

NAISS

National Academic Infrastructure
for Supercomputing in Sweden

A photograph of a server rack with green lights and cables. The image shows a close-up of the server units, with numerous green indicator lights glowing. Several thick, black cables are plugged into the front of the server units, and some are bundled together. The overall scene is dimly lit, with the primary light source being the green LEDs of the server hardware.

Annual report
2023

Executive summary

NAISS, the National Academic Infrastructure for Supercomputing in Sweden, commenced operations on 1 January 2023.

NAISS serves as the national infrastructure organisation entrusted with providing Sweden's researchers with the high-performance computing (HPC) resources, storage capacity, user support, AI and machine learning, and big data services necessary to maintain our country's position at the forefront of academic research. In 2023, NAISS received SEK 115 million in funding from the Swedish Research Council and SEK 35 million from our Swedish partner universities. Linköping University is the host of NAISS.

NAISS is by far the highest in demand and most widely used of all scientific research infrastructures in Sweden. During its inaugural year, NAISS successfully assumed the responsibilities and took over the resources from the previous organisation SNIC. NAISS has provided services to more than 7,000 individual researchers and allocated resources to more than 1,600 different scientific research projects. These projects are led by PIs from more than 30 Swedish universities and research institutes, collaborating with researchers from over 300 universities worldwide.

Research spans 32 different scientific fields, ranging from major users in physics, mechanics, chemistry, life sciences, and climate research, to emerging HPC areas such as history, political science, psychology, and economics. In 2023, researchers' computations and data analyses resulted in more than 1,300 scientific publications.

This extensive utilisation of NAISS resources underscores its pivotal role in supporting and driving innovative research initiatives across Sweden, as well as facilitating the efficient interpretation of results from our major experimental research facilities, such as MAX IV.

The user statistics presented on the following pages demonstrate the massive quantitative importance of NAISS for Swedish research, and the two research highlights show how NAISS enables scientific excellence, not least among young researchers.

One of NAISS's achievements during the year was the seamless transition of operational responsibility for all existing academic HPC systems from the former organisation, SNIC, without any disruptions for researchers. NAISS has thus facilitated access to more than 30 Pflops of computing power for research, along with large-scale storage solutions and data analysis services.

A key component of NAISS's success has been its efficient user support, now ensured through a collaborative agreement with 11 partner universities nationwide. This decentralised model maximises the value of NAISS resources by ensuring that researchers across Sweden are assisted by the best experts, regardless of their respective physical location. This is made possible even as NAISS trends towards centralising computer systems for economy-of-scale reasons.

Furthermore, on behalf of the government and the Swedish Research Council, NAISS has successfully secured significant investment in a European supercomputer in Sweden for the first time ever, through a granted application to EuroHPC JU (Joint Undertaking). The planned EUR 68 million investment in the Arrhenius supercomputer, with its approximately 40 Pflops, will provide a substantial increase of resources for Swedish computer-based research from 2025 onwards, enabling Sweden to truly step onto the international stage in HPC infrastructure.

In summary, the results from NAISS's first year of operation demonstrate its crucial role in enabling groundbreaking research and innovation in Sweden. With continued support and strategic partnerships, we look forward to further strengthening Sweden's position as a leading nation in advanced data-driven research across all scientific fields.

Linköping in March 2024

Björn Alling
Acting Director, NAISS





Alvis (CTH)

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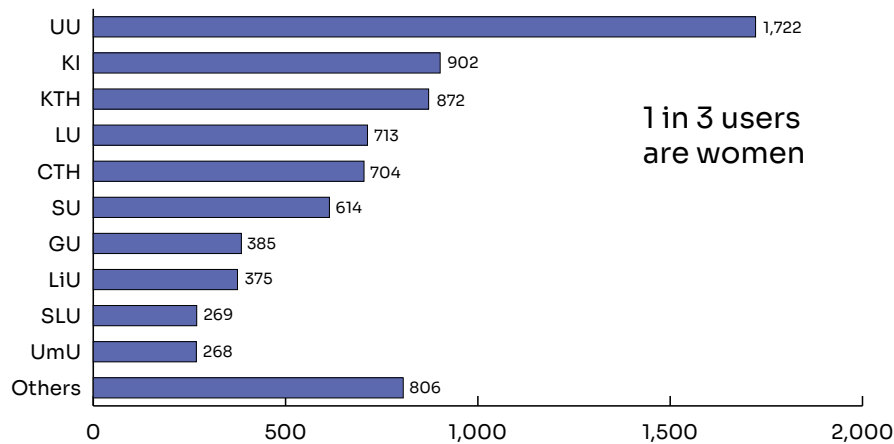
Layout: Jonathan Pakvis

