

The Swedish EuroCC Hub for High-Performance Computing

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

WHO WE ARE

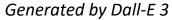




ENCCS empowers Swedish **industry, academia and the public sector** to leverage **HPC, AI, HPDA and QC** efficiently and effectively.











- Meetings on a weekly basis with new potential EuroHPC users
- What is available? Which system is best for me and my group? How do we apply? What are the requirements? How can we get started? Is it really free?
- One-stop shop if ENCCS can't help you, we hopefully know someone who can





- Meetings on a weekly basis with new potential EuroHPC users
- What is available? Which system is best for me and my group? How do we apply? What are the requirements? How can we get started? Is it really free?
- One-stop shop if ENCCS can't help you, we hopefully know someone who can



### ADAPTING AI-TECHNOLOGY For use in Archives

- Image segmentation models
- Text-recognition

Make scanned images searchable





- P	
13%. Juliji a aubra fidan harnda orderer fan a Saturne Janua understadu and in Madeira	Sin 1 11 1787 hafeable dannender attring dore IIII . 1.
Jaterne Jahres under Statione In Sendinen or anterne as the Materia Hafre attaljo Scool Hinderlar atta kierne Jos Seagan Kierfaur Halme fan opertierae. Strop 1828	har and a fing the solution of the Ston who har as honged the and the out
B. P. P. B.	The second
Brutentang ILB Lecenstral	fur for hall in a france of Million a fair the firm the the firm the test of test of the test of t
Street Stroet Stranger Stallacht	And the start of the line of the line for 25 This Section Salar 22 - 4.
Lippe un	The Jabriel Magner a the Sullimalt for 259.
Miller Miller	The t
the second	Horny Line Sector or Mallon, i advicting which we at the section of the section o
	Tunumin _ Cons that is
the state of the second of the second of the	Sura laigh Scatja bre Junor Scator happor Hater Mohay - Winder Las Scator hiombor Ho, or first and blim rating a Strong tholm Ven & Tebruarie UBS
MARTIN STATISTICS	Buitentary
A	



## BATTERIES FOR Stationary Energy Storage

Optical inspection by using Al-based machine vision

- Speed up model training time
- Larger image datasets

- Beginner/intermediate/advanced level
- HPC, AI, HPDA, Quantum Computing
- Domain specific training
  - CFD
  - Quantum Chemistry
  - Biomolecular Simulations
- Workshops, Hackathons, Bootcamps, Seasonal schools
- Collaborations: Centres of Excellence, HPC centres, NCCs
- Public and open source training material, workshop recordings on YouTube

