# EuroCC National Competence Center Sweden: ENCCS

https://enccs.se

Contact: info@enccs.se

Dr. Lilit Axner

LUMI roadshow, 2021-01-22

EuroHPC Joint Undertaking

ENCCS EuroHPC National Competence Centre Sweden

EURO

UPPSALA UNIVERSITET

RI. SE

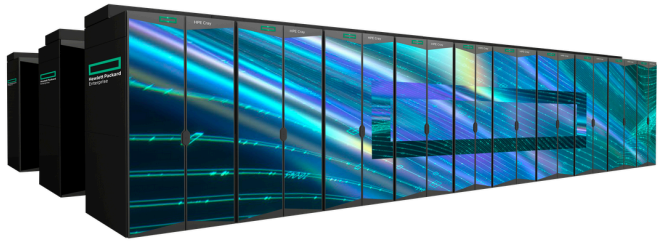
Swedish Research Council

VINNOVA Sweden's Innovation Agency

# EuroHPC JU: 3 (pre)exa-scale systems and 5 peta-scale systems

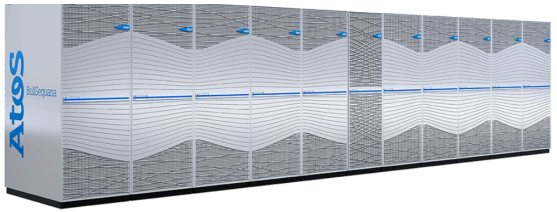
https://eurohpc-ju.europa.eu/discover-eurohpc

## LUMI, Finland (Sweden is consortium member)



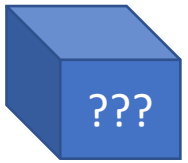
Cray EX supercomputer supplied by HPE
Sustained perf: 375 petaflops
Peak perf: 552 petaflops
64-core next-generation AMD EPYC™ CPUs, future generation AMD Instinct™ GPU

## Leonardo, Italy

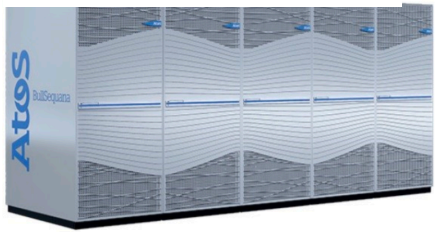


Supplied by Atos, based on the BullSequana XH2000,
Sustained perf: 249.4 petaflops
Peak perf: 322.6 petaflops
Intel Ice-Lake (Booster), Intel Sapphire Rapids (data-centric), NVIDIA Ampere architecture-based GPUs,

## (Pre)exa-scale system, Spain - yet to come




## PetaSC, Bulgaria

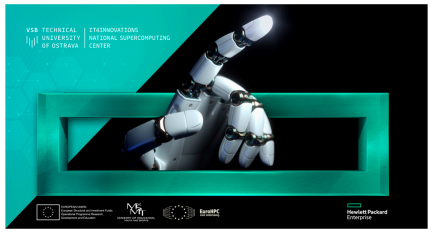


Supplied by Atos, based on the BullSequana XH2000, 4,44 petaflops, AMD EPYC 7H12 64core

## Vega, Slovenia

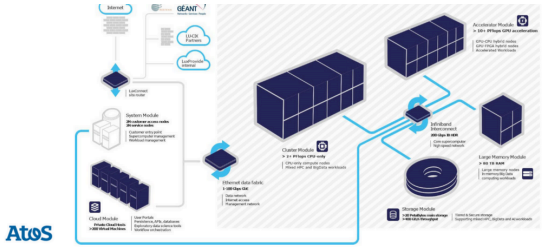
Supplied by Atos, based on the BullSequana XH2000, 6,8 petaflops, AMD EPYC 7H12 64core, 240 Nvidia A100 cards

## Karolina, Czech Rep.



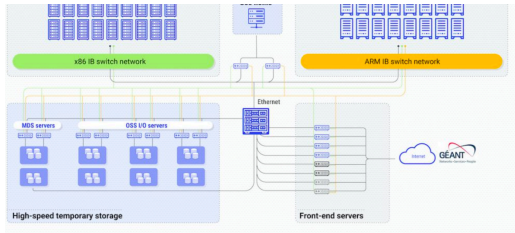
Supplied by HPE, based on an HPE Apollo 2000Gen10 Plus and HPE Apollo 6500, 9,13 petaflops

