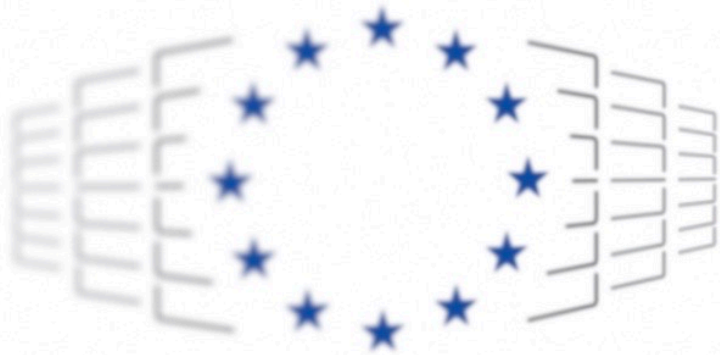


NIRD Inauguration

Dr. Lilit Anxer – ENCCS Director

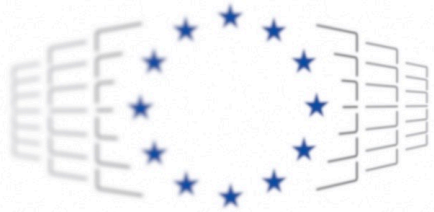




EuroHPC
Joint Undertaking

EuroHPC JU

- Developing a pan-European supercomputing infrastructure
- Supporting research and innovation activities



EuroHPC
Joint Undertaking



LUMI

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

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,

Vega

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

Karolina

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

MeluXina

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

Discoverer

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

Deucalion

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



EuroCC

- 33 countries
- Brings together expertise
- Increase national strengths in HPC, HPDA, AI



- Est. 01-09-2020



- Financing:



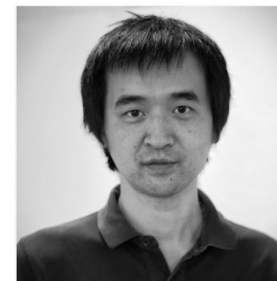
Staff



Lilit Axner, PhD
Director of ENCCS



Kjartan Thor Wikfeldt, PhD
Training Coordinator, Research Software
Engineer Domain expert in Materials
Science



Qiang Li, PhD
Research Software Engineer Domain
Expert in Climate modelling



Apostolos Vasileiadis, M.Sc
Dissemination Coordinator



Jeanette Nilsson, M.Sc
RISE project leader



Erik Ylipää, M.Sc
AI researcher



Industry



Academia

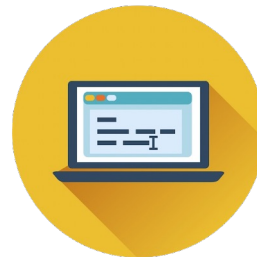


Public administration



Training

57
1300 (300)



Software support

12



HPC allocation help

43

Training

- Beginner/intermediate/advanced level
- HPC/AI/HPDA topics
- Focus on GPU programming: CUDA/HIP, SYCL, OpenMP, Julia/Python support
- Domain specific events
 - CFD
 - Quantum Chemistry
 - Biomolecular Simulations
- Hackathons/Bootcamps
 - NVIDIA
 - Intel
- Industry related events

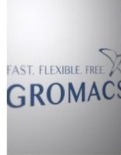


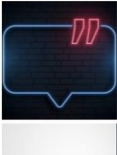
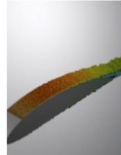