## HPC ACCESS | SUPPORT | TRAINING



Generated by Dall-E 3

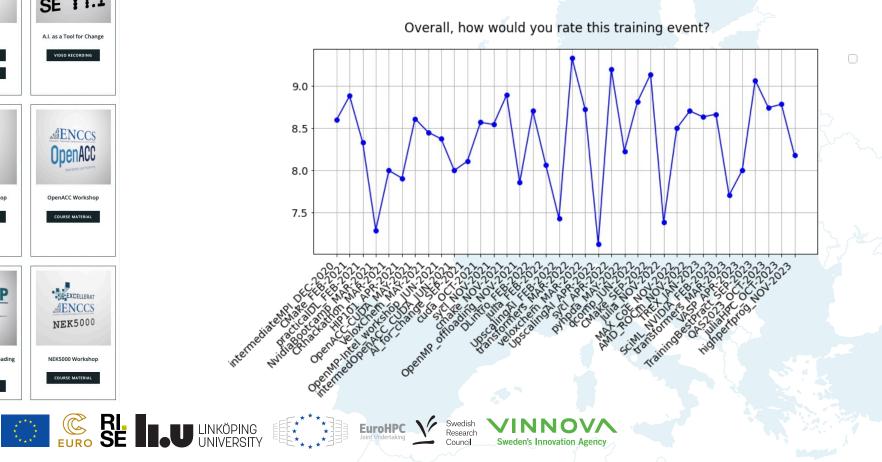
EuroHPC



#### **ENCCS** High-performance **ENCCS julia** with Python RE A.I SYCL ENCCS High-performance Julia for High Performance SYCL Workshop A.I. as a Tool for Change Data Analytics with Pytho Scientific Computing COURSE MATERIAL VIDEO RECORDING COURSE MATERIAL OURSE MATERIA VIDEO RECORDING VIDEO RECORDING *AENCCS* RI. ADVANCED: A.I. Workflows OpenACC LEARNING OpenVF0AM8 **AENCCS** Graph Neural Networks and Upscaling A.I. with **OpenFoam Workshop** OpenACC Workshop Transformer Workshop Containers COURSE MATERIAL COURSE MATERIAL COURSE MATERIAL COURSE MATERIAL VIDEO RECORDING EXCELLERAT OpenMP *AENCCS AENCCS* AENCCS MPI ENCCS CUDA NEK5000 Intermediate CUDA termediate MPI Worksh OpenMP for GPU Offload NEK5000 Workshop Workshop Workshop OURSE MATERIAL OURSE MATERIAL COURSE MATERIAL COURSE MATERIAL

## HPC ACCESS | SUPPORT | TRAINING

• Over 1500 people trained, ~10% from industry



## HPC ACCESS | SUPPORT | TRAINING

GPU programming: why, when and how? Search docs

☆ / GPU Programming: When, Why and How?

C Edit on GitHub

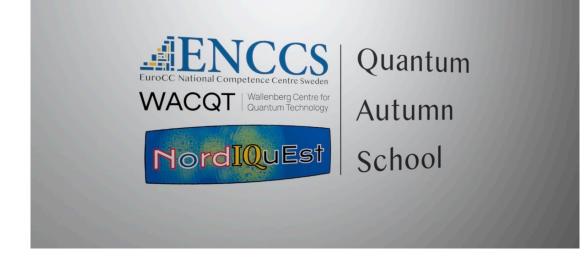
#### **GPU Programming: When, Why and How?**

Graphical processing units (GPUs) are the workhorse of many high performance computing (HPC) systems around the world. The number of GPU-enabled supercomputers on the Top500 has been steadily increasing in recent years and this development is expected to continue. In the near future, the majority of HPC computing power available to researchers and engineers is likely to be

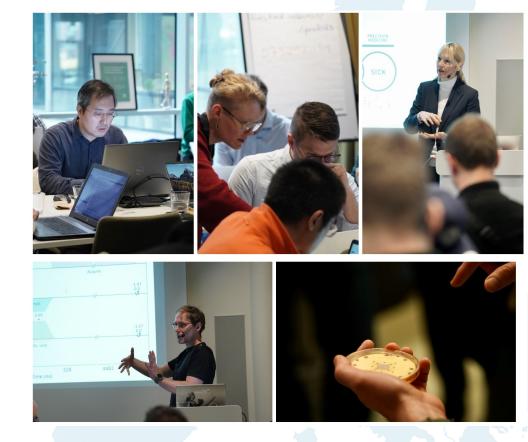
provided by GPUs or other types of accelerators. P crucial to developers of software run on HPC syste

- Collaborative effort with partners from Norway, Denmark, Finland and Lithuania
- Front page on Hacker News
- Best practice guide to be published
- To be developed into MOOC





- Hybrid event with 40 participants inperson and 40 online
- Speakers and instructors from academia and industry

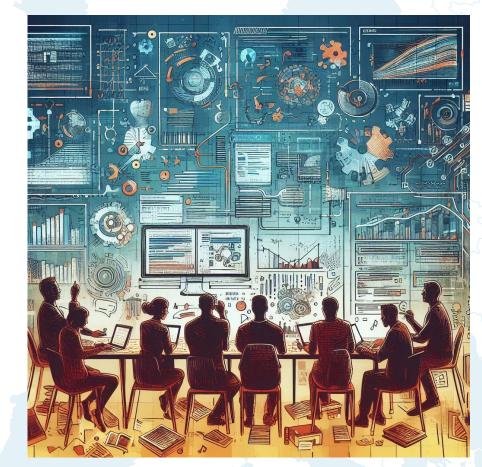






### HPC ACCESS | SUPPORT | TRAINING

- In phase 1 we contributed to academic software – GROMACS, VeloxChem, ICON, NEK5000 etc.
- In phase 2 we are transitioning to Proof of Concept projects
  - 3-6 month projects
  - 1-2 ENCCS experts
  - Matching contribution from client
  - Free of charge
  - Technology transfer