## MeluXina, Luxemburg



Supplied by Atos, based on the BullSequana XH2000, committed 10 petaflops HPL, 2+ petaflops HPL, AMD EPYC, NVIDIA A100

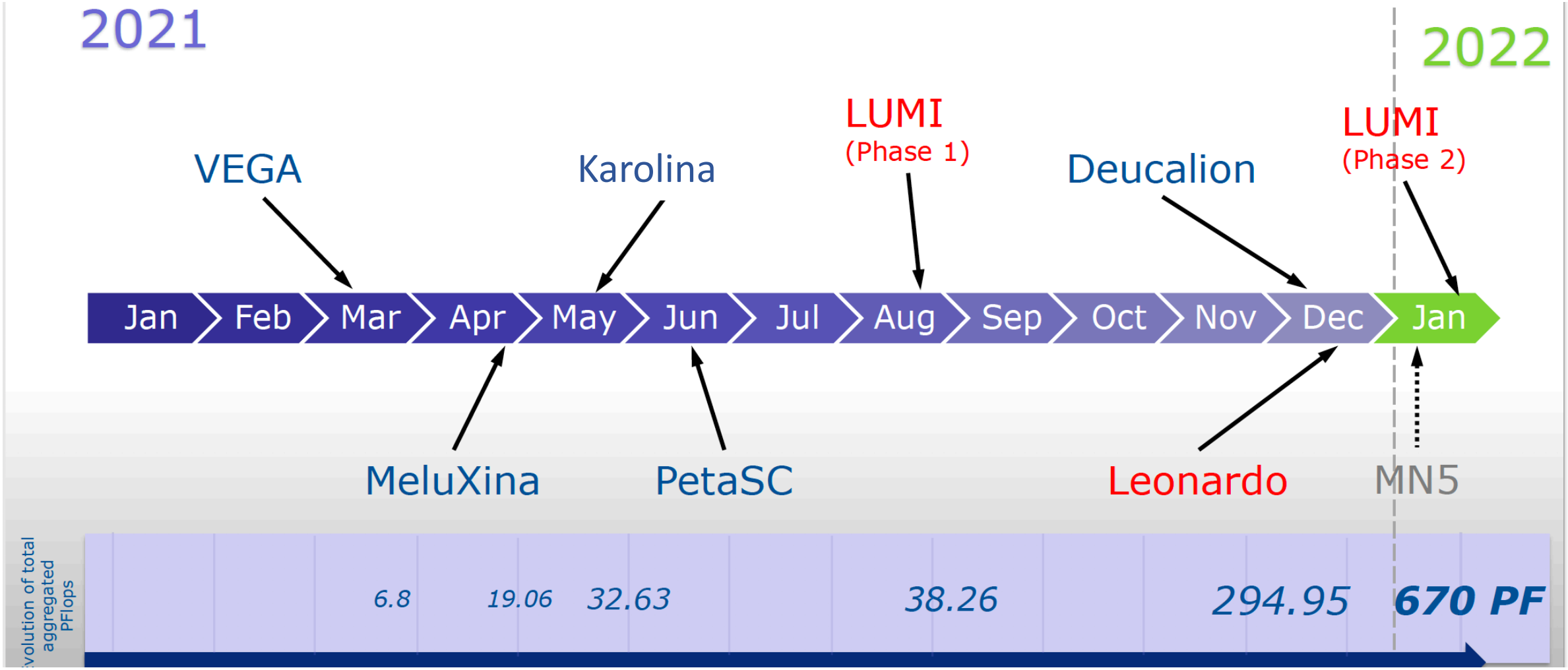
## Deucalion, Portugal




Heterogeneous 10 petaflops state-of-the-art system based on the x86 and the ARMv8 architectures.

