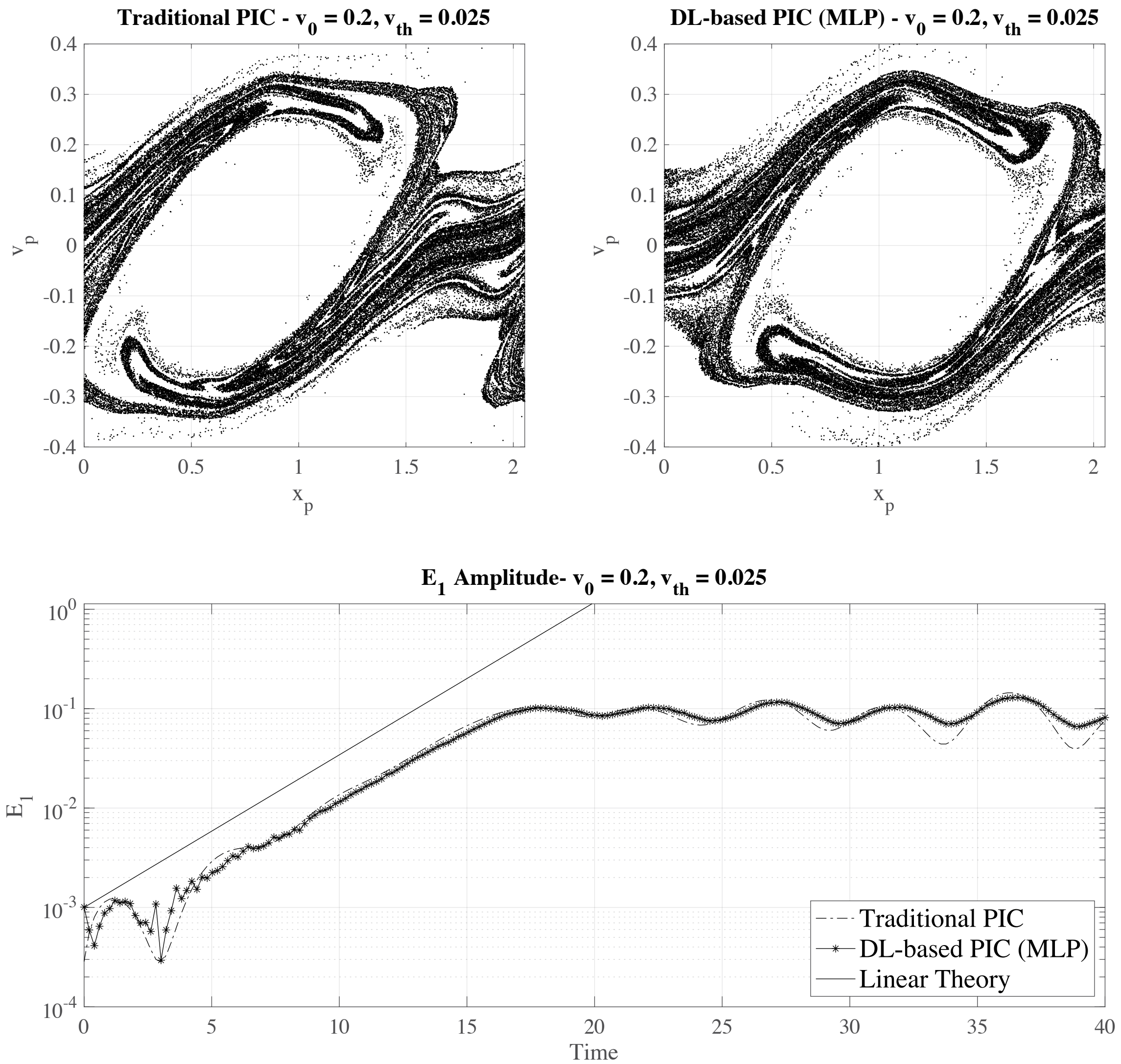
Our initial experiments showed that the MLP had a better mean absolute error on the test data, and it was also much faster to train, and therefore, we decided to focus our efforts on the DL-solver using the MLP. First, we validated



Above: Phase-space grids together with their associated electric fields
The DL-based PIC method uses these data sets to learn how to predict the electric field from the phase space.

