

# EuroCC National Competence Center Sweden: ENCCS

<https://enccs.se>

Contact: [info@enccs.se](mailto:info@enccs.se)

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Dr. Lilit Axner & Jeanette Nilsson

LUMI Roadshow, 2021-04-08



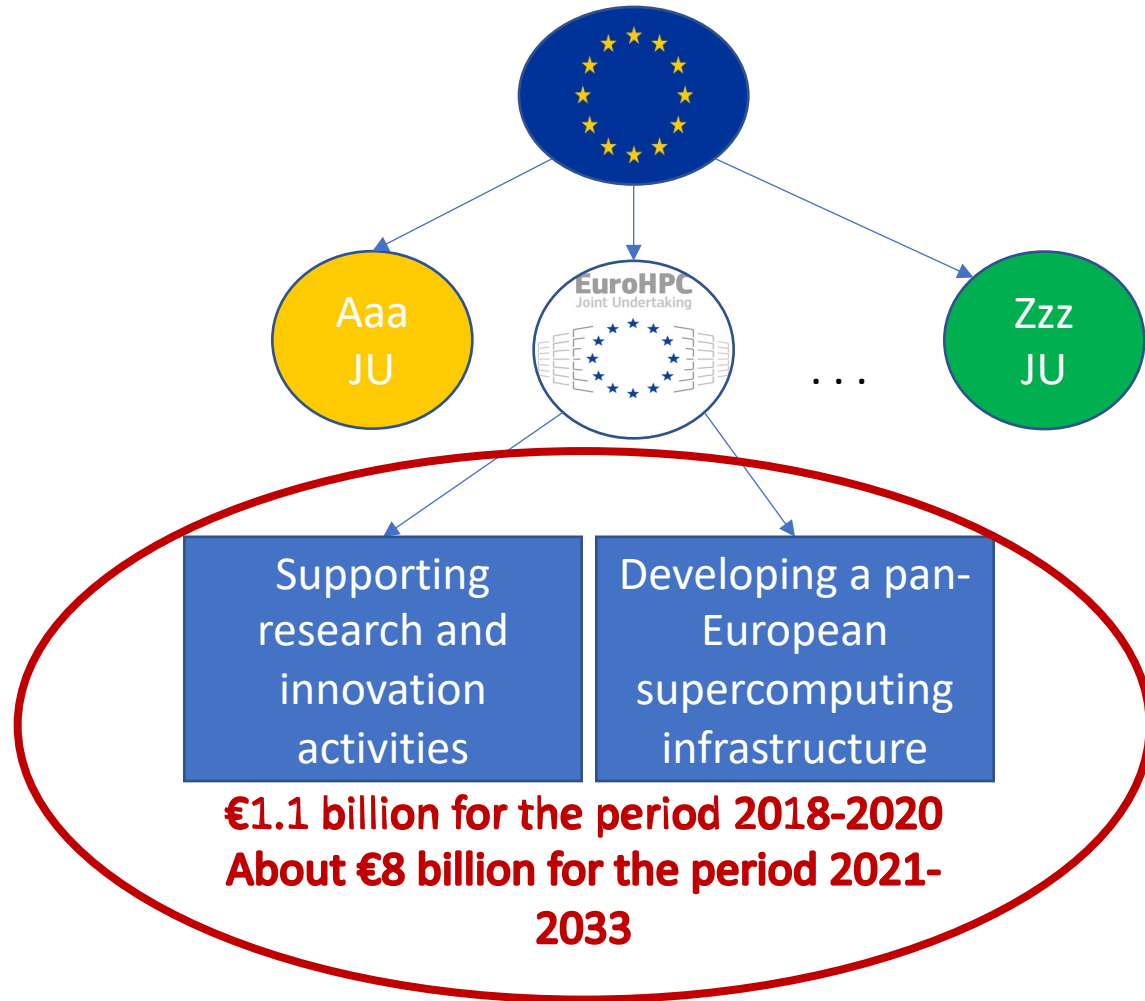
**EuroHPC**  
Joint Undertaking



Swedish  
Research  
Council

**VINNOVA**  
Sweden's Innovation Agency

# EuroHPC JU



The European High Performance Computing Joint Undertaking (EuroHPC JU) is a legal and funding entity, created in 2018, which enables the pooling of EU and national resources in high performance computing (HPC).

The EuroHPC Joint Undertaking is composed of public and private members:

Public members:

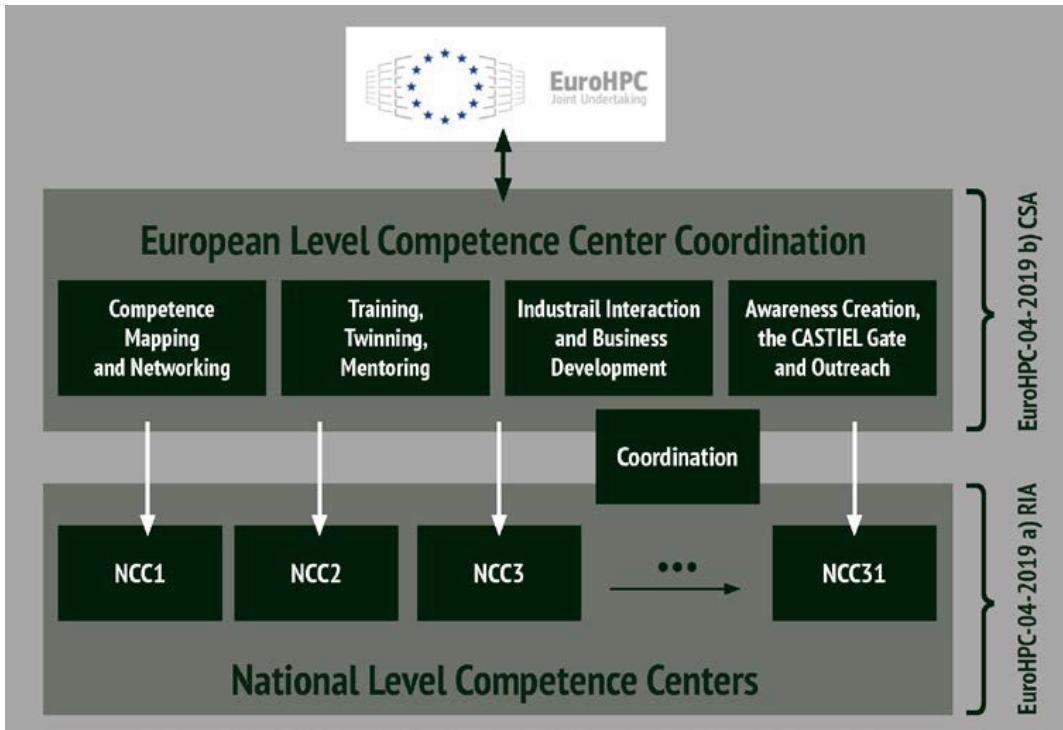
the European Union (represented by the Commission), Member States and Associated Countries that have chosen to become members of the Joint Undertaking are 32: Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Montenegro, the Netherlands, North Macedonia, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, Switzerland, and Turkey.