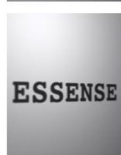

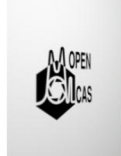


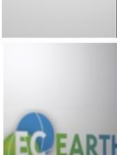
<https://enccs.se/training-resources/>

<p>High-performance Data Analytics with Python</p> <p>ENCCS</p> <p>High-performance Data Analytics with Python</p> <p>COURSE MATERIAL</p>	<p>Julia for High Performance Scientific Computing</p> <p>ENCCS</p> <p>Julia for High Performance Scientific Computing</p> <p>COURSE MATERIAL</p> <p>VIDEO RECORDING</p>	<p>SYCL Workshop</p> <p>ENCCS</p> <p>SYCL Workshop</p> <p>COURSE MATERIAL</p> <p>VIDEO RECORDING</p>	<p>AI as a Tool for Change</p> <p>ENCCS</p> <p>RI SE A.I.</p> <p>AI as a Tool for Change</p> <p>VIDEO RECORDING</p>
<p>Graph Neural Networks and Transformer Workshop</p> <p>ENCCS</p> <p>RI SE ADVANCED: DEEP () LEARNING.</p> <p>Graph Neural Networks and Transformer Workshop</p> <p>COURSE MATERIAL</p> <p>VIDEO RECORDING</p>	<p>Upscaling A.I. Workflows</p> <p>ENCCS</p> <p>Upscaling A.I. with Containers</p> <p>COURSE MATERIAL</p>	<p>OpenFoam Workshop</p> <p>ENCCS</p> <p>OpenFoam Workshop</p> <p>COURSE MATERIAL</p>	<p>OpenACC Workshop</p> <p>ENCCS</p> <p>OpenACC Workshop</p> <p>COURSE MATERIAL</p>
<p>Intermediate CUDA Workshop</p> <p>ENCCS</p> <p>CUDA</p> <p>Intermediate CUDA Workshop</p> <p>COURSE MATERIAL</p>	<p>Intermediate MPI Workshop</p> <p>ENCCS</p> <p>MPI</p> <p>Intermediate MPI Workshop</p> <p>COURSE MATERIAL</p>	<p>OpenMP for GPU Offloading Workshop</p> <p>ENCCS</p> <p>OpenMP</p> <p>OpenMP for GPU Offloading Workshop</p> <p>COURSE MATERIAL</p>	<p>NEK5000 Workshop</p> <p>ENCCS</p> <p>EXCELLERAT</p> <p>NEK5000</p> <p>NEK5000 Workshop</p> <p>COURSE MATERIAL</p>

Scientific Software Support

<https://enccs.se/supported-software/>

- Porting into GPUs
 - CUDA
 - HIP
- Optimizing for large scale (MPI)
- Providing best practices and know-how