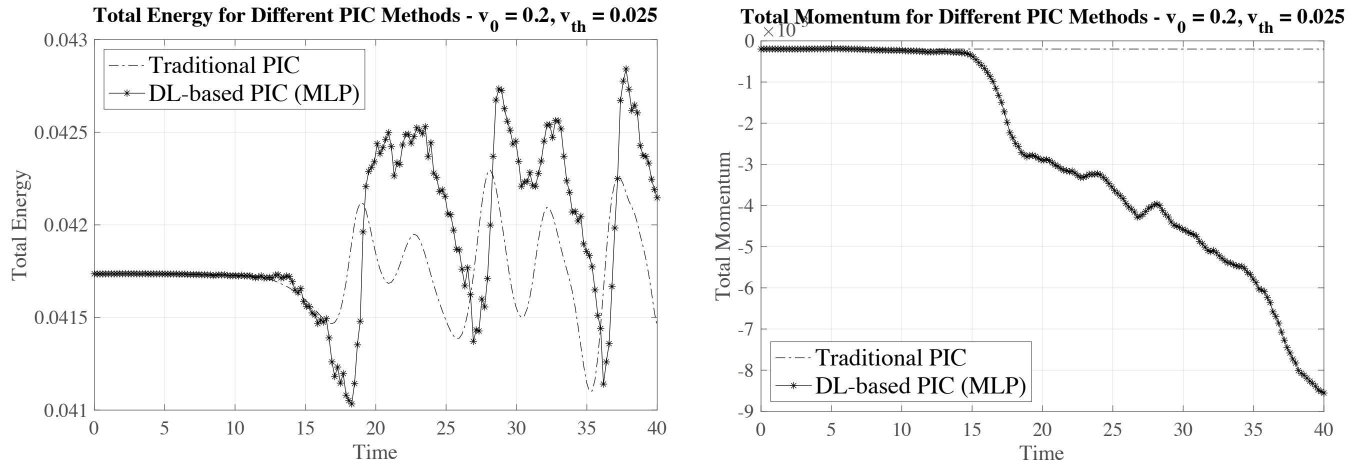
the results of the DL-based PIC method using a configuration that was not included in the initial data set. The top panel of the figure below shows the phase-space grid for the classical simulation and the DL approach. The x-axis represents space, and the y-axis is particle velocity. The phase-space plots are not exactly equal because the beam instability starts at different points in time in the two simulations. However, they show similar qualities – for example, how particles are distributed and the size of the phase-space hole – thereby indicating that both simulations produce similar results. Moreover, we validated the results of the DL-based PIC against the results of analytical theory, which provided us with the growth rate of the more unstable mode in the two-stream instability in the cold-beam $v_o >> v_{th}$ approximation. The bottom panel in the figure shows the electric field amplitude for the most unstable mode E_1 during the two-stream instability simulation. The solid line is the slope predicted by the linear theory, and the other two are the traditional PIC and the DL-based PIC, respectively. The plot shows how, during the linear phase of the instability (the first phase of the simulation when E_1 grows exponentially), both simulations follow the slope predicted by the linear theory, thus validating our results.

We also monitored how precisely the total energy and momentum were conserved in our simulations. The graph on the left of the figure on the next page shows the total energy for the classical PIC and the DL-based PIC. Both methods conserve the total energy with a maximum variation of approximately 2%, and therefore we can say that they have similar behaviour when it comes to energy conservation. The plot on the right in the figure above shows the evolution of the total momentum during the simulation. In this case, the traditional PIC conserves the momentum, whereas the DL-based approach does not conserve it.