Private members: representatives from the two participating private partners, the [European Technology Platform for High Performance Computing](#) (ETP4HPC) and the [Big Data Value](#) (BDVA) associations. The JU also relies on collaboration with key European actors such as [PRACE](#) (Partnership for Advanced Computing in Europe) and [GEANT](#) (the pan-European high-speed network for research and education).



The EuroCC activity will bring together the necessary expertise to set up a network of National Competence Centres in HPC across Europe in 33 (including UK) to provide a broad service portfolio tailored to the respective national needs of industry, academia and public administrations.

All of this to support and increase strongly the national strengths of High Performance Computing (HPC) competences as well as High Performance Data Analytics (HPDA) and Artificial Intelligence (AI).



# ENCCS

<https://enccs.se>

Start date: 1<sup>st</sup> of September

Host: Uppsala University

Physical address: KTH, Teknikringen 31, 5<sup>th</sup> floor

Third party: RISE <https://www.ri.se/en>

Financing: **EuroHPC JU, VR and Vinnova**

LinkedIn:

<https://www.linkedin.com/company/enccs>

Twitter:

[https://twitter.com/EuroCC\\_Sweden](https://twitter.com/EuroCC_Sweden)

Newsletter:

<https://enccs.se/newsletter>

**ENCCS**  
EuroCC National Competence Centre Sweden

Home News Events Training Industry Supported Software Proposal Support About Contact

## The Swedish EuroCC Hub for High-Performance Computing

**TRAINING**

Providing training on GPU usage, AI and HPC optimisations as well as on usage of HPC in scientific disciplines such as Life sciences, Chemistry, Climate modelling, Engineering and more.

**INDUSTRY**

Assisting SMEs and large businesses in delivering competitive benefits from advanced HPC and build awareness about HPC and AI/HPDA competences and identifying strategies for technology transfer from academia.

**EUROHPC JU SYSTEMS ACCESS PROPOSAL SUPPORT**

Helping researchers both in industry and academia with application forms to apply for access to EuroHPC JU (pre)exa-scale system application support.

**SUPPORTED SOFTWARE**

Support users move to pre-exascale systems. Set up mechanisms to educate users about technical requirements for scaling and provide consulting in HPC, GPU acceleration AI/HPDA and data handling.

European Union EURO UPPSALA UNIVERSITET RISE EuroHPC Joint Undertaking Swedish Research Council VINNOVA Sweden's Innovation Agency

### GROMACS at ENCCS

2020-09-29

GROMACS is one of the most widely-used codes in all of HPC, providing key mechanistic and energetic insight into numerous biological processes. It provided one of the two major computational