# EuroHPC Resources – Availability timeline

(Slide provided by FLOROS Evangelos - Programme Officer Infrastructure EU)



# EuroHPC Resources – Availability timeline

(Slide provided by FLOROS Evangelos - Programme Officer Infrastructure EU)

## Regulatory Framework

***EuroHPC Council Regulation***

- EuroHPC JU will be the owner or co-owner of the supercomputers it acquires
- the operation of those supercomputers is entrusted to **hosting supercomputing centres** located in the Union;
- the Union's share of access time to the EuroHPC supercomputers is **directly proportional to the financial contribution** of the Union;
- Centres of Excellence in HPC applications
- the Governing Board of the EuroHPC is responsible for defining the access rights to the Union's share of access time to the EuroHPC supercomputers

# EuroHPC Resources – Availability timeline

(Slide provided by FLOROS Evangelos - Programme Officer Infrastructure EU)

## General policy principles – based on Regulation (Art. 13)

- allocation of access time for **publicly funded R&I** activities based on a **fair and transparent peer review** process following continuously open calls
- the use of the Union's access time is **free of charge for R&I** applications
- applications will be **evaluated by independent experts**, using **Horizon 2020 principles** as a general guide
- the Governing Board may grant Union's access time without a call for expression of interest in **exceptional cases or in emergency and crisis management situations**
- the **Executive Director** is tasked with the **annual monitoring** of the Union's access time
- based on the results of this monitoring, the Governing Board may decide e.g. to re-adapt access times per category of activity or user, or propose additional support measures for providing fair access opportunities to users from all Member States and associated countries

# EU investment in 2021-2027

Worth €7.5 billion (in current prices), the Digital Europe Programme is a part of the next long-term EU budget that covers the 2021-2027 period. It will provide funding for projects in five crucial areas: supercomputing, artificial intelligence, cybersecurity, advanced digital skills, and ensuring the wide use of digital technologies across the economy and society.

# Why EuroCC  and thus ENCCS

The European High Performance Computing Joint Undertaking (EuroHPC JU) is a legal and funding entity, created in 2018 and located in Luxembourg.

Currently, the Joint Undertaking is supporting the following activities:

- **Developing a world-class supercomputing infrastructure**:

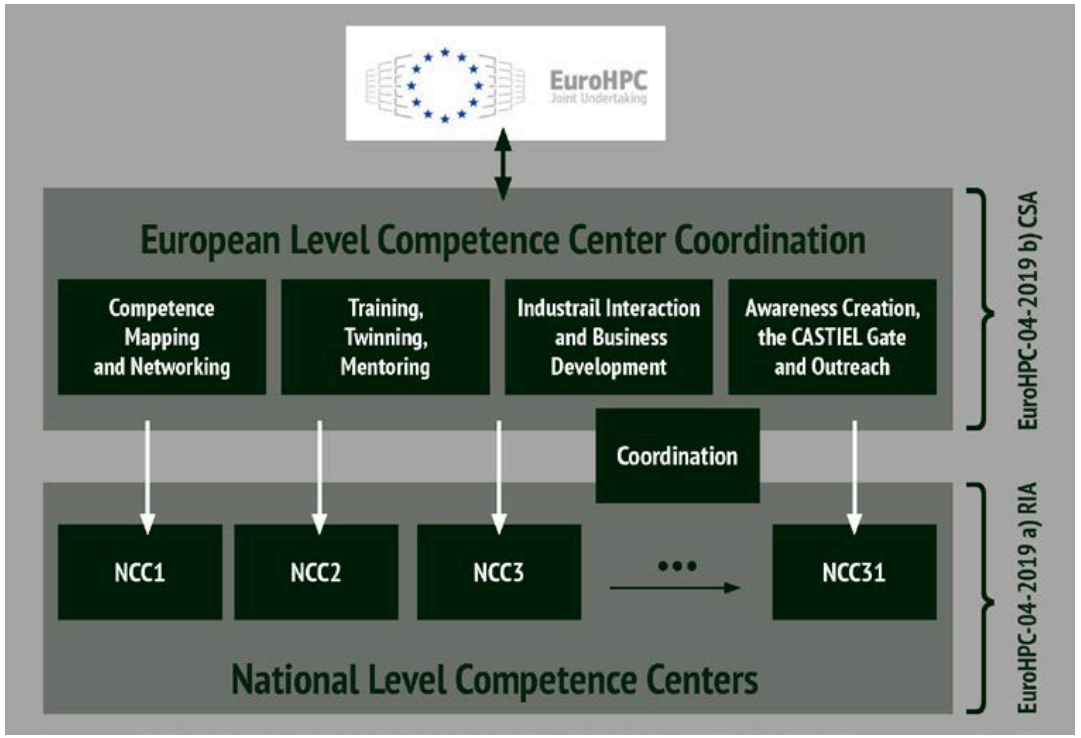
*Pre-exascale systems*: LUMI (AMD heterogeneous system in Finland), MareNostrum5, Leonardo (BullSequana XH2000 +NVIDIA system in Italy)