 <p>GROMACS PERSON RESPONSIBLE: MARK ABRAHAM</p> <p>GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles. It is primarily designed for biochemical simulations like proteins, lipids and nucleic acids that have a set of complex bonded interactions, but since GROMACS is extremely fast at calculating the nonbonded interactions that usually dominate simulations many groups are also using it for research on non-biological systems, e.g. polymers.</p> <p>LATEST DEVELOPMENTS</p>	 <p>BCPNNsSim PERSON RESPONSIBLE: Jing Gong and Arjen Zomorov</p> <p>BCPNNsSim is an open-source code for scalable parallel simulation of Bayesian Confidence Propagation Neural Networks. A BCPNN module features Bayesian-Hebbian synaptic plasticity as well as structural plasticity for unsupervised and supervised learning. The code has been applied successfully to simulation of reduced brain models of e.g. associative memory and to Machine Learning benchmarks like MNIST, SVHN and CIFAR-10. Current focus is on parallel implementation on GPU and clusters of GPUs via MPI. Extensions are planned for splitting units, stacked layers, and improved support for multi-network architectures.</p> <p>LATEST DEVELOPMENTS</p>
 <p>VeloxChem PERSON RESPONSIBLE: ROBERTO DI REMIGIO</p> <p>VeloxChem solves the Schrödinger equation to study the electronic structure of molecular systems. The program can compute molecular energies and simulate the response of molecules subject to external electromagnetic fields. VeloxChem is built to exploit the aggregate resources of computing systems: from laptops to clusters. It can handle thousands of atoms and leverages a hybrid Python/C++ programming paradigm for fast development without sacrificing performance.</p> <p>LATEST DEVELOPMENTS</p>	 <p>Swedish Language Models Person Responsible: Mark Abraham</p> <p>With https://www.voxo.ai/, ENCCS is helping build the next generation of Swedish language models from the BERT family. Currently we are training a DeBERTa large model for Swedish with only a small amount of data by using transfer learning from the equivalent English models. This project is running as a pilot access in the early life of the Berzelius AI supercomputer (https://www.vu.se/ai-system/berzelius/).</p> <p>LATEST DEVELOPMENTS</p>
 <p>NEK5000 PERSON RESPONSIBLE: JING GONG</p> <p>NEK5000 is an open-source code for the simulation of incompressible flow. Nek5000 is widely used in a broad range of applications, including the study of thermal hydraulics in nuclear reactor cores, the modeling of ocean currents and the simulation of combustion in mechanical engines. The Nek5000 discretization scheme is based on the spectral-element method. In this approach, the incompressible Navier-Stokes equations are discretized in space by using high-order, weighted residual techniques employing tensor product polynomial bases.</p> <p>LATEST DEVELOPMENTS</p>	 <p>Swedish Speech Synthesis Person Responsible: Mark Abraham</p> <p>Swedish Speech Synthesis With Voxo AI (https://www.voxo.ai/), ENCCS is using machine learning to develop Swedish-language speech synthesis machine-learning models based on the Tacotron2 family of speech-synthesis model architectures. It will be a key component of Voxo conversational assistants capable of providing information in real time in response to spoken natural-language questions. It will be capable of learning to pronounce jargon relevant to particular domains, such as banking. It will generate audio streams quickly so that users will be comfortable with natural conversation flow, without pauses for generating long replies. This project is using HPC time awarded via the PRACE SHARC project https://prace-1.eu/info-access/voxe-access/ on the German GPU-accelerated supercomputer JUWELS (https://www.fz-juelich.de/ias/isc/Software/voxe.html).</p> <p>LATEST DEVELOPMENTS</p>
 <p>ESSENSE PERSON RESPONSIBLE: QIANG LI</p> <p>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.</p> <p>LATEST DEVELOPMENTS</p>	 <p>Traffic Flow Optimization Person Responsible: Hossein Ehteshami</p> <p>Traffic flow is a major contributor to the emission of greenhouse gases. Municipalities around the world have invested in what is known as Intelligent Transportation Systems (ITS) to optimize the traffic flow and reduce the emission. Proactive traffic prediction can significantly help ITS to provide a better organization of the flow across cities. Machine learning methods have proved their usability in forecasting traffic flow, in a joint undertaking, Trafikverket, KTH, and ENCCS experts Mr. Christian Edgård, Assoc. Prof. Xiaoliang Ma, and Dr. Hossein Ehteshami aim to predict traffic along the E40 highway using deep learning (DL) methods. In the first part of the project, the traffic flow will be modeled using appropriate DL models. In the second part, the already verified DL models will be coupled to a traffic-based pollution theory in order to study the dynamic of traffic pollutants at the E40. The upcoming model will primarily be developed in "Trafficflow (Java API)" in combination with in-house codes.</p> <p>LATEST DEVELOPMENTS</p>
 <p>OpenMolcas PERSON RESPONSIBLE: Roberto Di Remigio</p> <p>OpenMolcas is a molecular electronic structure package focused on multiconfigurational methods. The program can compute molecular ground- and excited state energies with state-of-the-art accuracy for many complex electronic structure problems. OpenMolcas is open source (GPL, licensed) with an open development workflow. It is a large code, written in a mix of languages: primarily Fortran (77 and 90) with some C and external modules in C++. OpenMolcas has a large, international user base. It is among one of the most used software packages for multiconfigurational quantum chemistry, in Europe and around the world.</p> <p>LATEST DEVELOPMENTS</p>	 <p>Speech-to-Text (Swedish) Person Responsible: Hossein Ehteshami</p> <p>Sentiment analysis of texts and speech-to-text transformation are active areas of research and development in the field of Artificial Intelligence (AI). Two main ingredients of such endeavor are high-quality training data and a suitable deep neural network (NN) model, which uses the training data to tune its parameters. The reward is a system that not only can turn (almost) any speech to text but also "understand" the context and sentiment in it. Modern phones, laptops, and other gadgets are already using this technology to serve their owners. Nonetheless, most of the development in this field emerged around the English language model. Currently, there is a void for a Swedish counterpart. As a response to this void, the data lab (KSLab) at the National Library of Sweden (Kungliga Biblioteket) developed the KB-SERT model, the Swedish trained transformer model based on Google BERT architecture. KB-SERT, trained on the vast amount of high-quality data solely available at KB, proved to be a game-changer in this area* and add a sentence that that ENCCS is assisting KB in this project that will run on Vega.</p> <p>LATEST DEVELOPMENTS</p>
 <p>ICON PERSON RESPONSIBLE: QIANG LI</p> <p>ICON is a highly versatile next generation global climate model. The model solves the equations of motion for the atmosphere and ocean and couple these together with unresolved processes such as small scale turbulence, cloud microphysics and radiation. The model code has been designed with parallelization in mind allowing scientists to achieve unprecedented kilometer-scale resolutions, enabling simulations of individual clouds and ocean eddies even on global grids.</p> <p>LATEST DEVELOPMENTS</p>	 <p>EC-Earth PERSON RESPONSIBLE: QIANG LI</p> <p>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, ice, 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 a core partner leading the development and other Swedish partners from the universities of Lund, Stockholm, Gothenburg and Luleå. The model in its different configurations and resolutions is used for climate change projections, predictions and process studies.</p> <p>LATEST DEVELOPMENTS</p>