More



# ENCCS Staff (incl. RISE)

12 People + 1 more in May 2021



**Lilit Axner, PhD**

Director of ENCCS



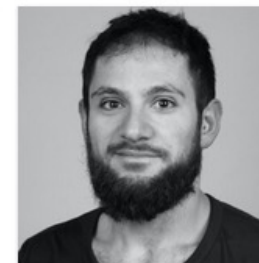
**Kjartan Thor Wikfeldt,  
PhD**

Training Coordinator



**Mark Abraham, PhD**

Research Software Engineer Domain  
Expert in Life Sciences



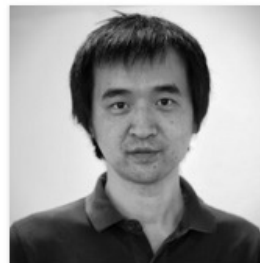
**Roberto Di Remigio,  
PhD**

Research Software Engineer Domain  
Expert in Chemistry



**Jing Gong, PhD**

Research Software Engineer  
Domain Expert in  
Computational Fluid Dynamics



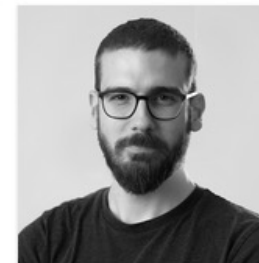
**Qiang Li, PhD**

Research Software Engineer  
Domain Expert in Climate  
modelling



**Artem Zhmurov, PhD**

Research Software Engineer  
Domain Expert in Life Sciences



**Apostolos Vasileiadis,  
M.Sc**

Dissemination Coordinator



**Jeanette Nilsson, M.Sc**

RISE project leader



**Tor Björn Minde**

Head of Lab RISE ICE Data



**Erik Ylipää**

AI researcher



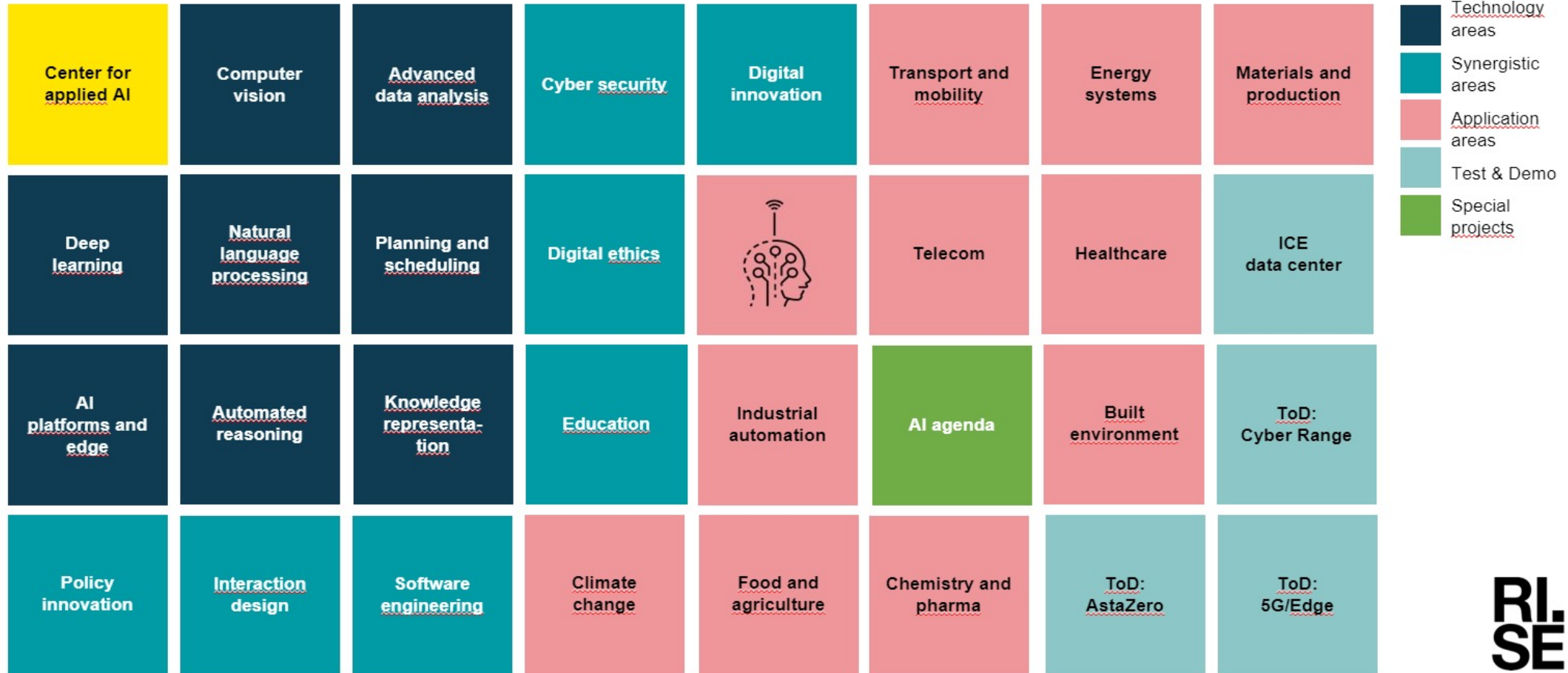
**Johan Kristiansson**

AI researcher

# RISE Research Institutes of Sweden

Bioekonomi	Brand & risk	Cement & betong	Certifiering	Cirkulär ekonomi
Design	Elektronik	Energi & bränslen	Förpackning	Glas
Hälsa, vård & omsorg	ICT och Telecom	Jordbruk & livsmedel	Kemi, material & ytor	Life Science
Maritim	Maskinteknik	Mekanik	Metrologi & mätteknik	Papper och massa
Processutveckling	Samhällsbyggnad	Säkerhet	Transport	Trä
Vatten	Produktion	Korrosion	Arbetsmiljö	Kompositer
Tillverkningsprocesser	Metaller	Additiv tillverkning	Gjutning	Textil

# AI at RISE

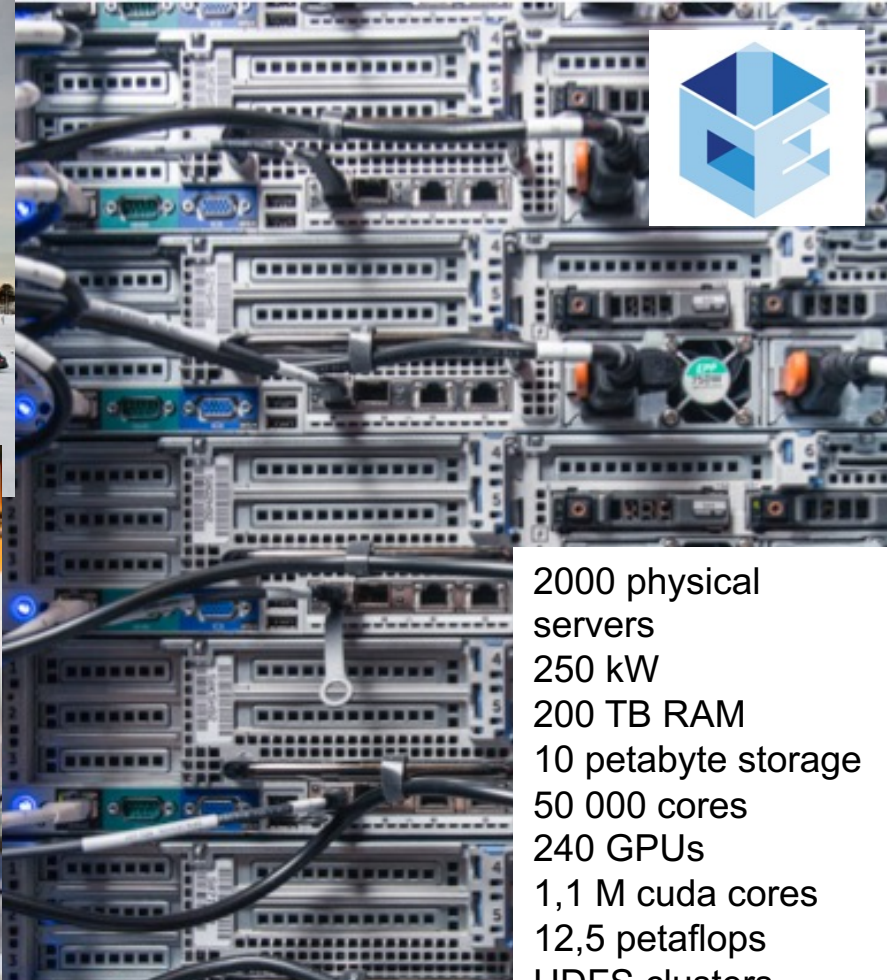
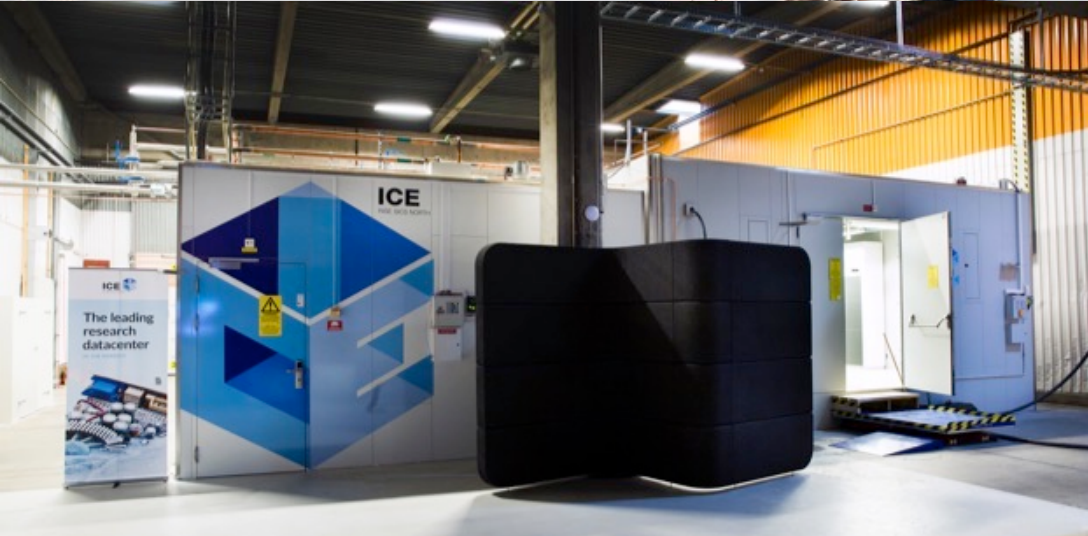