*Petascale systems*: Bulgaria, Czech Republic, Luxemburg, Portugal, Slovenia

- **Supporting research and innovation activities**:

Through its research and innovation agenda, the EuroHPC JU is also strengthening the European knowledge base in HPC technologies and bridging the digital skills gap, notably through the creation of a network of national HPC Competence Centres (EuroCC). The Competence Centres act locally to ease access to European HPC opportunities in different industrial sectors, delivering tailored solutions for a wide variety of users.

EURO




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: 1st of September

Host: Uppsala University

Physical address: KTH, Teknikringen 31, 5th 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

Newsletter:

https://enccs.se/newsletter

# ENCCS
# Staff (incl. RISE)

11 People + 2 more in 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

**Tor Björn Minde**

SME Expert

**Erik Ylipää**

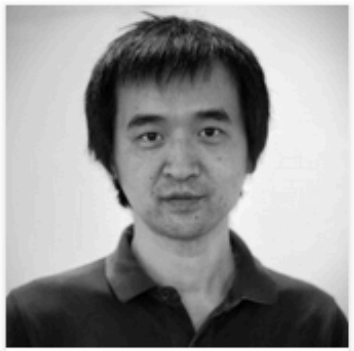
AI researcher

**Johan Kristiansson**

AI researcher

**Jing Gong, PhD**

Research Software Engineer Domain Expert in Computational Fluid Dynamics



**Qiang Li, PhD**

Research Software Engineer Domain Expert in Climate modelling

**Jeanette Nilsson, M.Sc**

SME Coordinator

**Apostolos Vasileiadis, M.Sc**

Dissemination Coordinator

# The Ocean of Computing Resources & The Ocean of Questions

LUMI EuroHPC JU part

PRACE Tier-0 resources

EuroHPC JU peta-scale resources

PRACE Tier-1 resources

Industry part of PRACE Tier-1 resources

LUMI national part

Industry and Pub Sec. part of EuroHPC JU resources

EuroHPC JU other (pre)exa-scale resources

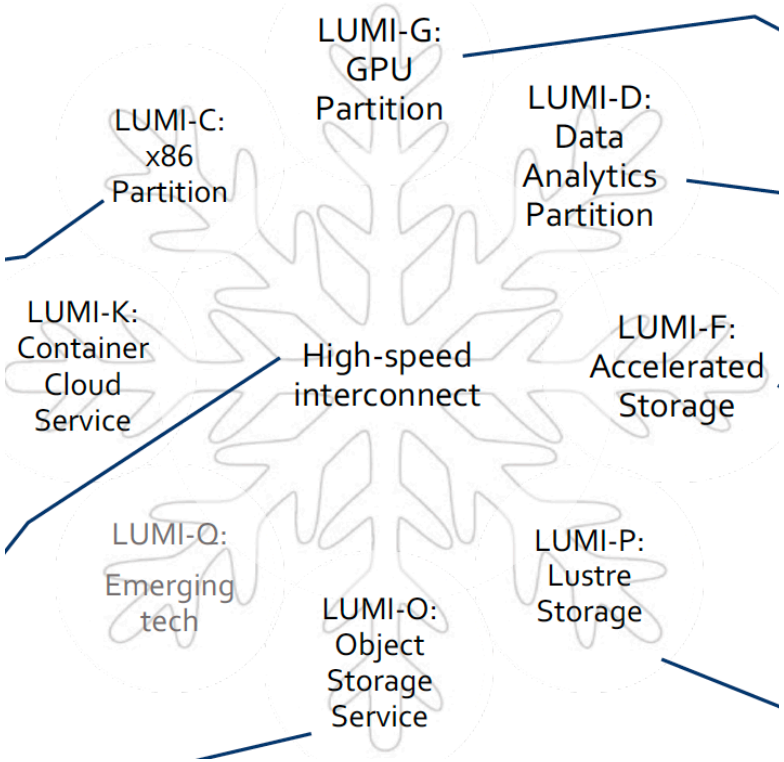
PRACE DECI resources

- 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 ?