Proposal support

<https://enccs.se/proposal-support/>

- Choosing type of access
- Assisting in writing the proposal
- Follow up to assist and give know-how after access has been gained

 <p>EuroHPC JU Extreme Access</p> <p>For getting a large amount of compute time (12 to 24 month access)</p> <ul style="list-style-type: none">✓ CPU Hours: ≈ 80 million✓ GPU hours: ≈ 55 million <p>GO TO CALL</p>	 <p>EuroHPC JU Regular Access</p> <p>For getting a large amount of compute time (12 month access)</p> <ul style="list-style-type: none">✓ CPU Hours: ≈ 20 million✓ GPU hours: ≈ 2 million <p>GO TO CALL</p>	 <p>EuroHPC JU Development Access</p> <p>For developing your solution or software (6-12 month access)</p> <ul style="list-style-type: none">✓ CPU Hours: 2 560 000✓ GPU hours: 384 000 <p>GO TO CALL</p>	 <p>EuroHPC JU Benchmark Access</p> <p>For benchmarking and small tests (3-month access)</p> <ul style="list-style-type: none">✓ CPU Hours: 896 000✓ GPU hours: 128 000 <p>GO TO CALL</p>
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How do you go about applying?

In this video we explain how a company, public authority or researcher can apply for access to EuroHPC JU supercomputers.

Need more tailored help?

[PROPOSAL SUPPORT](#)




Success Stories



**Göteborgs Universitet
Accesses Karolina**

The NLU team at AI Sweden has gained access to VEGA to experiment with a Swedish GPT model.

[Read more →](#)



AI Sweden Accesses VEGA for a Second Time

The NLU team at AI Sweden has gained access to VEGA to experiment with a Swedish GPT model.


[Read more →](#)



Swedish National Archives Gain Access to VEGA

With assistance from ENCCS, the Swedish National Archives (Riksarkivet) successfully applied for access to the EuroHPC supercomputer Vega hosted by IZUM in Slovenia.

[Read more →](#)



Traffic Flow and Deep Neural Networks

Modelling traffic flow on a specific part of the E45 using deep neural networks. The results give a hint at the most appropriate models for such modeling.


[Read more →](#)



Successful application of Compular to the FF4EuroHPC program

Compular develops cutting-edge analysis tools for molecular dynamics simulations. The awarded project will fund a computational experiment in partnership with Stiftelsen Chalmers Industriteknik, Enerpoly, and ENCCS.


[Read more →](#)



Thermo-Calc Software AB to access VEGA

The project leverages the power of HPC and first-principles-based calculations to accelerate the development of CALPHAD thermodynamic and kinetic databases that bring the feasibility of alloys-by-design to reality.

[Read more →](#)



Compular AB Accesses Karolina Supercomputer

Compular has successfully applied for access to EuroHPC JU supercomputer Karolina!