**RI  
SE**



# RISE ICE datacenter

Infrastructure and Cloud research & test Environment



- 15 projects, from the ground to the cloud
- 25 employees
- 3 MEUR turnover
- Established 2016



Stakeholders: Ericsson, ABB, Vattenfall, Facebook, LTU, Region North

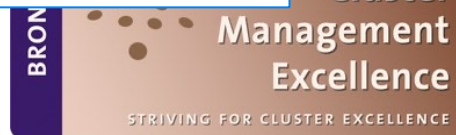


2000 physical servers  
250 kW  
200 TB RAM  
10 petabyte storage  
50 000 cores  
240 GPUs  
1,1 M cuda cores  
12,5 petaflops  
HDFS clusters  
OpenStack ECC  
OCP servers

A full-scale research datacenter and test environment with the objective to increase knowledge, strengthen the AI & DC ecosystems and attract researchers.



DATA CLOUD  
GLOBAL AWARDS  
2019



# ENCCS

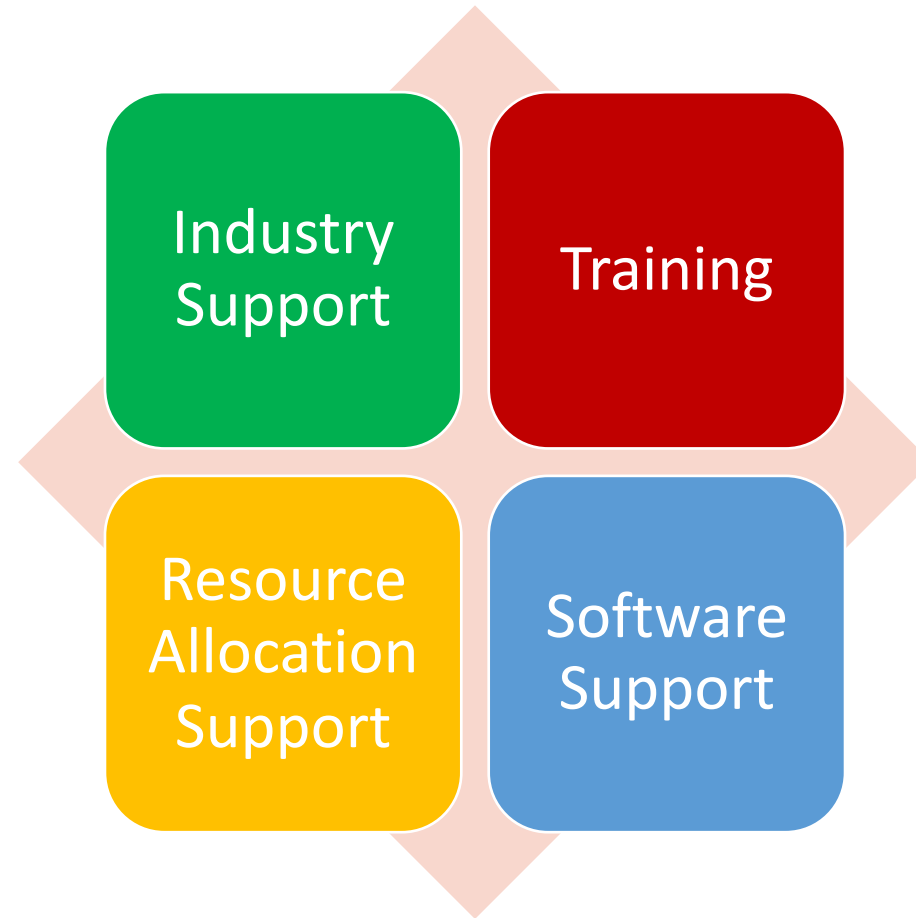
ENCCS is exploring the user **needs and gaps of knowledge** within HPC, AI and HPDA for **academia, industry and public sector**



# ENCCS: For whom, why and how

ENCCS - for three types of users	ENCCS for three types of techniques	ENCCS – gives three types of services
<ol style="list-style-type: none"><li>1. Swedish Academia</li><li>2. Swedish Industry: (small, medium and large)</li><li>3. Swedish Public Sectors</li></ol>	<ol style="list-style-type: none"><li>1. HPC</li><li>2. HPDA</li><li>3. AI</li></ol>	<ol style="list-style-type: none"><li>1. Help to access computing resources</li><li>2. Extensive training and training material</li><li>3. Help to enhance your software</li></ol>

# ENCCS activity division



# ENCCS for industry and the public sector

1. Explore and map the needs of industry (both large industries and SMEs) and the public sector in HPC/AI/HPDA
2. Identify the hurdles on the way to use HPC/HPDA/AI
3. Find solutions to eliminate these hurdles (even case by case)
4. Help industry and the public sector to use EuroHPC JU and/or PRACE systems for HPDA/AI/HPC

Industry  
Support

# Industry and Public Sector support

HPC AI

Machine Learning

DATA Analytics



## Assisting small & medium enterprises, as well as large businesses **free of charge**.

**Building awareness in the industry about HPC and AI/HPDA competences nation-wide and identifying strategies for technology transfer from academia.**

ENCCS focuses on industry usage of HPC and AI/HPDA targeting EuroHPC in collaboration with academia, with particular focus on assisting SMEs in deriving competitive benefits from advanced HPC. HPC and AI/HPDA usage from industry involvement in large research infrastructures such as ESS, SciLifeLab, ESRANGE and MAX IV will also be in scope, and a HPC industry eco-system will be developed in the task. Seminars showing best practises and examples of industry use of HPC and computing-focused business will be organized to support the eco-system.