……

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

LUMI famouse snowflake



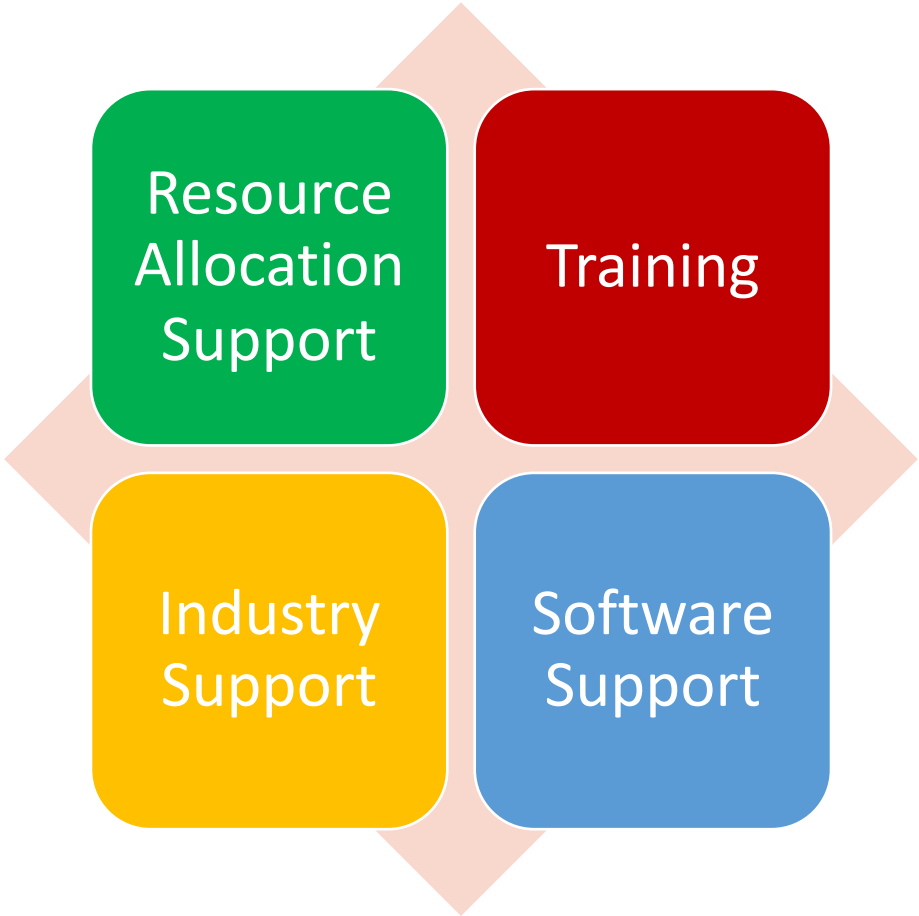

ENCCS Helps with preparation of applications and workflows for LUMI

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: For whom, why and how

| ENCCS - for three types of users | ENCCS for three types of techniques | ENCCS – gives three types of services |
|---|---|---|
| 1. Swedish Academia<br>2. Swedish Industry: (small, medium and large)<br>3. Swedish Public Sectors | 1. HPC<br>2. HPDA<br>3. AI | 1. Help to access computing resources<br>2. Extensive training and training material<br>3. Help to enhance your software |

# ENCCS activity division



# Resource Allocation Support

ENCCS
EuroCC National Competence Centre Sweden

Home | News | Events | Training | Industry | Supported Software | Proposal Support | About | Contact