[Read more →](#)



Computational design for quantum technologies

Associate Professor Biplab Sanyal from the physics department of Uppsala University has gained access to Karolina supercomputer.

[Read more →](#)



ERCO Pharma AB Accesses VEGA

We are pleased to announce that ERCO Pharma AB has successfully applied.

[Read more →](#)



Vinnova to Use Vega EuroHPC JU System

With the awarded HPC time on the Vega EuroHPC JU petascale system within EuroHPC JU development call, Vinnova intends to further develop this AI tool for analysis of new types of government agency documents and enhance it with new features.


[Read more →](#)



Drug Research and HPC. Moroxite AB & Forcelab AB Access VEGA System

Moroxite develops targeted drug delivery strategies for breakthrough therapies. Forcelab provides in silico insight into the drug development pipeline. The access to VEGA will help the companies advance their in silico drug discovery program and accelerate the testing of drug delivery methodologies.


[Read more →](#)



National Library of Sweden Has Now Access to VEGA

The National Library of Sweden has been awarded development access to the Vega EuroHPC JU system for the development of speech-to-text transformation software.


[Read more →](#)



Why does the Royal Library of Sweden need HPC? [Video]

RISE NLU Group will train English BERT model using multiple GPUs on the EuroHPC JU system Vega.

[Read more →](#)



RISE Accesses VEGA

RISE NLU Group will train English BERT model using multiple GPUs on the EuroHPC JU system Vega.

[Read more →](#)



Icarus Simulations AB Accesses EuroHPC JU system Vega

In the project, Icarus aims to focus on development for industrial and commercial applications in the aviation, marine and, automotive industry.



EnginZyme Successful Application

Cell-free synthetic biology helps to harness the power of nature's catalysts, enzymes. This gives a unique insight to address many challenges facing the chemical industry in the 21st century, both by accelerating the industry's transition to sustainability and by innovating solutions for other industries through novel chemical products.

[Read more →](#)



Northvolt to Be the First Industrial Actor to Access a EuroHPC System

In partnership with ENCCS, Northvolt will investigate the use of classical and reactive molecular dynamics and quantum chemical simulations to devise bottom-up design strategies for improved batteries.


[Read more →](#)



Creo Dynamics Successful Application

Study of high-pressure hydrogen (H2). The overall aim of the project is to derive a best practice recommendation for transient Computational Fluid Dynamics (CFD) simulations of H2 high pressurized tanks.

[Read more →](#)



VOXO ENCCS



PRAGE

northvolt



Skellefteå, Sweden



Simulations of the electrochemistry relevant for battery development

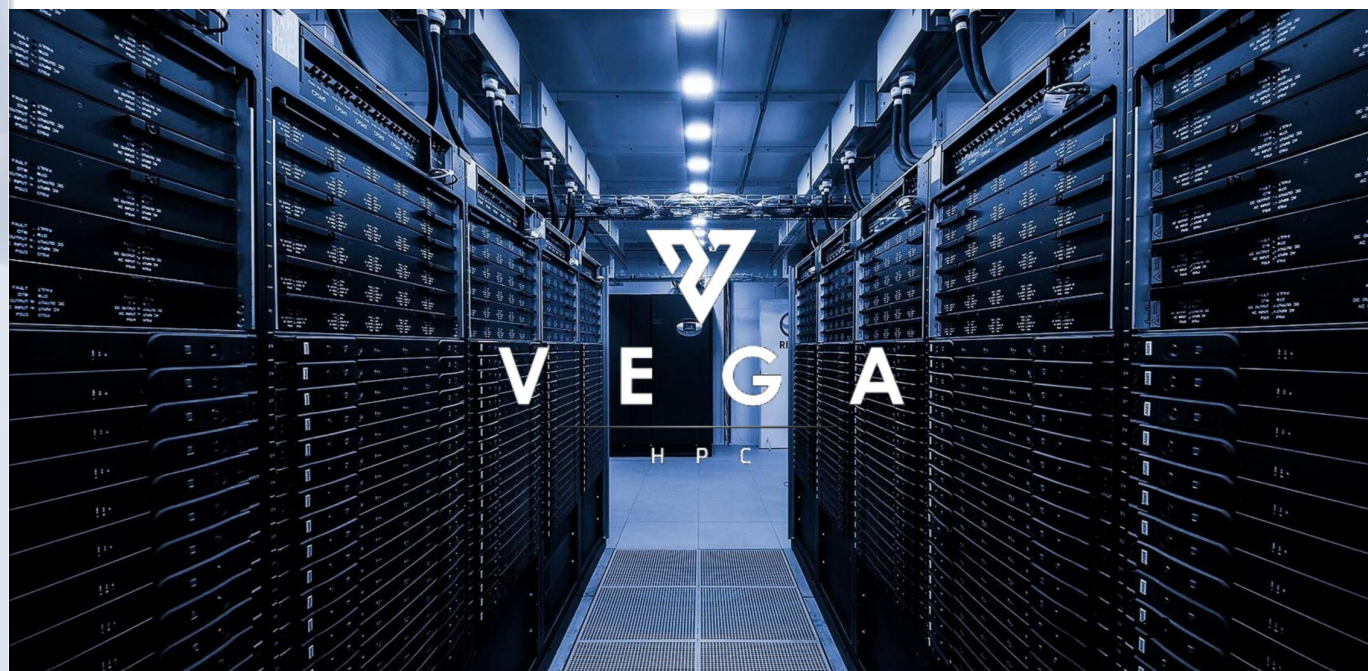
Use of classical and reactive molecular dynamics and quantum chemical simulations to devise bottom-up design strategies for improved batteries