Cover photo: Tetralith, LIU

Photographers: Charlotte Perhammar (Björn Alling), Thor Balkhed (Tetralith), Henrik Sandsjö/Chalmers University of Technology (Alvis), Olov Planthaber (Florian Trybel)

Statistical highlights

7,630 unique users



32 research areas

Top 7 research areas

- 1 Physics + Materials
- 2 Mechanics, CFD*
- 3 Chemistry
- 4 Biology
- 5 Climate etc
- 6 Medicine
- 7 Computer Science

*Computational Fluid Dynamics

Other areas include

- History
- Political Sciences
- Economy
- Agriculture
- Psychology

~ 30 Pflops available computational resources

including LUMI-SWE

>1,300 publications

(Scopus funding search NAISS OR SNIC)

1,924 projects

55 Large	
University/Institute	Projects
UU	12
SU	10
LiU	10
KTH	8
CTH	5
LU	5
SMHI	2
GU	1
LTU	1
Nordita	1

433 Medium	
University/Institute	Projects
UU	92
KTH	73
CTH	47
LU	33
KI	32
LiU	31
SU	29
SLU	21
GU	20
UmU	15
Others	40

1,096 Small	
University/Institute	Projects
UU	285
KTH	144
KI	130
SU	99
CTH	85
LU	78
GU	69
SLU	61
LiU	50
UmU	39
Others	56

340 Sensitive	
University/Institute	Projects
KI	132
UU	124
GU	18
LU	17
UmU	16
Others	33

Compute allocations on top three NAISS resources

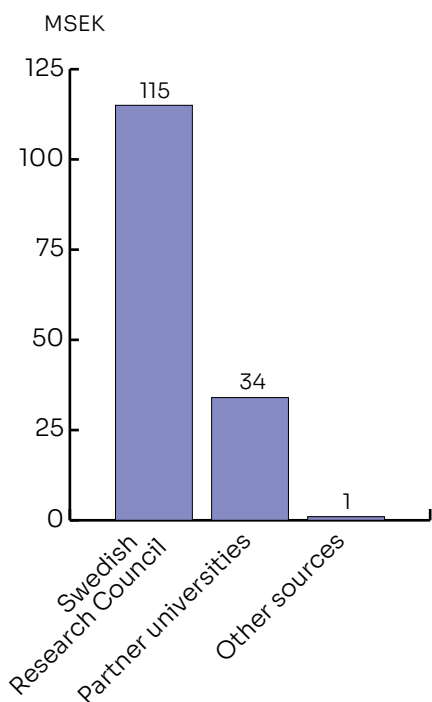
Dardel CPU	
University/Institute	xM core hours
KTH	268
UU	146
LiU	114
SU	84
LU	56
CTH	43
Nordita	28
LTU	14
GU	9
Others	36

Tetralith CPU	
University/Institute	xM core hours
KTH	111
LiU	96
UU	90
SU	60
CTH	50
LU	36
SMHI	31
GU	15
LTU	10
Others	22

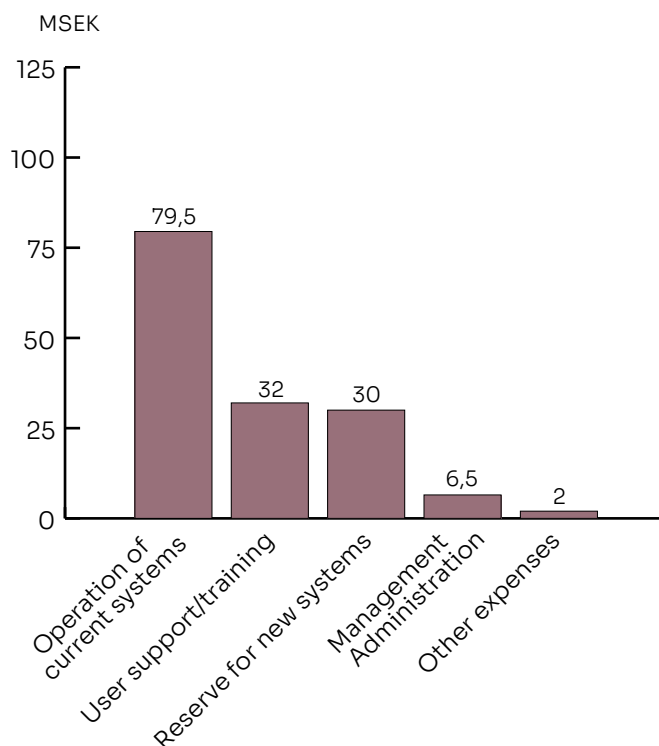
Dardel GPU	
University/Institute	x1000 GPU hours
KTH	636
UU	540
SU	188
LiU	96
LU	60
LTU	48
Others	12