## 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.

OPEN CALLS

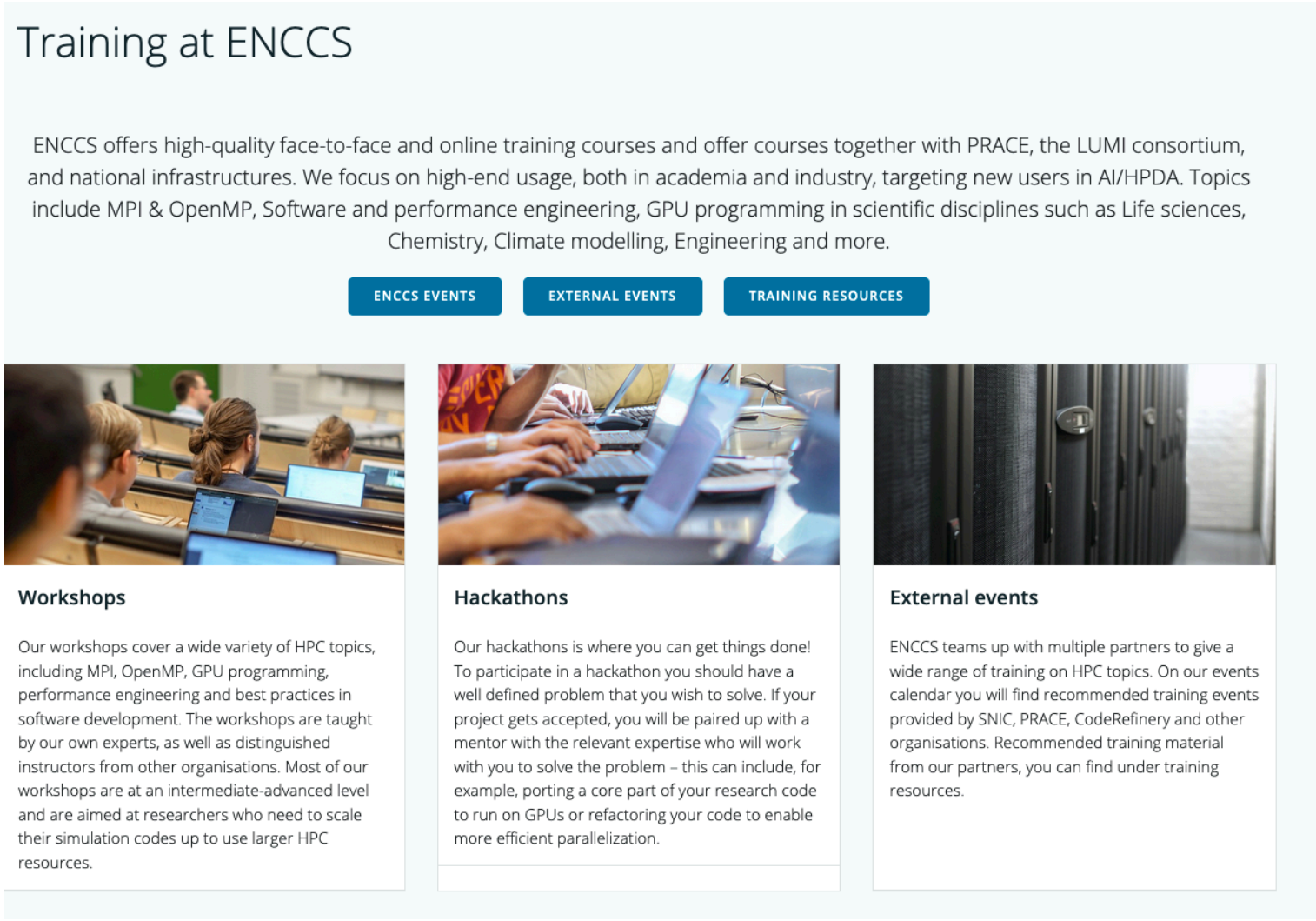
## Succesful Swedish Applications

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

# 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 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

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

# 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 | **LUMI roadshow & ENCCS introduction** | 1 Day |
| 2021-02-09 | ENCCS CMake training | 2 Half days |
| 2021-02-16 | ENCCS/CSC Practical **Deep learning** | 2 Days |
| 2021-03-08 | NVIDIA/ENCCS Bootcamp “**AI for Science**” | 2 Days |
| 2021-03-24 | **AI for beginners** in collaboration with RISE (especially for SMEs) | 1 Day |
| 2021-04-08 | **LUMI roadshow & ENCCS introduction** | 1 Day |
| 2021-04-12 | ENCCS Heterogeneous computing with HIP | 4 Half days |
| 2021-04-21 | ENCCS/RISE **Industry day** in collaboration with KTH/PDC | 1 Day |
| 2021-05-04 | OpenACC/CUDA training for beginners | 2 Days |
| 2021-05-26 | **AI for beginners** in collaboration with RISE (especially for SMEs) | 1 Day |
| 2021-06-01 | OpenMP **hackathon** with Intel | 3 Days |
| 2021-06-15 | OpenMP training (GPU aspects) | 2 Days |
| 2021-06-18 | **AI for beginners** in collaboration with RISE (especially for SMEs) | 1 Day |
| 2021-06-28 | Advanced OpenACC/CUDA training | 2 Days |