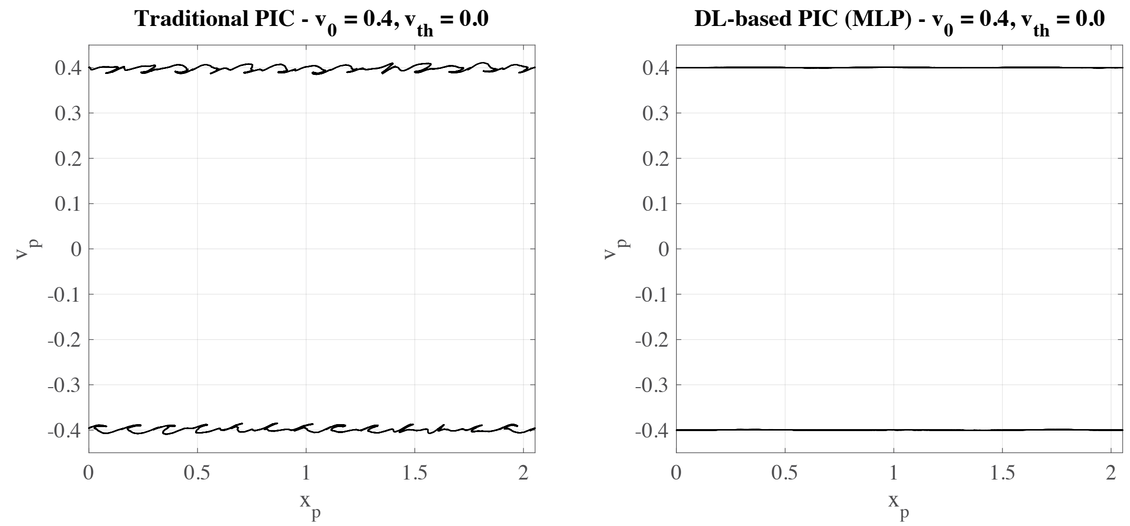
Above: Phase space for PIC and DL-based PIC, and electric field amplitude of the most unstable mode for PIC, DL-based PIC, and analytical calculations

Below: Total energy and momentum conservation during simulation time of the two-stream instability for the classical PIC and the DL-based PIC approaches



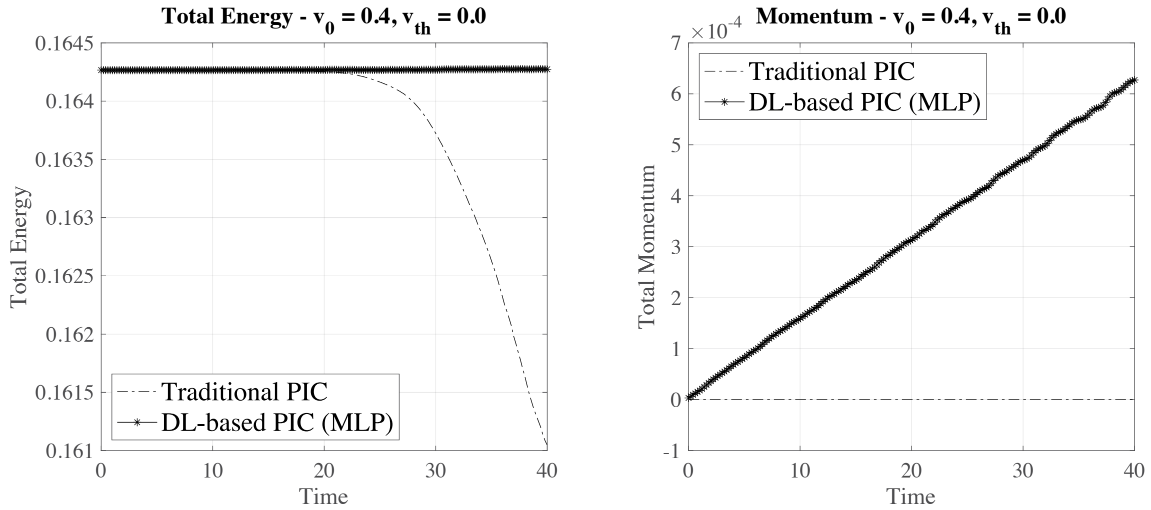
As a final experiment, we simulated a system that is stable against the two-stream instability where the two beams should continue to stream. The figure below shows the phase space for both versions at timestep 40. It can be noticed that the classical PIC exhibits a non-physical behaviour, visible in ripples pictured in the phase space. This is called cold-beam instability, and it is a well-known numerical instability that affects momentum and energy conservation in PIC methods. As can be seen in the figure, the DL-based approach is not affected by this cold-beam instability. This numerical instability can also be seen in the total energy conservation of the traditional PIC (left picture of the figure on the next page). While the numeral instability is not present in the DL-based PIC, it still does not conserve the momentum, as can be seen in the right plot of the figure on the next page.

As we have seen in this article, Deep Learning is a promising field that can open new paths to develop novel PIC methodologies. We have demonstrated that our new DL-approach produces correct results, and it is stable against the cold-



Above: Phase space for the traditional PIC and DL-based PIC simulating the two-stream instability when v_o = ±0.4 The traditional PIC presents a numerical instability shown as ripples in the plot.