- ✓ Consulting and support to improve software performance and adapt to AI/HPDA solutions
- ✓ Assisting in accessing the new (pre-)exascale resources
- ✓ Organising tailored training in HPC, AI and HPDA for your enterprise

OPEN CALLS FOR INDUSTRY



Voxo

Voxo AB is a Stockholm-based startup that specializes in extracting, analysing and visualising voice data. Their services are used



Airinnova

Airinnova is a start-up company with a key competency in the automation of high-fidelity computational fluid dynamics (CFD) analysis



Creo Dynamics

Creo Dynamics is a Swedish engineering company with core competence in fluid dynamics, acoustics and structural dynamics



The Swedish Aeronautical Institute

The Swedish Aeronautical Institute focuses on three areas: Research-,



Ingrid Cloud

Ingrid Cloud is built on a groundbreaking Computational Fluid Dynamics (CFD) framework, which

# Training needs and ENCCS training material

## ENCCS training for academia, industry and public sector:

1. Intermediate and advanced level HPC training (if needed beginners level)
2. Beginner/intermediate/advanced level courses on Deep learning incl. AI/HPDA
3. Hackathons/Bootcamps
4. Industry related events
5. Training on writing (pre)exa-scale application sessions (**attend the session tomorrow**)

**The ENCCS training material is always online for use on the bases of acknowledgment of ENCCS – permissive license.**



# Training

- HPC training/workshops on Intermediate and Advanced level
- AI/HPDA straining from beginners to advanced level
- Survey of needs
- Collaborative training/workshops
- Hackathons
- Bootcamps

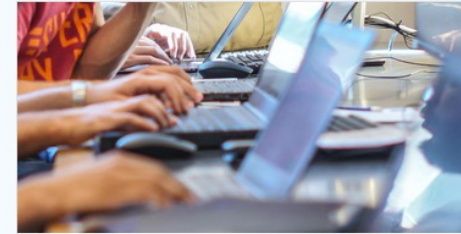
## Training at ENCCS

ENCCS offers high-quality face-to-face and online training courses and offer courses together with PRACE, the LUMI consortium, and national infrastructures. We focus on high-end usage, both in academia and industry, targeting new users in AI/HPDA. Topics include MPI & OpenMP, Software and performance engineering, GPU programming in scientific disciplines such as Life sciences, Chemistry, Climate modelling, Engineering and more.

[ENCCS EVENTS](#)[EXTERNAL EVENTS](#)[TRAINING RESOURCES](#)

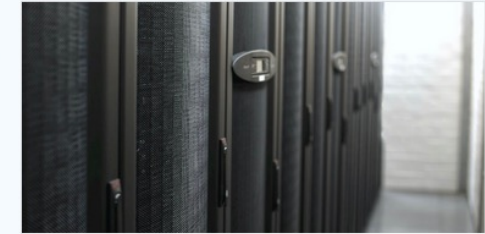
### Workshops

Our workshops cover a wide variety of HPC topics, including MPI, OpenMP, GPU programming, performance engineering and best practices in software development. The workshops are taught by our own experts, as well as distinguished instructors from other organisations. Most of our workshops are at an intermediate-advanced level and are aimed at researchers who need to scale their simulation codes up to use larger HPC resources.



### Hackathons

Our hackathons is where you can get things done! To participate in a hackathon you should have a well defined problem that you wish to solve. If your project gets accepted, you will be paired up with a mentor with the relevant expertise who will work with you to solve the problem – this can include, for example, porting a core part of your research code to run on GPUs or refactoring your code to enable more efficient parallelization.



### External events

ENCCS teams up with multiple partners to give a wide range of training on HPC topics. On our events calendar you will find recommended training events provided by SNIC, PRACE, CodeRefinery and other organisations. Recommended training material from our partners, you can find under training resources.

# ENCCS training material is public under the [Creative Commons Attribution license \(CC-BY-4.0\)](https://creativecommons.org/licenses/by/4.0/)

## Training Resources

### MPI & OpenMP

Introduction to MPI in C, Fortran and Python

[Introduction to MPI](#)

Intermediate topics on MPI

[Intermediate MPI](#)

A mini app simulating weather-like flows for training in parallelizing accelerated HPC architectures

[miniWeather](#)

### General Training Material

CMake hands-on material

[CMake](#)

CodeRefinery training material

[Training material](#)

HLRS HPC training

[HLRS](#)

### GPU Programming

NVIDIA Deep Learning Institute

[Deep learning](#)

### AI and Deep Learning

Practical Deep Learning

[Introduction to deep learning](#)

Swedsoft courses and seminars

[Swedsoft](#)

### Domain and language specific material

GROMACS GPU performance

[GROMACS](#)

Running LAMMPS on HPC systems

[LAMMPS on HPC](#)