# Industry and Public Sector support

AI

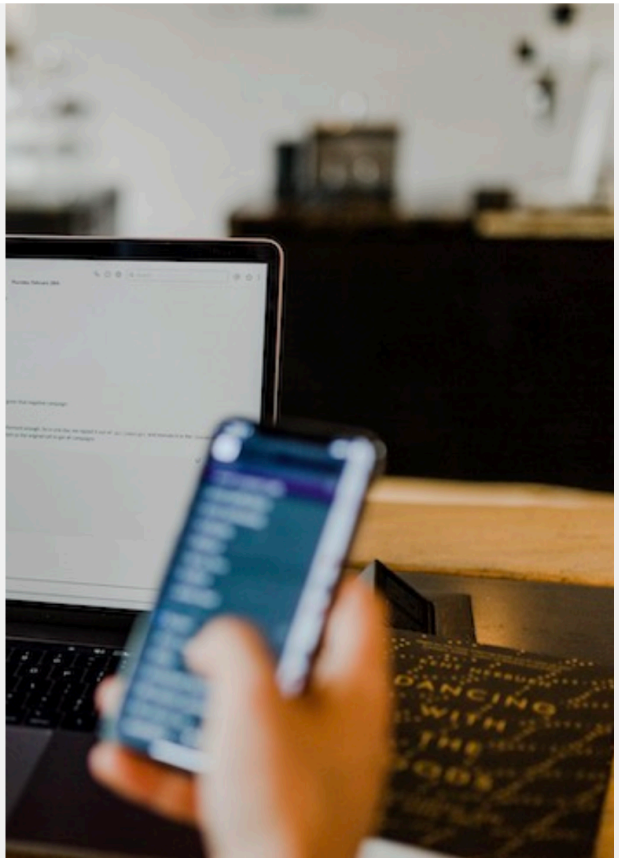
Machine Learning

DATA Analytics

HPC

ENCCS
EuroCC National Competence Centre Sweden

Home | News | Events | Training | Industry | Supported Software | Proposal Support | About | Contact



## 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

airinnova
Engineering Solutions and Innovations

### 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

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

SVENSKA FLYGTEKNISKA INSTITUTET
Swedish Aeronautical Institute

### The Swedish Aeronautical Institute

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

ingrid cloud
SMART WIND SIMULATIONS

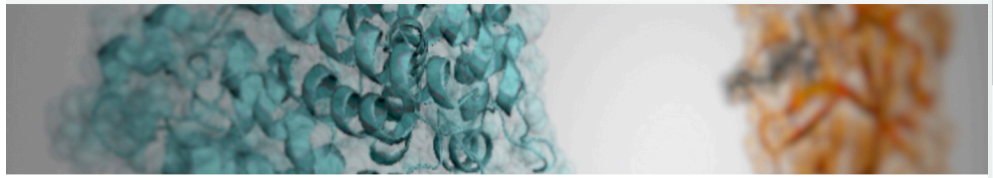
### Ingrid Cloud

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

# Scientific Software support

ENCCS
EuroCC National Competence Centre Sweden

Home | News | Events | Training | Industry | Supported Software | Proposal Support | About | Contact