Financial summary

Revenues (150 MSEK)



Expenditures (150 MSEK)



Description of NAISS operations

Arrhenius

NAISS, together with LiU, applied to EuroHPC JU (Joint Undertaking) for a mid-range system in Sweden, Arrhenius. Support for this application came from the Swedish Research Council and the Swedish government. EuroHPC JU approved the application in June 2023. The Swedish co-financing for Arrhenius was secured during the autumn of 2023 through guarantees from the Swedish Research Council and with government support. Negotiations with EuroHPC regarding hosting agreements and other contracts are ongoing and expected to be finalised in April 2024. Gert Svensson has been appointed project manager for the Arrhenius project. Work on preparing procurement and other related matters is underway.

Establishment of a Steering Committee and management team

NAISS was established administratively as a centre at LiU through a decision by LiU's Vice-Chancellor on 13 February 2023. An interim Steering Committee, which had been working since the summer of 2022, was formally constituted simultaneously, consisting of Jan-Eric Sundgren (chair from the turn of the year), Matts

Karlsson, Lars Börjesson, Anders Ynnerman, Charlotte Platzer-Björkman, and Patrik Norman (replacing Mikael Östling). The process of appointing a regular Steering Committee with broad expertise and ties to the research community continued, and the Steering Committee was appointed by LiU's Vice-Chancellor starting from 1 April 2023.

This Steering Committee consists of

Chair

- Jan-Eric Sundgren, Senior Advisor, Association of Swedish Engineering Industries

Members

- Erik Lindahl, Deputy Chair, Professor Biophysics, Royal Institute of Technology
- Marianne Sommarin, Professor Emerita Plant Biochemistry, Umeå University
- Anders Ynnerman, Professor Scientific Visualisation, Linköping University
- Susanne Aalto, Professor Radio Astronomy, Chalmers University of Technology
- Bengt Persson, Professor Bioinformatics, Uppsala University
- Thorsten Mauritsen, Associate Professor Meteorology, Stockholm University



The regular Steering Committee held 10 meetings in 2023.

Björn Alling, Associate Professor in Theoretical Physics at LiU, was appointed Acting Director of NAISS by LiU's Vice-Chancellor on 13 February 2023. The Acting Director has appointed leading management roles to Anna Jänis, Head of Administration, LiU, Niclas Andersson, Technical Director, LiU, Gert Svensson, Deputy Technical Director, KTH, Torben Rasmussen, User Support Manager, LiU, Henric Zazzi, Deputy User Support Manager, KTH, and Joachim Hein, Training Manager, LU.

Building trust with universities and other organisations

NAISS operates under maximum transparency and aims for a close dialogue with all parties: users, the Research Council, managements of partner universities, staff and associated staff, and other interested partners. This is critical to build trust in our new organisation. NAISS's chairperson has engaged in dialogue with university vice-chancellors and their deputies to understand their expectations of NAISS and vice versa. The Acting Director of NAISS has attended several URFI (the University Reference Group for Research Infrastructure) meetings, and, through them, negotiated Collaboration Agreements for user support (see below).

NAISS User Forum was held in Linköping on 5-6 December, where all users/researchers were in-

cluded. Some 40 people attended in person and approximately 50 virtually. An All-Hands staff meeting was held simultaneously with approximately 80 participants.

Newsletters from NAISS's chairperson to university managements have been sent four times. Newsletters from the Acting Director of NAISS to staff within NAISS's operational area have been sent eight times. Newsletters from NAISS to all users have been sent during the autumn. NAISS has a clear national perspective and a steering committee with broad representation across scientific disciplines and home universities. In order to build national trust and support, it continues to be important for NAISS to demonstrate independence in decision-making from the old HPC centres, including LiU's centre NSC.

A seamless transition from SNIC to NAISS

From a user perspective, the transition from SNIC to NAISS has worked as intended. NAISS has assumed responsibility for funding all SNIC systems that were to continue operating, supported by partners at various university HPC centres. Thanks to our partner universities, user support has also worked interimsitically in the same manner as previous years, while the new branch structure for user support has been developed and negotiated.