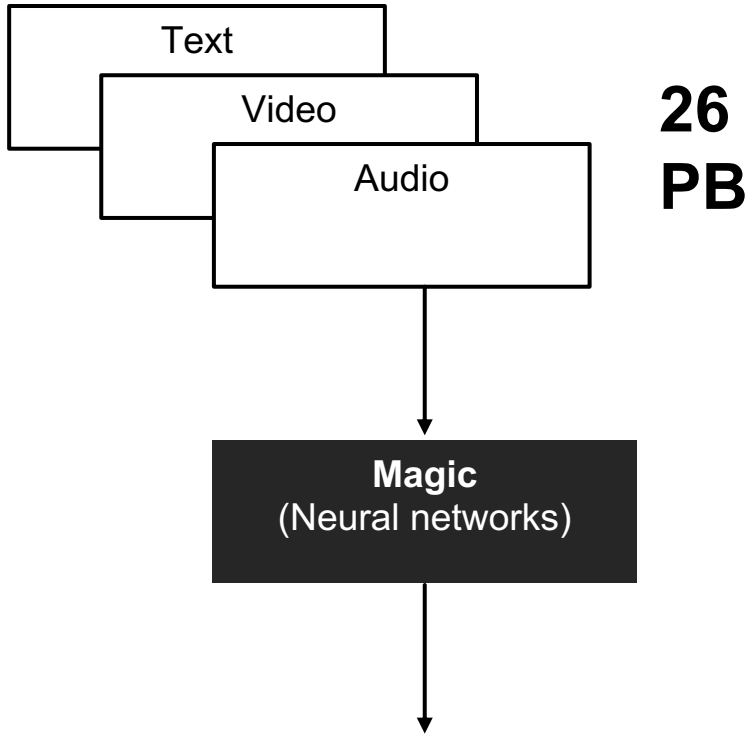
Software used:

- **Lammps** (for reactive force field simulations)
- **GROMACS**
- **psi4** (for sapt simulations)
- **ADF**