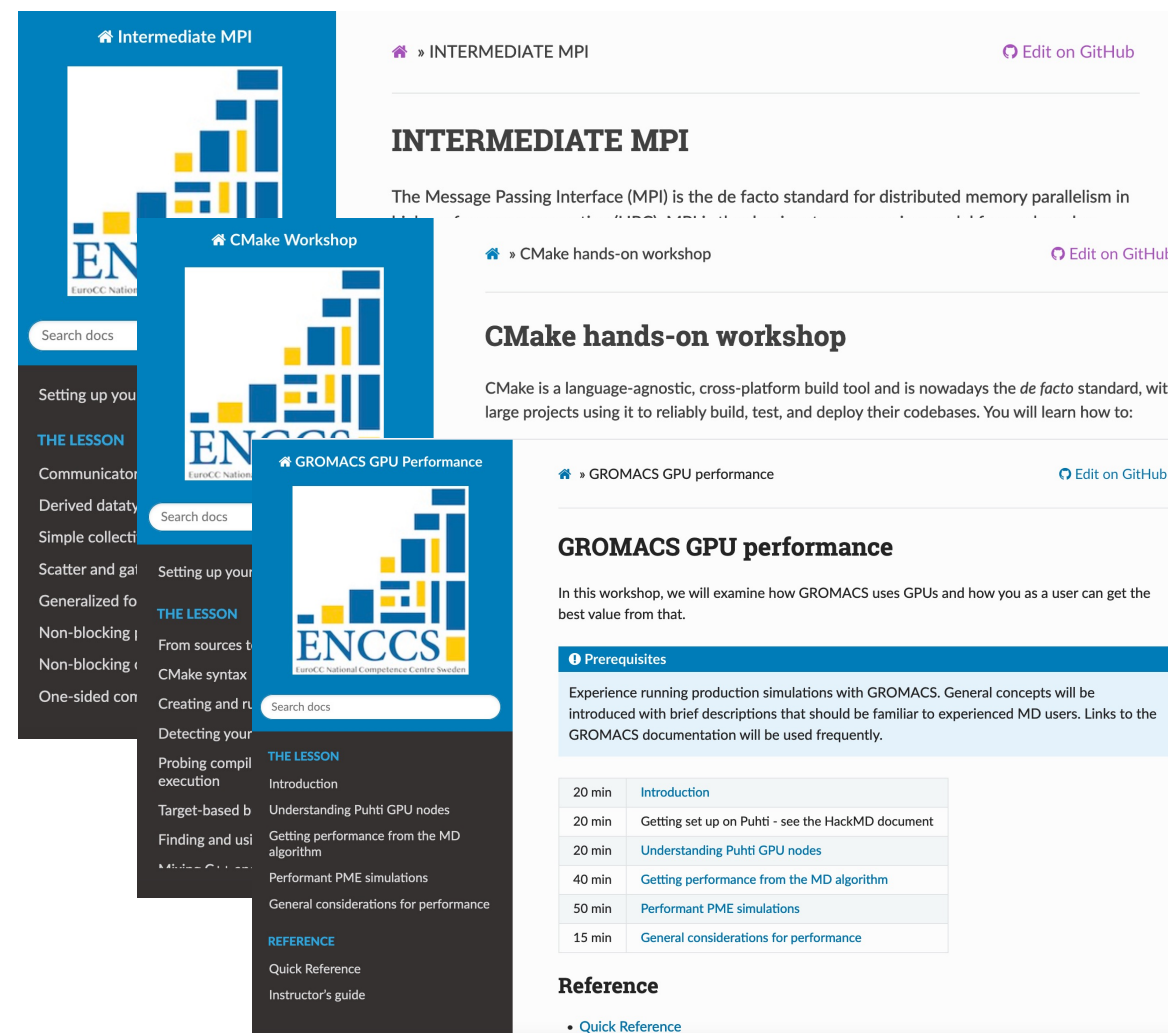
High-performance Python

[HPC Python](#)

### Performance engineering

Performance Optimisation and Productivity

[Parallel Programming and Performance Tools](#)



The collage displays three overlapping screenshots of ENCCS training resources. The top-left screenshot shows the 'Intermediate MPI' page, which describes MPI as the de facto standard for distributed memory parallelism. The top-right screenshot shows the 'CMake hands-on workshop' page, stating that CMake is a language-agnostic, cross-platform build tool. The bottom-right screenshot shows the 'GROMACS GPU performance' page, which includes a table of prerequisites and a reference section. The ENCCS logo is visible on the left side of the collage.

**Intermediate MPI**

The Message Passing Interface (MPI) is the de facto standard for distributed memory parallelism in HPC.

**CMake hands-on workshop**

CMake is a language-agnostic, cross-platform build tool and is nowadays the *de facto* standard, with large projects using it to reliably build, test, and deploy their codebases. You will learn how to:

**GROMACS GPU performance**

In this workshop, we will examine how GROMACS uses GPUs and how you as a user can get the best value from that.

**Prerequisites**

Experience running production simulations with GROMACS. General concepts will be introduced with brief descriptions that should be familiar to experienced MD users. Links to the GROMACS documentation will be used frequently.

Duration	Topic
20 min	Introduction
20 min	Getting set up on Puhti - see the HackMD document
20 min	Understanding Puhti GPU nodes
40 min	Getting performance from the MD algorithm
50 min	Performant PME simulations
15 min	General considerations for performance

**Reference**

- [Quick Reference](#)

## SAVE the DATE

(Some dates are preliminary, follow our newsletter for updates <https://enccs.se/newsletter>)

DATE	Event	Duration
2021-01-12	BioExcel/ENCCS training “Advanced topics with GROMACS”	4 Half days
2021-01-22	<b>LUMI roadshow &amp; ENCCS introduction</b>	1 Day
2021-02-09	ENCCS CMake training	2 Half days
2021-02-16	ENCCS/CSC Practical <b>Deep learning</b>	2 Days
2021-03-08	NVIDIA/ENCCS Bootcamp “ <b>AI for Science</b> ”	2 Days
2021-03-17 & 24	CodeRefinery software testing hackathon	2 Days
2021-03-31	<b>AI for beginners</b> in collaboration with RISE (especially for SMEs)	1 Day
2021-04-08	<b>LUMI roadshow &amp; ENCCS introduction</b>	1 Day
2021-04-16	<b>HIP101</b> ENCCS/CSC course	1 Day
2021-04-27	HiDALGO UAP modelling for <b>HPDA</b>	1 Day
2021-05-04	OpenACC/CUDA training for beginners	2 Days
2021-05-06	VeloxChem training	2 Days
2021-05-20	Ophidia training with CMCC for <b>HPDA</b>	1 Day
2021-06-01	OpenMP <b>hackathon</b> with Intel	3 Days
2021-06-15	OpenMP training (GPU aspects)	2 Days
2021-06-28	Advanced OpenACC/CUDA training	2 Days

# Resource Allocation Support



## Successful Swedish Applications

There have been multiple successful applications from Swedish organisations from multiple scientific areas that can be seen in the pages below.

[PREPARATORY ACCESS](#)[PROJECT ACCESS](#)

## EuroHPC JU Systems Access Proposal Support

ENCCS is working on removing possible bottlenecks in user management, resource allocation, and lacking experience that prevents projects from utilizing EuroHPC resources, whether it is due to technical challenges, policies (e.g. national vs. European infrastructure) or legislation.



ENCCS offers hands-on advice to users writing EuroHPC applications and share experience from previous successful projects, e.g. about technical proposal requirements, and assists users requiring new technical access mechanisms to EuroHPC resources.