New systems

The focus of the planning for new systems has been the Arrhenius system, in partnership with EuroHPC JU (see below). NAISS decided to grant the sensitive data resource Bianca in Uppsala an extended operational time until 31 December 2026 to ensure that the sensitive data part of Arrhenius can come into operation and replace Bianca without any interruption for users. Rackham users have started migrating to Dardel. Tetralith is to be replaced by Arrhenius.

Five-year technical-scientific roadmap and strategic plan

NAISS initiated work on these plans at the end of 2023. NAISS's medium and long-term strategy will be discussed and anchored nationally during the spring of 2024, and a plan will be adopted before the summer of 2024.

Hardware consolidation

The process towards consolidation of hardware has been initiated. Lennart Johnsson, Profes-



Dardel (KTH)



Tetralith (LiU)

son in Computer Sciences, Mathematics, and Electrical & Computer Engineering, University of Houston, has led a working group consisting of academic HPC experts from around Sweden. They have compiled the basis and requirements profile for the future NAISS data centre. However, Arrhenius needed to be handled separately due to time and experience criteria set by the EuroHPC JU.

All universities were asked if they had a suitable data centre for Arrhenius that met these requirements, e.g. on the availability of electricity and cooling. Only LiU responded positively. The data centre investigation will resume in 2024 with the aim of having full freedom to find the best data centre for NAISS resources beyond Arrhenius.

Resource allocations and the National Allocation Committee (NAC)

The NAC has continued the good and appreciated work that its predecessor SNAC carried

out during the SNIC era. Based on peer reviews and scientific and technical assessments, the Allocation Committee has allocated resources to researchers who have registered applications. Allocations have been in the form of large, medium, and small projects for computation and storage, reflecting the sizes of the research groups, the type of computations they perform, the assessed needs, and a compromise with other applicants, as resources are usually over-applied.

Allocations have been awarded on the NAISS resources Dardel, Tetralith, Bianca, Alvis, Rackham, Science Cloud, Swestore, and other storage facilities. Additionally, the Swedish part of LUMI in Finland has been allocated in a similar manner through NAC. Large compute projects are typically in the order of a few million core-h/month on the largest computational resources. Medium compute projects are in the order of 500,000 core-h/month, while small projects are up to 10,000 core-h/month on the same resources.

The chairperson of NAC has been Professor Paul Erhart, Materials Science, CTU. Peter Munger from LiU has been the Secretary of NAC and convener of the technical experts working group NAC-WG that is supporting NAC.

Sensitive data services

Arrhenius will offer services for sensitive data, which will mean a significant expansion of available resources for researchers in fields such as bioinformatics, medicine, and social sciences.

In 2023, NAISS decided to extend the operation of Bianca, the NAISS-SENS resource for sensitive data, until 31 December 2026 as a bridging solution to avoid interruptions in available resources ahead of the commissioning of Arrhenius' part for sensitive data, which is planned for the first part of 2025. This decision was made in consultation with Uppsala University, which will also make its own parallel investment.

User support

NAISS is establishing a distributed user support organisation via NAISS branches in partnership with Sweden's universities. Collaboration agreements have been signed between NAISS and the following 11 institutions regarding support and funding for this initiative: LiU, KTH, SU, KI, CTH, UmU, SLU, GU, UU, LU, and LTU.

Bilateral branch agreements are under negotiation between NAISS and KTH, UmU, UU, CTH, and LU. KI and SU will not become branches, but are supporting the organisation on a level equal to that of branch universities. KI and SU have also signed special user support agreements with NAISS.

NAISS's user support will be structured as a unified organisation with a national responsibility and equal service to all researchers in Sweden. However, through the distributed function, the best experts to support users can be recruited or retained regardless of whether they currently work in locations such as Linkoping, Stockholm, Umea, Uppsala, Lund, or Gothenburg.

A unified system for handling user inquiries, tickets, and other needs is under development. The goal is for all users to receive assistance from the best experts, regardless of which university they belong to.

NAISS's responsibility is to provide user support at the basic and intermediate levels, while the most advanced user support will

be financed and managed by the universities according to their assessments and needs. However, NAISS will coordinate this work. To achieve this, the plan is to organise NAISS staff partially according to research areas, enabling a comprehensive overview of the entire country's research and advanced user support in each specific area.

The importance of the user perspective, and user support in particular, is being safeguarded by the standing User Support Advisory Committee (USAC) that has just been elected, based on nominations from the NAISS User Forum held in December 2023. The chair of USAC is Marie Skepo, Professor in Chemistry, Lund University.