## 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 allocatio

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


## 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.

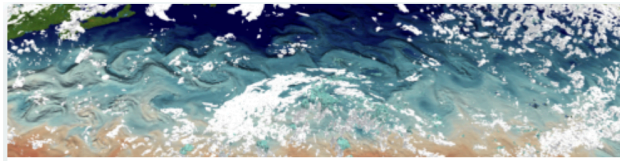
Learn more

## 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



## VeloxChem – Successful Preparatory Access Application

by ENCCS on December 15, 2020

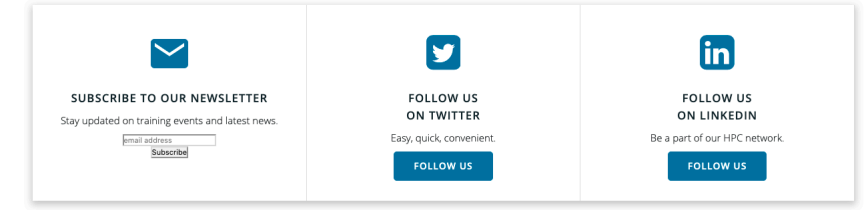
Roberto Di Remigio has successfully secured a preparatory access PRACE allocation on the newly installed JUWELS Booster system for ENCCS work on VeloxChem. JUWELS Booster is an upgrade module to the JUWELS Cluster supercomputer and is the fastest supercomputer in Europe. This allocation will be used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

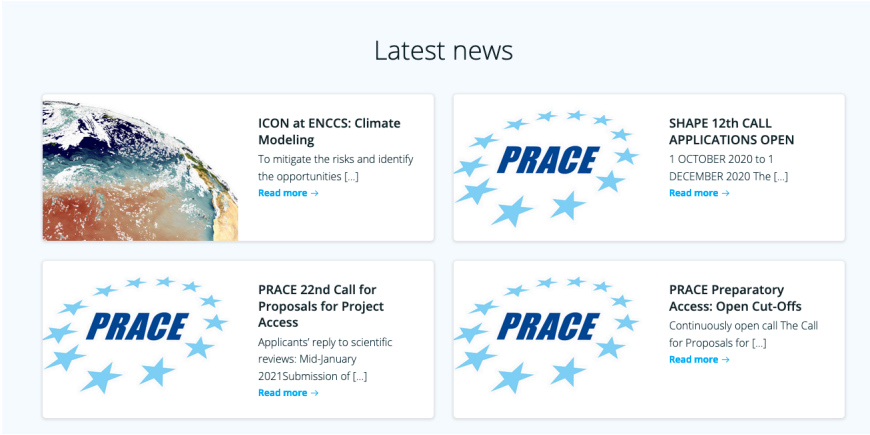
## ICON at ENCCS: Climate Modeling

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.

# User awareness (especially industry and public sector)

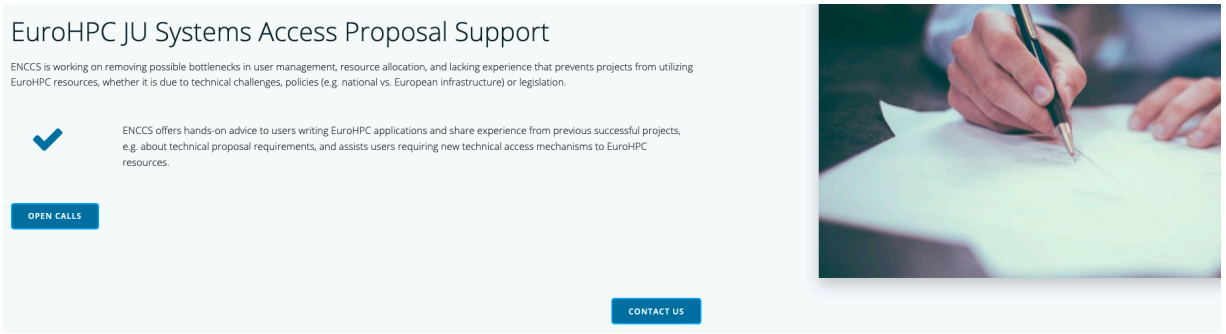



## Knowledge Mapping - Sweden

- Webpage
- Communications channels: Email, Twitter, LinkedIn
- Newsletter
- Movies (soon to come)

- Brainstorming meetings with you
- Site visits
- Awareness events (Business day)
- Statistics and observations of HPC/AI/HPDA usage



# ENCCS

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

# 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 roadshow Sweden
# 8 April 2021

LinkedIn:
https://www.linkedin.com/company/enccs

Twitter:
https://twitter.com/EuroCC_Sweden

Newsletter:
https://enccs.se/newsletter

Thank you!

EuroHPC Joint Undertaking

ENCCS
EuroHPC National Competence Centre Sweden

EURO

UPPSALA UNIVERSITET

RI. SE

Swedish Research Council

enccs.se