Below: Total energy and momentum conservation for the traditional PIC and DL-based PIC methods simulating the two-stream instability when v0 = ± 0.4



beam instability. However, these are just the first steps towards the integration of DL techniques into PIC methods. More studies such as spectral error analysis of the electrical field values are needed in order to have a better understanding of such DL-based PIC methods. Furthermore, the use of other networks architectures should be explored. For example, using ResNets or Physics-Informed Neural Networks (PINN) would allow us to include energy and conservation law equations into the network itself, thereby increasing the physical accuracy of the system. Future work would also include characterising the performance of this new DL approach, as well as extending the model to 2D and 3D systems.

References

1. K. J. Bowers, B. J. Albright, L. Yin, W. Daughton, V. Roytershteyn, B. Bergen, and T. Kwan, "Advances in petascale kinetic plasma simulation with vpic and roadrunner," in Journal of Physics: Conference Series, vol. 180, no. 1. IOP Publishing, 2009, p. 012055.
2. S. Markidis, G. Lapenta, and R. Uddin, "Multi-scale simulations of plasma with iPIC3D," Mathematics and Computers in Simulation, vol. 80, no. 7, pp. 1509–1519, 2010.
3. J.-L. Vay, A. Almgren, J. Bell, L. Ge, D. Grote, M. Hogan, O. Kononenko, R. Lehe, A. Myers, C. Ng et al., "Warp-x: A new exascale computing platform for beam–plasma simulations," Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 909, pp. 476–479, 2018.
4. X. Guo, W. Li, and F. Iorio, "Convolutional neural networks for steady flow approximation," in Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining, 2016, pp. 481–490.
5. R. Pradhan, R. S. Aygun, M. Maskey, R. Ramachandran, and D. J. Cecil, "Tropical cyclone intensity estimation using a deep convolutional neural network," IEEE Transactions on Image Processing, vol. 27, no. 2, pp. 692–702, 2017.
6. S. Markidis, (2021). The old and the new: Can physics-informed deep-learning replace traditional linear solvers?, Frontiers in Big Data, 92.
7. T. Ichimura, K. Fujita, M. Hori, L. Maddegedara, N. Ueda, and Y. Kikuchi, "A fast scalable iterative implicit solver with Green's function-based neural networks," in 2020 IEEE/ACM 11th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA). IEEE, 2020, pp. 61–68.
8. X. Aguilar and S. Markidis, "A Deep Learning-Based Particle-in-Cell Method for Plasma Simulations," 2021 IEEE International Conference on Cluster Computing (CLUSTER), 2021, pp. 692-697, doi: 10.1109/Cluster48925.2021.00103.

Dardel Update

Gert Svensson, PDC

The first phase of Dardel, the new Swedish National Infrastructure for Computing (SNIC) flagship system at PDC, recently passed the final acceptance test with flying colours. At the time of writing, PDC is in the process of migrating all the researchers who have been working on Beskow and Tegner over to using Dardel, and is also accepting new users who have not previously used PDC's systems.

Current Status of First Phase

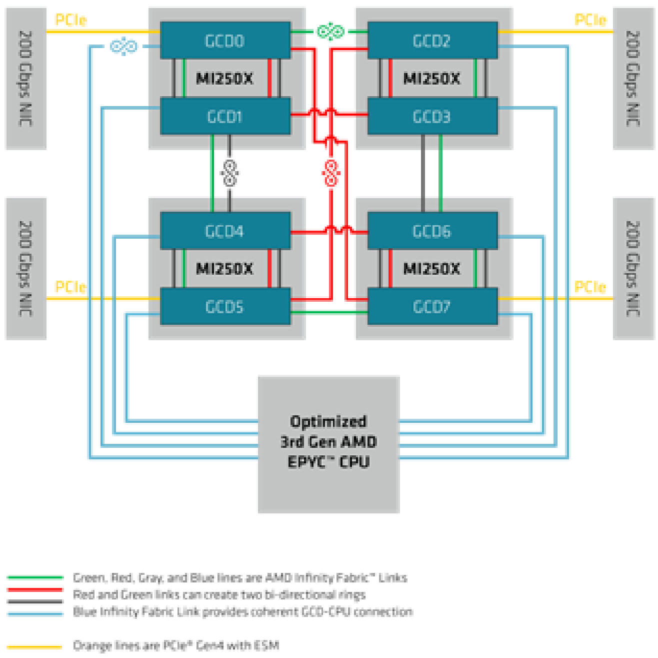
In the final acceptance test, which started at the beginning of October, several research groups were selected to test the first phase of Dardel by running real applications on the system for one month. During that period, the system had to function so that it was available at least 98% of the time to pass the test, which it did! After the acceptance test, additional system software and applications were installed while the test users continued to work on the system.