User training and education

NAISS training activities for users were initiated in early 2023 under the leadership of Joachim Hein, Lund University. Courses have been organised regularly, ranging from basic HPC routines and best practices for the most used software packages to more advanced on-demand courses. Training events are highlighted in regular training newsletters to all users.

Communication work

Updates on the build-up of NAISS and current activities have been sent out regularly via email by Jan-Eric Sundgren (to university managements) and Bjorn Alling (to staff within the HPC field and NAISS users). NAISS launched its website in mid-2023. It was updated with full functionality in early 2024. The work of adding more information and documentation of services is ongoing.

In January 2024 NAISS hired a communications officer to develop its communication. He will be responsible for supporting the management's communication with users, the general public and other groups, as well as website functionality and content. He will also create a long-term communication plan.

International work

In addition to the work with EuroHPC JU regarding Arrhenius, NAISS has played a leading role in the Nordic e-Infrastructure Collaboration, NeIC. NAISS is also active in other collaborations within our field in the Nordic region, for example with Sigma2 in Norway and CSC in Finland, where CSC is responsible for the operation of Europe's largest computer, LUMI.

Research highlights



Tuuli Lappalainen

Professor, KTH

Director of the Genomics Platform and the National Genomics Infrastructure of SciLifeLab

Senior Associate Faculty Member at the New York Genome Center

Publication

T Lappalainen et al. "Genetic and molecular architecture of complex traits."

<https://pubmed.ncbi.nlm.nih.gov/38428388/>

Prior to relocating to Sweden in May 2021, Tuuli Lappalainen was an Associate Professor with tenure at the Department of Systems Biology at Columbia University, where she now holds an adjunct position.

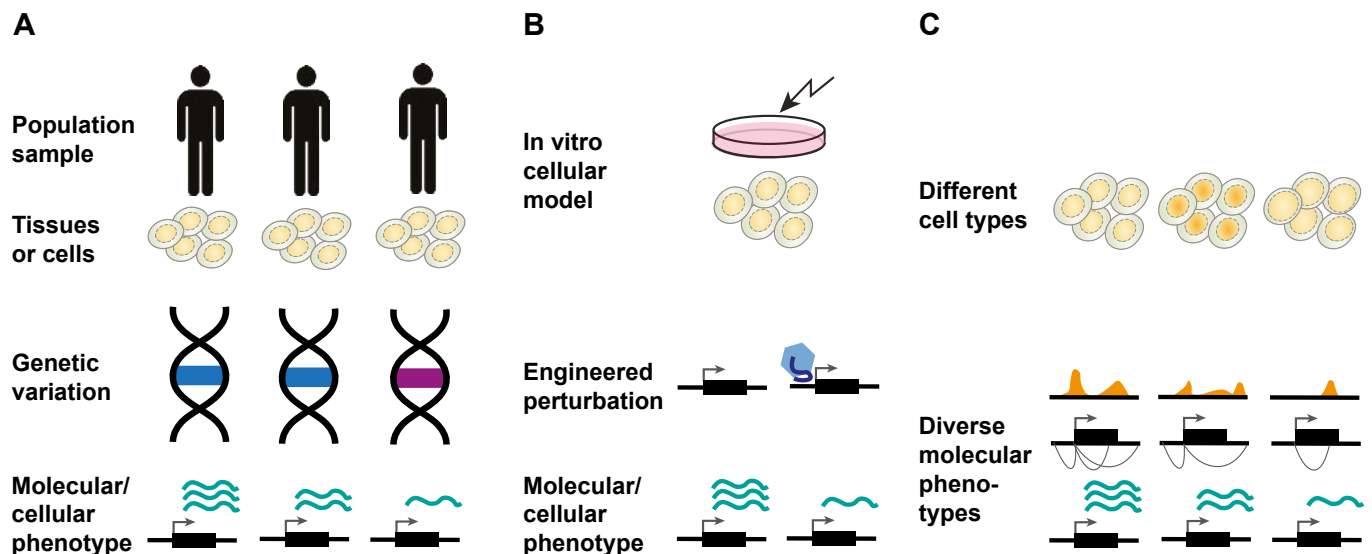
She is one of the international leaders in human genetics and functional genomics, and she has participated in and co-led several major consortium projects in this field.

She has received multiple recognitions and awards for her work, including the international Leena Peltonen Prize in Human Genetics in 2018 and the Göran Gustafsson Prize in Molecular Biology in 2022. She received the ERC Consolidator grant in 2022 and has received millions of dollars of grant funding from the US National Institutes of Health.