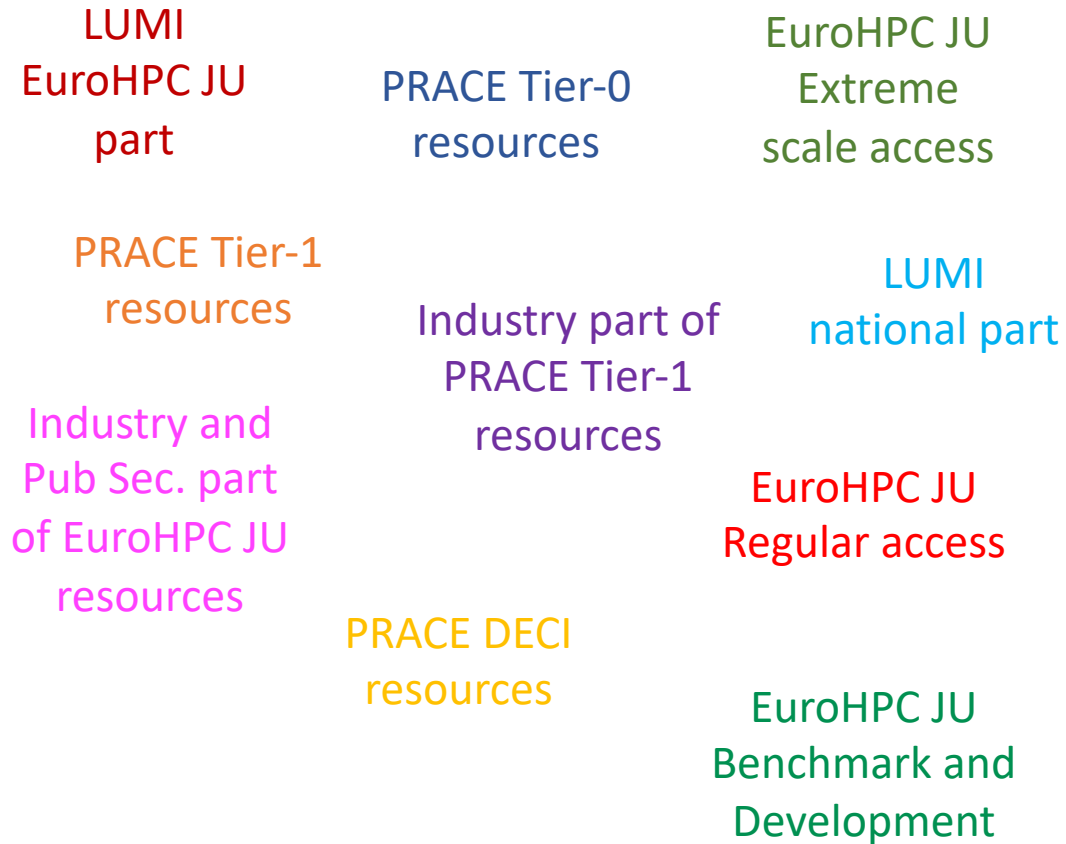
For more information on Access Policy please follow this [link](#). The document provides a high-level framework of an Access Policy for the allocation of the Union's share of the supercomputers co-funded by the Joint Undertaking.

[OPEN CALLS](#)

Resource  
Allocation  
Support



# The Ocean of Computing Resources & The Ocean of Questions



- Where to apply?
- Which resource suits me best?
- How to fill in the application?
- What criteria of my software should I consider and how?
- What can I develop with the resources?
- What do I gain from it ?
- Is there a business plan to follow?
- How are my results protected?
- Will my data be secure?"
- What is my gain of it ?
- .....



# Successful applications during the seven months of ENCCS existence

1. Prof. Rickard Armiento (**LiU**)- Preparatory access PRACE allocation for work on [VASP](#)
2. CEO Johan Wadenholt & Dr. Mark Abraham – PRACE SHAPE allocation for **Voxo AB**
3. CEO Dr. Mengmeng Zhang & Dr. Jing Gong – PRACE Preparatory TYPE-A for **Airinnova AB**
4. Prof. Thorsten Mauritsen (**SU**) & Dr. Qiang Li - PRACE Preparatory TYPE-A for work on [ICON](#)
5. Prof. Patrick Norman (**KTH**) & Dr. Roberto Di Remigio - PRACE Preparatory TYPE-B for work on [VeloxChem](#)
6. Prof. Philipp Schlatter & Dr. Jing Gong – PRACE Preparatory TYPE-B for for work on [Nek5000](#)
7. Dr. Walter Villanueva (**KTH**) & Dr. Jing Gong – PRACE Preparatory TYPE-C for for work on [Nek5000](#)

# Scientific Software support

## GROMACS 2021 beta release

by ENCCS on October 23, 2020

The GROMACS team has made available a preview of version 2021. Most new features and performance are finalized, and the team would like users to try things out and help find any rough edges. You can see the announcement with download links at <https://gromacs.bioexcel.eu/t/first-gromacs-2021-beta-release-available/986>. Please post there if you have feedback, good or bad!



## NEK5000 – Successful Preparatory Access Application

by ENCCS on December 16, 2020

Jing Gong has successfully applied for a preparatory access PRACE allocation

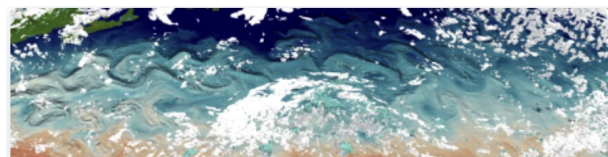
Exascale HPC architectures are increasingly prevalent in the Top500 list, with processors optimized for floating-point calculations. We have previously pre-



## VeloxChem – Successful Preparatory Access Application

by ENCCS on December 15, 2020

Roberto Di Remigio has successfully secured a preparatory access PRACE allocation on the newly installed JUWELS Booster system for ENCCS work on VeloxChem. **JUWELS Booster** is an upgrade module to the JUWELS Cluster supercomputer and is the **fastest supercomputer in Europe**. This allocation will be used to investigate an alternative algorithm for the computation of electron repulsion integrals.



## ICON at ENCCS: Climate Modeling

by ENCCS on October 7, 2020

To mitigate the risks and identify the opportunities associated with climate changes, we first need to understand what these changes are. Climate Models are essential tools that are based on our knowledge about the Earth and allow scientists to study the various complex phenomena happening in our earth system. The earth system model provides a numerical test bed to study hypotheses on environmental changes and can be used to conduct research on the climate dynamics on different time scales ranging from hours to millennia.

Software  
Support

## ESSENSE

**PERSON RESPONSIBLE:**  
**QIANG LI**

ESSENSE is a research code for flow calculations by solving the compressible Navier-Stokes equations. Using a high order finite difference method in combination with summation-by-parts operators and weak boundary conditions makes it possible to efficiently and reliably handle large problems on structured grids for reasonably smooth geometries.

[Learn more](#)

## EC-Earth

**PERSON RESPONSIBLE:**  
**QIANG LI**

EC-Earth is a global climate model system based on the idea to use the world-leading weather forecast model of the ECMWF (European Centre of Medium Range Weather Forecast) in its seasonal prediction configuration as the base of climate model. The model system can be used in several configurations including the classical climate model (atmosphere, soil, ocean, sea ice) and Earth System configurations (adding atmospheric chemistry and aerosols, ocean bio-geo-chemistry, dynamic vegetation and a Greenland ice sheet). The model is developed by the European EC-Earth consortium with SMHI as core partner leading the development and other Swedish partners from the universities of Lund, Stockholm, Gothenburg and Uppsala. The model in its different configurations and resolutions is used for climate change projections, predictions and process studies.