By the time this article is published, the process of transferring users from Beskow and Tegner should be in full swing. After discussions with the principal investigators for each allocation, researchers will be moved over gradually from Beskow and Tegner to Dardel. Files will be transferred, allocation by allocation, from the old to the new disks.

Status of Second Phase (GPU-partition)

The second phase of Dardel will be a partition of the system featuring GPUs. This partition has been delayed due to worldwide shortages and delays in the electronics industry, however, the plan is for the second phase of Dardel to be installed in mid-March 2022. This GPU-partition will use AMD Instinct® MI250X GPUs and will have 56 GPU nodes – each with a special version of a 64-core AMD CPU, known as the 7A53 (Trento) and only available from Hewlett Packard Enterprise (HPE) – plus four MI250X GPUs connected by AMD's Infinity Fabric® as shown in the figure above. Each GPU node will have 512 GB of shared fast HBM2E memory. The memory is cache-coherent, which will simplify programming. In principle, each MI250 consists of two separate GPU devices (similar to the K80s in Tegner). The performance of the MI250X is impressive at up to 95.7 TFLOPS in double precision when using special matrix operations, giving Dardel a theoretical peak performance of over 21 PFLOPS. HPE guarantee a High-Performance Linpack (HPL) performance for the entire GPU-partition of at least 8.2 PFLOPS!

Below: GPU node architecture



Type of nodes	Memory	Number of CPU nodes						Number of GPU nodes
		SNIC initial	Industry	Scania	SU Dept. of Astronomy	SNIC extra	Total	
Thin	256 GB	**488**	**36**				524	
Large	512 GB	**20**		236	12	48	316	56
Huge	1 TB	**8**					8	
Giant	2 TB	**2**				8	10	
Total		**518**	**36**	236	12	56	858	56

Above: This table shows the number and types of nodes that will be in the Dardel system after both phases and all the currently-planned extensions are installed. The coloured boxes indicate the nodes that have already been installed.

EuroCC National Competence Centre Sweden

AI February at ENCCS

Lilit Axner, ENCCS

Have you considered getting acquainted with artificial intelligence (AI), machine learning or deep learning? Or maybe you have been using them in your software solutions for a while now and would like to deepen your knowledge?

In either case, you are more than welcome to attend the series of ENCCS training events dedicated to AI, deep learning and machine learning that will be starting on the 26th of January 2022 and running through all of February 2022.

In recent years we have seen an exponential growth in the interest shown by researchers (whether within academia, industry or the public sector) regarding AI, machine learning and deep learning. Some researchers are switching from traditional simulations to machine learning methods; some only use machine learning for data analysis, while others combine both of these approaches.

ENCCS was established to help Swedish researchers along these paths. This year we offered a series of five training events based on your feedback to our surveys. However, we promise to cover further topics in this exciting journey within AI in the coming year. The training topics that will be covered in January and February next year are:

- AI as a Tool for Change,
- Upscaling AI with Containers,
- Advanced Deep Learning with Graph Neural Networks and Transformers,
- Julia for High-Performance Scientific Computing, and
- Introduction to Deep-Learning.

You are welcome to register for these at https://enccs.se/news/2021/11/ai-february-2022, and to keep updated on new training events run by ENCCS, please register for our newsletter: https://enccs.se/newsletter.

Swedish HPC Business Day 2021

Lilit Axner, ENCCS

On the 5th of October, ENCCS, for the first time, organized the Swedish HPC Business Day face to face event in collaboration with its third-party RISE, and PDC. The event was a big success and attracted 16 companies and public organizations. At the event, the participants shared their experiences and wishes of using HPC. They described the advantages of using HPC for their businesses and discussed the hurdles they face connected to the lack of hardware, lack of experience with HPC application software and legal aspects. The attendants were a good mixture of participants who already had a vast experience of using HPC as well as those who would like to use it and are exploring the possibilities. Below we highlight some of the presentations during the event.