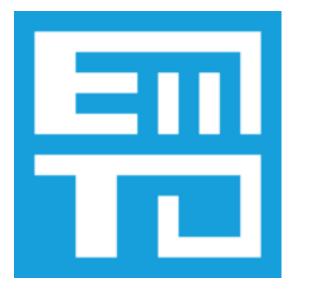
Generated by Dall-E 3

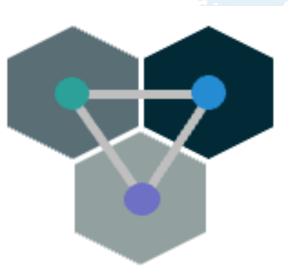






### HPC ACCESS | SUPPORT | TRAINING



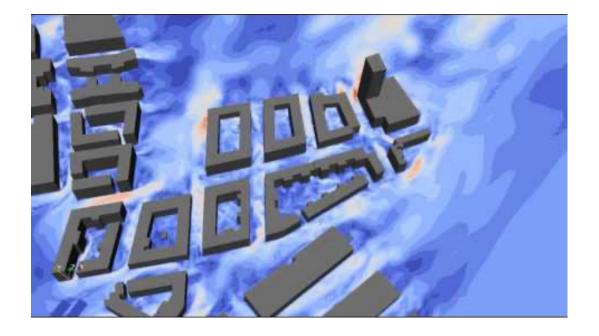


**EMTO-CPA** is an all-electron density functional theory code based on the Exact Muffin-Tin Orbitals formalism

**Colonies** is an open-source framework designed to facilitate seamless execution of computational workloads across cloud, edge, devices, or High-Performance Computing (HPC).







## SLB-ANALYS ANALYSE AIR Pollution flow USING Meluxina Supercomputer

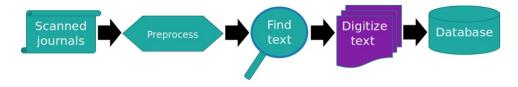
Simulate wind fields for wind comfort simulations and dispersion of air pollutants in complex urban environments

- Simulating larger urban area becomes possible
- Time-to-solution is greatly reduced
- Better results used for air quality assessment





## DIGITIZATION OF TABULAR DATA



Ar dagen den L	i Jan unti manad 1927.	Las dagen den	, Tanuari mind 1927.
Timme på Baron. Torra Våta term. <sup>N</sup> of n baron. term. <sup>V</sup> ata term. <sup>3</sup>	Viln der Sityrka Rässing Bisgraka retek. Sikk Sjön Maximi Minimi Nederbörd	Timme parts Barron. Toma trias MA 16 March 194	
2 fm.			
8. tm. + 11,0 747.9 - 15.6 7 10	N 599 K 0.6 5.	8.10. Ale 747.0 15.6 7.10	
2 em. +10,0 SUS -163 7 10 10	MAG 5 9 9	2 cm 160 10 5 163 7 10 10	
7 om. + 9. 4 753, 6 -15, 8 6 3 3	1 3 5 9 x - 0.9 S.	2 m + 9 x 7536 - 15 2 6 3 . 3	
3 em,	Peres I	<u></u>	
*) Pyrstationer kunna i deena keluran krikoa watteniemperetaron. Väder -	lekstelegram	S. Providence Ascess 2 dente automa informationen. Väder-	lekistelegram
Snötläcke kJ. 8 fm.	Bid gruppen &u gruppen Sie gruppen Gie gruppen Avaler kt	Sedtlete M. 8 fm.	
Bart eller snöt,	2 80	East eller solt.	
Tjockiek i cm. 8 fm. 51832 51166	0229× 7070× 96×9× 8,20	0 m 51532 51166	112.29× 70401 06×91 820
2 em. 54202 51166	0429× 7650× 2,16	Tjocklek i cm. 2 cm. 542.0.0. 51166	04291 75301 2.15
7 em. 5743230166	03192 63632 01295 9,21	2 m 579 32 30166	03192 5363 8 01295 221
Nederbördens beskaffenhet och tiden för densamma:	Tiden 15r dimma: Statesting and Statesting	Nøderbördens beskallinshet och liden för densammas	Tiden für dimma:
	Övriga anm. (åska, norrsken, frost m. m.)	and the second second second second second	Orriga ann. (Eska, narraken, troat m. m.)
1		17	