[Learn more](#)

# Scientific Software support – progress is reported in blog posts every 2 months



by ENCCS

December 15, 2020

## NEK5000 and LUMI GPU Partitions

One of main tasks for the ENCCS project is to enable Nek5000 to run on LUMI GPU partitions [...]



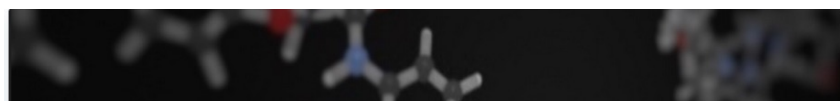
by ENCCS

November 24, 2020

## Improving GROMACS for API-driven simulations

The lead developer for the GROMACS Python API (gmxapi – see <https://academic.oup.com/bioinformatics/article/34/22/3945/5038467>), Dr Eric Irrgang of Prof. Peter [...]

[read more →](#)



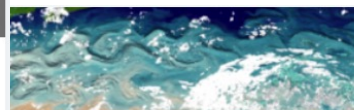
by Roberto Di Remigio

March 9, 2021

## How We Package VeloxChem with conda-build

We recently achieved two important objectives in our collaboration with VeloxChem: We helped port the code to compile [...]

[read more →](#)



by ENCCS

October 7, 2020

## ICON at ENCCS: Climate Modeling

To mitigate the risks and identify the opportunities associated with climate changes, we [...]



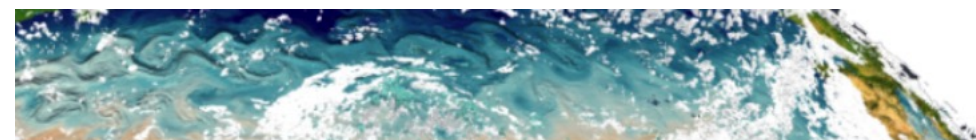
by ENCCS

September 30, 2020

## NEK5000: Simulating incompressible flow in complex geometries

Nek5000 is an open source code for simulations of incompressible flows in complex geometries. It is widely used [...]

[read more →](#)



by ENCCS

by ENCCS

October 23, 2020

## GROMACS 2021 beta release

The GROMACS team has made available a preview of version 2021. Most new features and performance are finalized, [...]

[read more →](#)



by ENCCS

January 18, 2021

## Second VeloxChem Progress Meeting

The new year starts with a progress update on the ergonomics aspects of the work of ENCCS with [...]

by ENCCS

November 10, 2020

## First GROMACS Progress Meeting

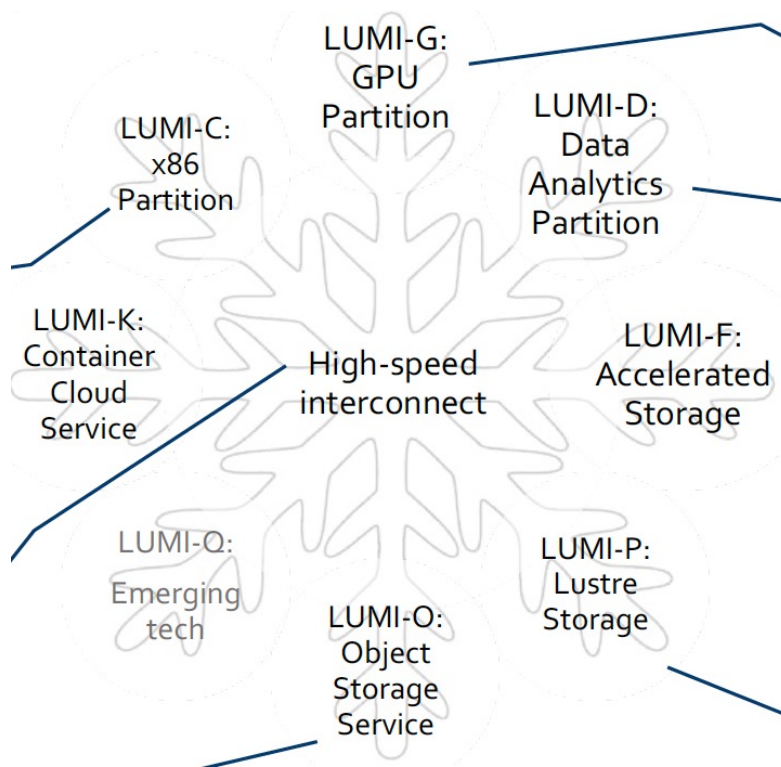
On Nov 6, the first ENCCS developer progress meeting was held. We took an in-depth look at the [...]

[read more →](#)

# HEEEELP!!! - “No problem, ENCCS is here to provide the expertise needed to make good use of LUMI!”

ENCCS Helps with preparation of applications and workflows for LUMI

## LUMI famouse snowflake



1. Combining CPU and GPU nodes within one job – perhaps only part of the application needs to be GPU-enabled
2. Refactorizing and modernizing your code
3. Employing modern frameworks and libraries
4. Writing a well-scaling MPI code first and accelerate it with GPUs
1. Converting CUDA codes to HIP, OpenACC codes to OpenMP



## ENCCS Vision

**Our vision is to establish an HPC Competence Centre as a single reference and contact point for academia, industry and public administration.**

**All activities should be focused and orchestrated as a single know-how/knowledge -transfer hub both for academia, public sector and industry (including SMEs).**



# Future plans

Our future plans are based on the

1. Changes of the Swedish HPC ecosystem
2. Constantly developing needs of the HPC/AI/HPDA users (academy, public sector and industry)
3. Developments of the international and, first of all, EU HPC ecosystem

Create a sustainable and flexible roadmap for the ENCCS' future activities!

Always be “User-centric”!!!

# SAVE The DATE: Next LUMI & the other JU systems event in Sweden 8 September 2021

LinkedIn:

<https://www.linkedin.com/company/enccs>

Twitter:

[https://twitter.com/EuroCC\\_Sweden](https://twitter.com/EuroCC_Sweden)

Newsletter:

<https://enccs.se/newsletter>

Thank you!



**EuroHPC**  
Joint Undertaking



EuroHPC National Competence Centre Sweden



**EURO**



UPPSALA  
UNIVERSITET



Swedish  
Research  
Council

[enccs.se](https://enccs.se)