Love Börjeson, director of KBLab, the Swedish National Library, presented their work on a new generation of artificial neural network models for language understanding. KBLab's models serve as a way to transfer the full potential of KB's collection to the Commons, thereby contributing to the digital transformation of society, and ultimately supporting high-quality research and democratic development. Dr. Börjeson mentioned that to be able to analyze 17 billion parameters for the current model architecture, KBLab need a very large HPC system such as Vega, and the next step of analyzing 175 billion parameters models would be possible only through access to such large systems as the upcoming LUMI system in Finland. KBLab is the first public administration in Europe that successfully applied and received access to the EuroHPC JU systems thus putting Sweden on the front line. Dr. Börjeson expressed his gratitude to ENCCS for proposing and assisting KB-Lab in its successful journey on the Vega system.

However, KB-lab was not the only organization ENCCS assisted in using HPC. Another presenter at the event was NorthVolt AB, currently making amazing progress in environmentally friendly battery production. With The help of ENCCS, NorthVolt AB is the first company accessing the EuroHPC JU systems in Europe to optimize in silico the main components of a cell battery: anode, cathode, electrolyte, and membrane. Matteo Ambrosetti, advanced material engineer at NorthVolt AB, proudly presented the progress they made in their battery research since accessing the Vega system in Slovenia and emphasized the importance and cost efficiency of HPC.

Mattias Chevalier from Scania presented the results of ten fruitful years of collaboration with PDC. Scania has been working with PDC since 2011, which has led to a significant increase in the size and speed of the HPC systems at KTH during that period. Scania highly appreciates the HPC system access at PDC and the support given to them by PDC. It is vital for Scania to have this opportunity to replace many physical experiments with simulations, thus decreasing their research and development costs drastically thanks to HPC.

EUMaster4HPC

Dirk Pleiter, PDC

A consortium of European partners led by the University of Luxembourg has been selected by the EuroHPC Joint Undertaking to design and implement the first pan-European high-performance computing (HPC) pilot master's programme. EuroHPC is an organization that was created by the European Union, thirty member states and several private members to establish a European exascale computing infrastructure. To ensure that this infrastructure is used as effectively as possible, it is essential to advance education and training in HPC and its applicability to high-performance data analytics (HPDA) and artificial intelligence (AI). EuroHPC has recognised this and is therefore investing 7 million euro into this new project, which is called EUMaster4HPC.

EUMaster4HPC will support the training of two cohorts of students through joint- and double-degree master's programmes and finance the necessary mobility. The students will be trained at two or more sites, which broadens the scope of topics they will receive training on. Furthermore, they will have the opportunity to use upcoming pre-exascale systems like LUMI, which is in part funded by Sweden, and to visit leading supercomputing centres for internships.

EUMaster4HPC will also work on a common curriculum for master's studies in HPC. KTH will be involved in this effort, together with a number of other leading universities in this field. In addition, representatives from private organizations and supercomputing centres will assist with this work. Establishing these master's studies at a European level will make them significantly more attractive for students in the future.

PDC Summer School

Dirk Pleiter, PDC

The PDC Summer School is an annual event that is designed for researchers (from the government, academic or business/industry arenas) and graduate students who want to learn the skills necessary for using high-performance computing (HPC) resources for their research. This year the summer school ran from the 23rd of August to the 3rd of September and, due to the ongoing global pandemic, it had to be an online event.

The school covers a broad range of topics and, in particular, aims to enhance practical skills, so it includes both lectures and hands-on labs. Additional enlightening talks gave participants opportunities to gain exposure to the state-of-the-art for modern HPC architectures, as well as computational science areas that leverage HPC systems.

As well as many local researchers from KTH, Linköping University, Stockholm University, and the Karolinska Institute, there were also participants from the Swedish Institute of Space Physics, Uppsala University and Lund University, as well as from farther afield, including the Tallinn University of Technology in Estonia, Utrecht University in the Netherlands, the University of Bologna in Italy, and the National Biotechnology Development Agency in Nigeria.