Tuuli Lappalainen's research programme seeks to understand molecular mechanisms of genetic risk for human diseases. The lab does not study any particular disease but rather the core processes that are shared across different traits and diseases.

Her research group's main approach is computational integration of large-scale human genome data with gene expression data and other molecular data from large human cohorts.

The powerful computational infrastructure provided by NAISS (and previously SNIC) is an essential resource for this work. In particular, the infrastructure must be designed for protected human genetic data, and compliant with international standards and regulations. The Bianca infrastructure provided by NAISS is thus essential for the research in the Lappalainen lab.



Different approaches for interrogating functional effects of genetic variants (Tuuli Lappalainen)



Florian Trybel

Assistant Professor in Theoretical Physics, LiU

Publications

Laniel, Trybel et al. "Synthesis of Ultra-Incompressible and Recoverable Carbon Nitrides Featuring CN_4 Tetrahedra." *Advanced Materials* (2023): 2308030.

<https://dx.doi.org/10.1002/adma.202308030>

Laniel, Trybel et al. "Structure determination of ζ -N₂ from single-crystal X-ray diffraction and theoretical suggestion for the formation of amorphous nitrogen." *Nature Communications* 14.1 (2023): 6207

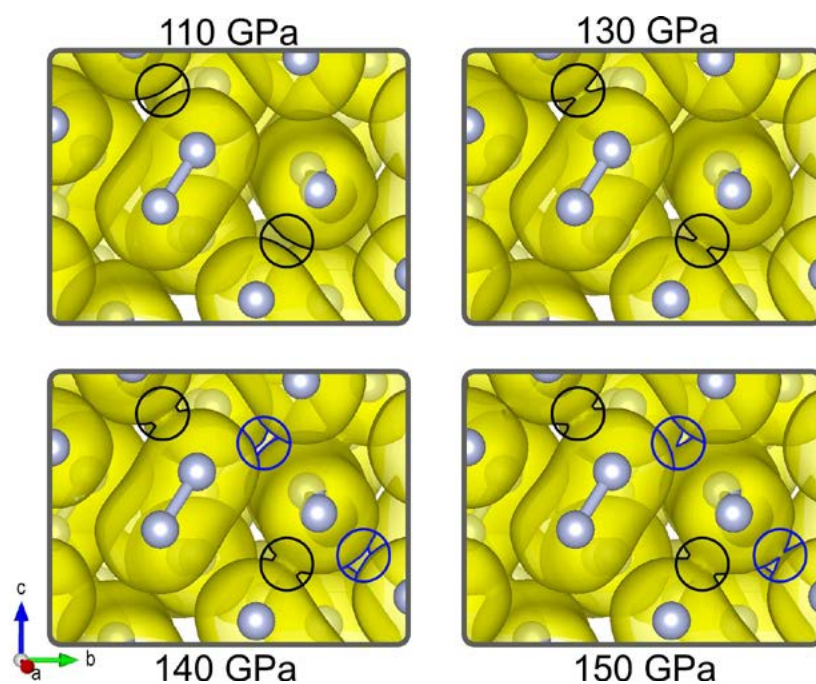
<https://www.nature.com/articles/s41467-023-41968-2>

Florian Trybel's research aims at understanding the stability and properties of new hydrogen and nitrogen-bearing materials featuring promising functionalities that can so far only be synthesised at extreme pressure and temperature conditions of millions of times the atmospheric pressure and thousands of Kelvin. He uses density functional theory and, increasingly often, machine learning-accelerated computations.

"I am working in close multi-disciplinary collaborations with experimental scientists, which in my opinion are indispensable in state-of-the-art high-pressure research. This surprisingly rare synergy enabled us recently to find promising new materials and resolve mysteries in high-pressure chemistry."

Within this collaborative research network they achieved the long sought-after recovery of polymeric C-N materials from high-pressure synthesis and theoretically described many of their properties. They were furthermore able to refine the previously unknown crystal structure of the high-pressure ζ polymorph of nitrogen, where DFT calculations revealed an interconnected network of charge density progressively forming under further compression. For this research, NAISS resources were essential.

"In the coming years, I will be able to extend this research to more complex materials, thanks to the support from the European Research Council (ERC). I am looking forward to the new NAISS system Arrhenius and further exploring the GPU capabilities of Dardel and the Swedish share of LUMI with the help of NAISS user support."



Charge density channels progressively forming under strong compression in ζ -N₂ (Florian Trybel)

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