2 268 000 CPU & GPU Core Hours

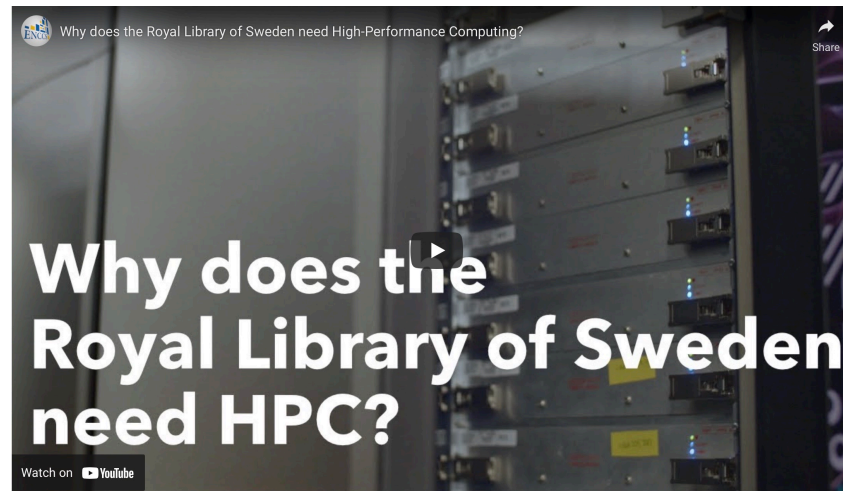
northvolt





Swedish speech-to-text models
(Based on Google-BERT)

10 000 000 GPU core hours
(Regular Access, Meluxina)



Adapting AI-technology for use in archives

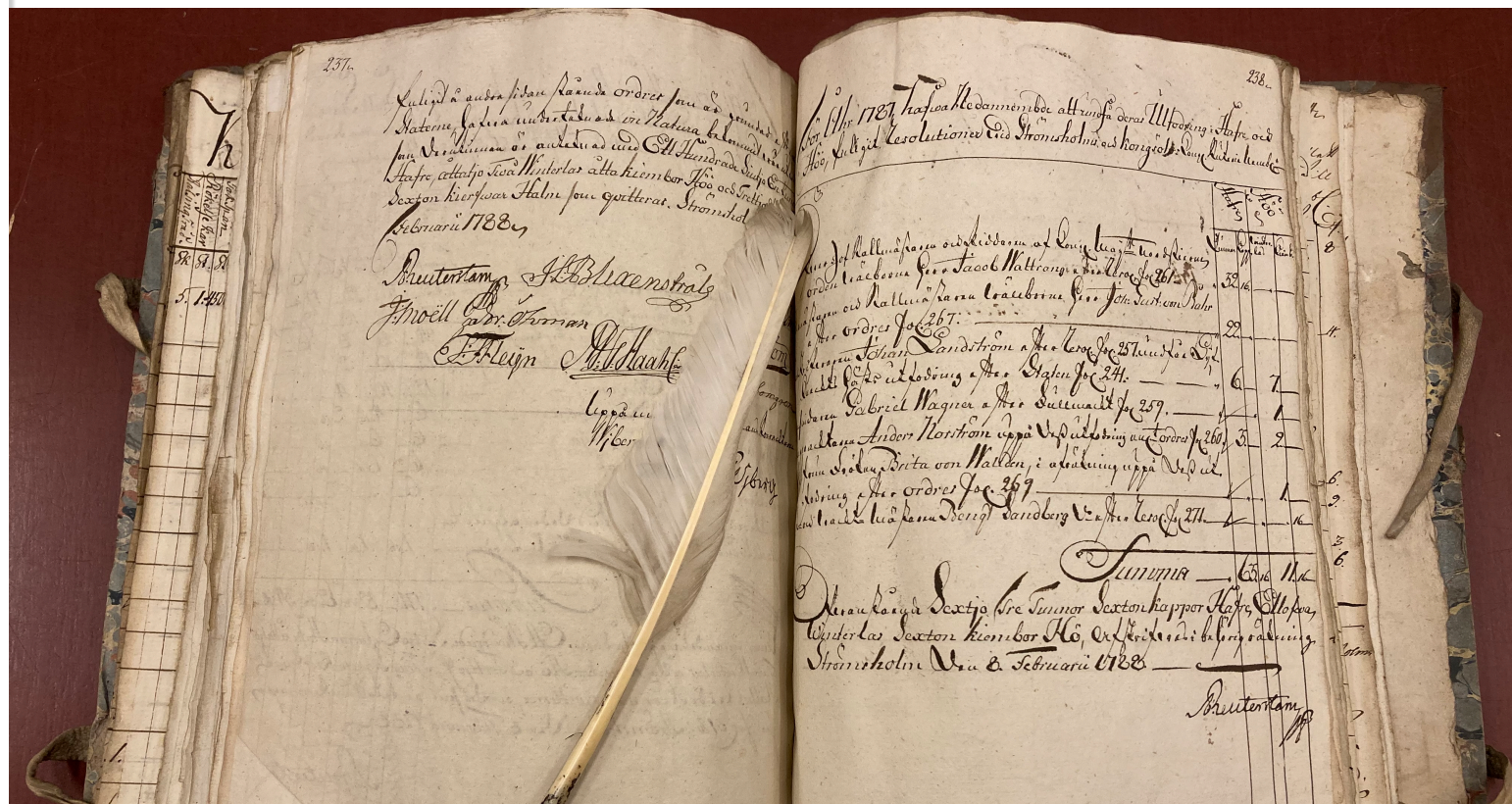
- Image segmentation models
- Text-recognition