PRACE & EuroHPC JU Join Forces to Enable Excellent Research on HPC

Lilit Axner, ENCCS

The PRACE research infrastructure https://prace-ri.eu was established in 2010 as a collaborative effort which included most European countries. Since then, PRACE has developed and established itself as a successful research infrastructure. It offers world-class high-performance computing (HPC) resources and services through an established peer review process (solely based on scientific excellence), with a strong training and support programme which is highly respected by the European user communities and valued by stakeholders and policymakers. The European High Performance Computing Joint Undertaking (EuroHPC JU, https://eurohpc-ju.europa.eu) is a legal and funding entity, created in 2018 and located in Luxembourg. The EuroHPC JU enables the European Union and the countries participating in the EuroHPC JU to coordinate their efforts and pool their resources to make Europe a world leader in supercomputing.

Since June 2019, high-level coordination meetings involving members of PRACE (the council chair, vice-chair, managing director, and council delegate) and EuroHPC (the governing board chair, vice-chair, and executive director) have been held to align activities, and discuss and define roles in the European HPC ecosystem. A joint working group on access policies was established with experts from PRACE, EuroHPC and the Infrastructure Advisory Group (INFRAG). The objective of the working group was to prepare an access policy document for the EuroHPC Governing Board https://eurohpc-ju.europa.eu/sites/default/files/2021-03/Decision 06.2021 - Access policy.pdf.

In 2021, the EuroHPC JU delegated part of the implementation of the access policy to PRACE. For this, the EuroHPC JU relied on the structure established by PRACE (which includes the necessary committees, expert databases and IT tools) to implement the evaluation and application process. PRACE implemented these processes under the guidance of the EuroHPC JU Executive Director. The task of coordinating the different actors involved in the access and evaluation procedures was performed by the PRACE Access Resource Committee, which assumed the role of the EuroHPC JU Access Resource Committee, with the JU Executive Director joining the PRACE committee for this task. The task of determining the final allocation of resources was not delegated to PRACE and is being undertaken by the JU's Resource Allocation Panel. The portal for European HPC services is still under development, however, it already serves as a one-stop shop for exploring HPC access, training and other offerings – see https://hpc-portal.eu.

EBRAINS News

Mikael Djurfeldt, PDC

The Swedish brain research community has recently participated in a VR needs inventory to support the establishment of a Swedish EBRAINS node. The EBRAINS research infrastructure is the continuation of the Human Brain Project, an EU flagship project, and is viewed by the European Commission as a catalyser for future brain research.

PDC is taking part in the EBRAINS HealthDataCloud which is a GDPR-compliant new service for sensitive medical brain data. This enables large-scale analysis of hospital data to better understand the complexity behind diseases like Alzheimer's and Parkinson's.

The full dataset of the Jülich-Brain Atlas has been published. It contains cytoarchitectonic maps of more than 200 areas of the human brain, including cortical areas and subcortical nuclei that capture the variability between individual brains.

The NEST Desktop, a web-based GUI for the NEST Simulator that helps users without programming skills to run simulations on laptops or supercomputers, has been published in eNeuro.

AI Sweden Initiative

Fredrik Viksten & Niclas Fock, AI Sweden

AI Sweden Infrastructure Network Group

AI Sweden is the Swedish national centre for applied artificial intelligence (AI). It is supported by the Swedish government, as well as the public and private sectors across the country. The mission of the initiative is to accelerate the use of AI for the benefit of Sweden, both from the perspective of everyone living in Sweden, and in terms of Sweden in relation to the rest of the world. Since its inception, AI Sweden has gathered more than a hundred partners from all parts of the Swedish AI ecosystem: authorities, regions, municipalities, academia and institutes, start-ups and small to medium-sized enterprises (SMEs), as well as large national and multinational corporations.

To achieve its mission, AI Sweden runs projects of national interest in areas such as information-driven healthcare, AI solutions for the Swedish language, data-driven journalism, and AI to help tackle climate change. As competence is key, AI Sweden also facilitates targeted training provided by, and designed for, its partners, and also enables training for the general public, in particular via an organization known as the Data Factory. This organization was initially established physically in Gothenburg and, over the last year, it has been expanding and spreading across more sites. The Data Factory enables AI Sweden partners to make their data available to others and to access existing data produced by others, as well as to make use of computing power and storage capacity early in their key AI projects.