- Meteorological agencies possess troves of archival observational data
- SMHI will train machine learning model to read different forms of tabular data
- Result will enable better understanding of climate – especially occurrence of extreme weather events



## **SUCCESS STORIES**



EuroCC National Competence Centre Sweden



## THANK YOU!



EURO EURO EUROHPE SE LIGUE Swedish Research Council Sweden's Innovation Agency

🖂 in 🔽

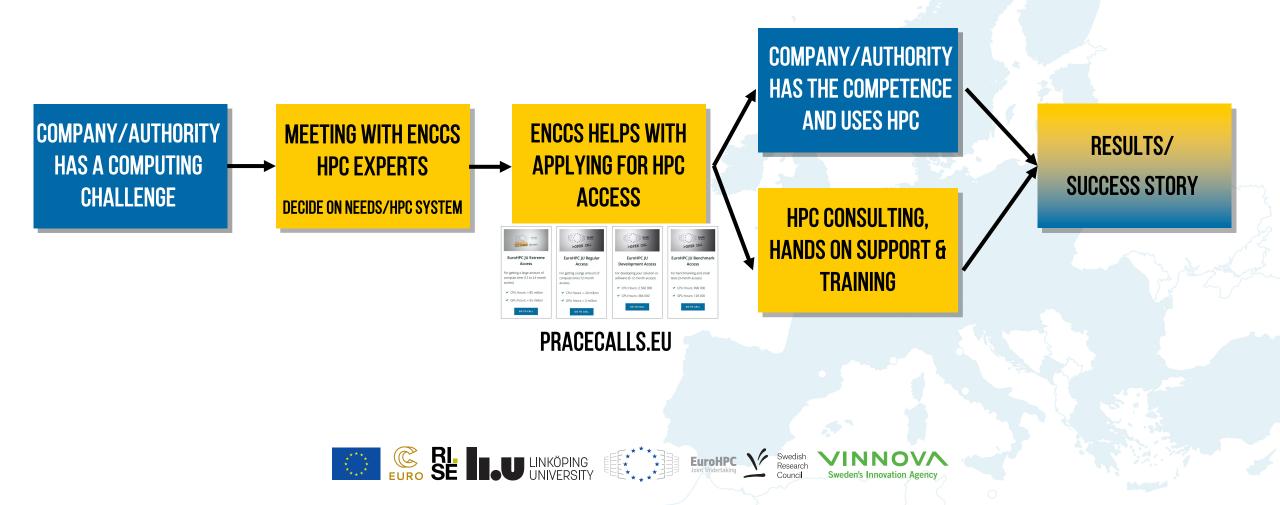
The Swedish EuroCC Hub for High-Performance Computing

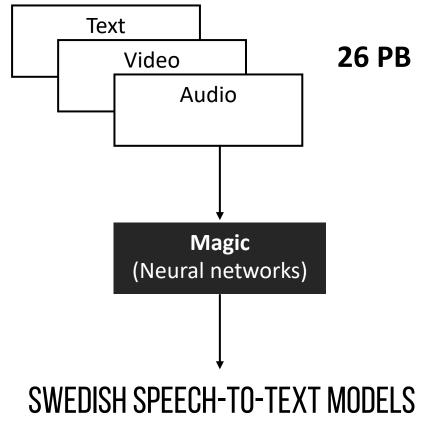
#### We help you access and use CPUs/GPUs on European Supercomputers for Free

WHO WE ARE





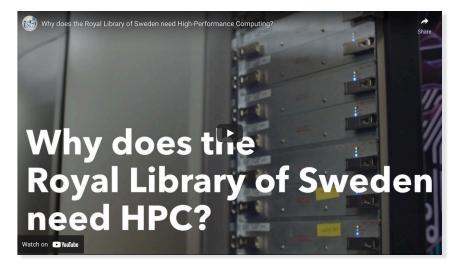




(Based on Google-BERT)



National Library of 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

# northvolt