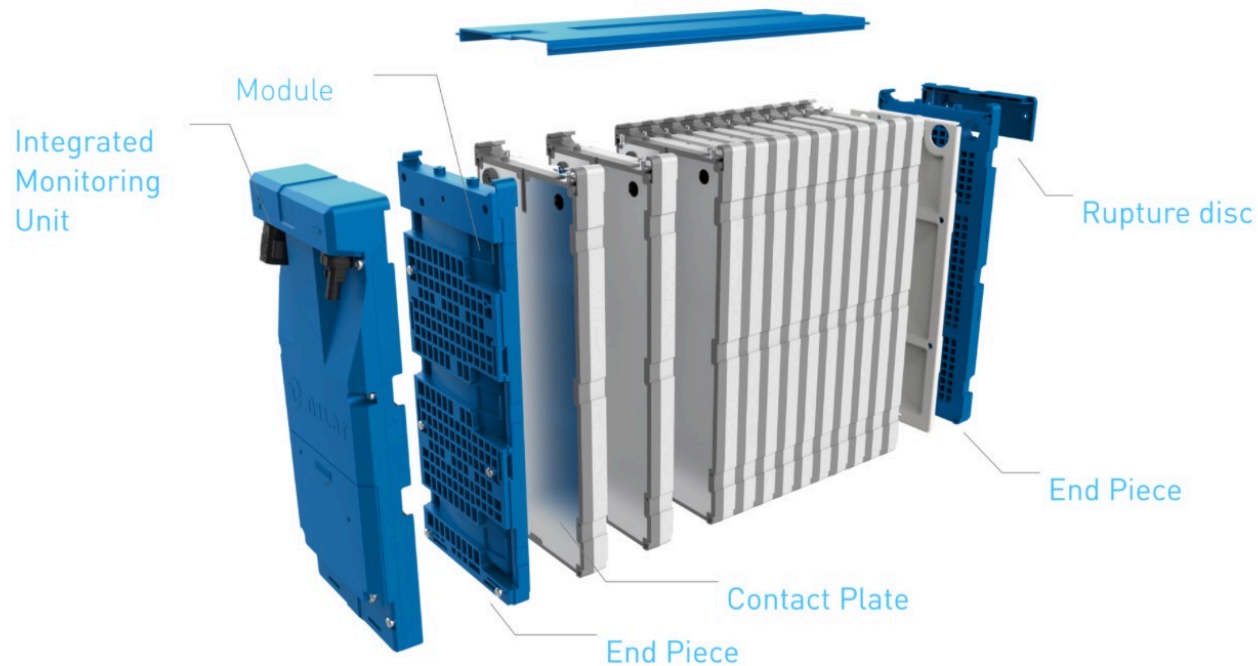
Make scanned images searchable

**384 000 GPU core hours
(Development Access, VEGA)**



Riksarkivet





Batteries for Stationary Energy Storage

Optical inspection by using AI-based machine vision

- Speed up model training time
- Larger image datasets

**384 000 GPU core hours
(Development Access, VEGA)**



Collaborations with more than 24 companies and institutions

Thank you!



EuroCC National Competence Centre Sweden



The Swedish EuroCC Hub for High-Performance Computing

We help you access and use CPUs/GPUs on European Supercomputers for Free

WHO WE ARE