AI Sweden is not a research institute, but rather facilitates the entire AI ecosystem, and therefore wants to contribute to a culture of sharing, cooperation, and action between partners in Sweden. All the project's initiatives are undertaken in collaboration with the AI Sweden partners. AI Sweden is funded by Vinnova (the Swedish government innovation agency) as well as by its partners. The organization has around forty employees working at its offices in Stockholm, Gothenburg, Lund, Örebro, Luleå, Sundsvall, Skellefteå, Linköping and Karlskrona.

Why an Infrastructure Network Group?

The ecosystem of the storage and compute infrastructure is growing across Sweden. For those working within AI-related businesses, this is obviously very positive and an important foundation for developing data factory solutions and accelerating the use of AI nationwide. As a response to the growing need to share learning and knowledge about this topic and to boost collaborative efforts, in spring 2021 AI Sweden decided to create an expert group for infrastructure know-how among Swedish AI computer centres.

The purpose of the infrastructure network group is to share knowledge and experience relating to how to build and operate larger, multi-user AI centres for research and development or for providing services. The network group works to identify common challenges, needs and interests. It will accumulate knowledge in the domain in order to accelerate the use of secure, efficient operations. The idea is to increase the possibilities for collaboration between partners working on similar projects or already owning an infrastructure, and to connect key resources across Sweden.

An initial meeting was held late in spring 2021, and the network group now holds regular network meetings about once a month. Quite early on, the group itself decided to limit the scope and member focus to publicly-funded AI data centres in Sweden. AI Sweden has several private corporate partners, and a parallel group for these partners would be considered if sufficient interest in a similar network forum arises. External to the expert group(s), there is an infrastructure ecosystem consisting of AI Sweden partners that are suppliers of hardware, software and solutions.

The infrastructure network group today consists of representatives from the National Supercomputer Centre (NSC) at Linköping University, PDC at KTH, Chalmers Center for

Computational Science and Engineering (C3SE), Helsingborg city, RISE ICE Data Center, RISE Centre for Applied AI, Statistics Sweden (SCB), Swedish Tax Agency (Skatteverket), Vinnova, Swedish University of Agricultural Sciences (SLU), National Library of Sweden (KB), Gothenburg School of Economics, Wallenberg AI, Autonomous Systems and Software Program (WASP), EuroCC National Competence Centre Sweden (ENCCS) and many more, and is open to further members.

The Infrastructure Expert Group is sharing knowledge relating to a broad range of infrastructure-related topics, building on technical knowledge and learning from the previous experiences of AI Sweden and all the participating partners. The overall idea was initially to discuss things such as:

- building infrastructure, hardware and peripherals;
- safety and security policies, cyber and information security;
- user models and policies for accessing common resources;
- scheduling, scaling, efficient use of overcapacity;
- user interfaces;
- studies of usage and user patterns; and
- training and learning within ethics and technologies

During one of the first network meetings, a workshop was set up to identify the most important topics and challenges based on input from the participating member representatives. The outcome of the workshop was a list of areas that, since then, has been guiding the network administration in planning events. The areas include:

- trends in hardware and software;
- federated learning and edge computing;
- scheduling, job handling and large data transfers;
- security and sensitive data;
- machine learning operations (MLOps); and
- current topics of research and use-case studies.

So far, the following topics have been covered:

- Lessons from building the AI Sweden infrastructure – Asymptotic.AI;
- Outlook Europe – EuroCC/ENCCS;
- Security for ML/ML for security – RISE;
- Local government and AI usage – HPE; and
- NLP models: Data, requirements and lessons from BerzeLiUs and ENCCS – RISE/AI Sweden & the Swedish Royal Library.

If you work at one of AI Sweden's partners in a position relevant to any of the topics that are being addressed, please contact Niclas Fock (niclas.fock@ai.se) or Fredrik Viksten (fredrik.viksten@ai.se) at AI Sweden to lend your expertise to the endeavour.

HPC Sources

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

HPC in Sweden and Scandinavia

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

European HPC ecosystem

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

A selection of projects that PDC is involved with

- BioExcel CoE
  https://bioexcel.eu
- TREX
  https://trex-coe.eu
- EBRAINS
  https://ebrains.eu
- PerMedCoE
  https://permedcoe.eu
- EXCELLERAT
  https://www.excellerat.eu
- EOSC-Nordic
  https://eosc-nordic.eu
- DICE
  https://www.dice-eosc.eu
- HPC-Europa3
  http://www.hpc-europa.eu

HPC news sources

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