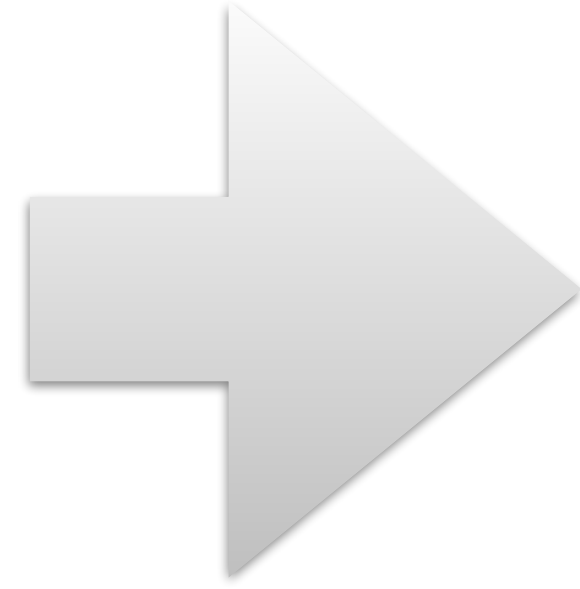


NSC introduction to Tetralith/Sigma

National Supercomputer Centre (NSC), Linköping University

NAISS training, online @NSC 15th Apr 2025, 10:00 - 12:00

Information / Schedule



https://www.nsc.liu.se/support/Events/NSC_intro_Apr2025/

- this presentation as .pdf
- everything underlined is a link

10:00 Introduction to Tetralith/Sigma (Weine Olovsson)

~10:45 Using Python (Hamish Struthers)

~11:00 Using VSCode and Jupyter Notebook (Xuan Gu)

~11:15 Using GPUs (Torben Rasmussen)

~11:30 Open session, questions?

National Supercomputer Centre (NSC)

NSC is part of:

- **NAISS** National Academic Infrastructure for Supercomputing in Sweden (branch)
- **li.u** LINKÖPING UNIVERSITY liu.se

1983 - SAAB buys Cray1



SAAB



1989 - NSC first supercomputer centre in Sweden / SAAB partner

1996 - SMHI partner



2016 - MET Norway partner



Meteorologisk
institutt



NAISS

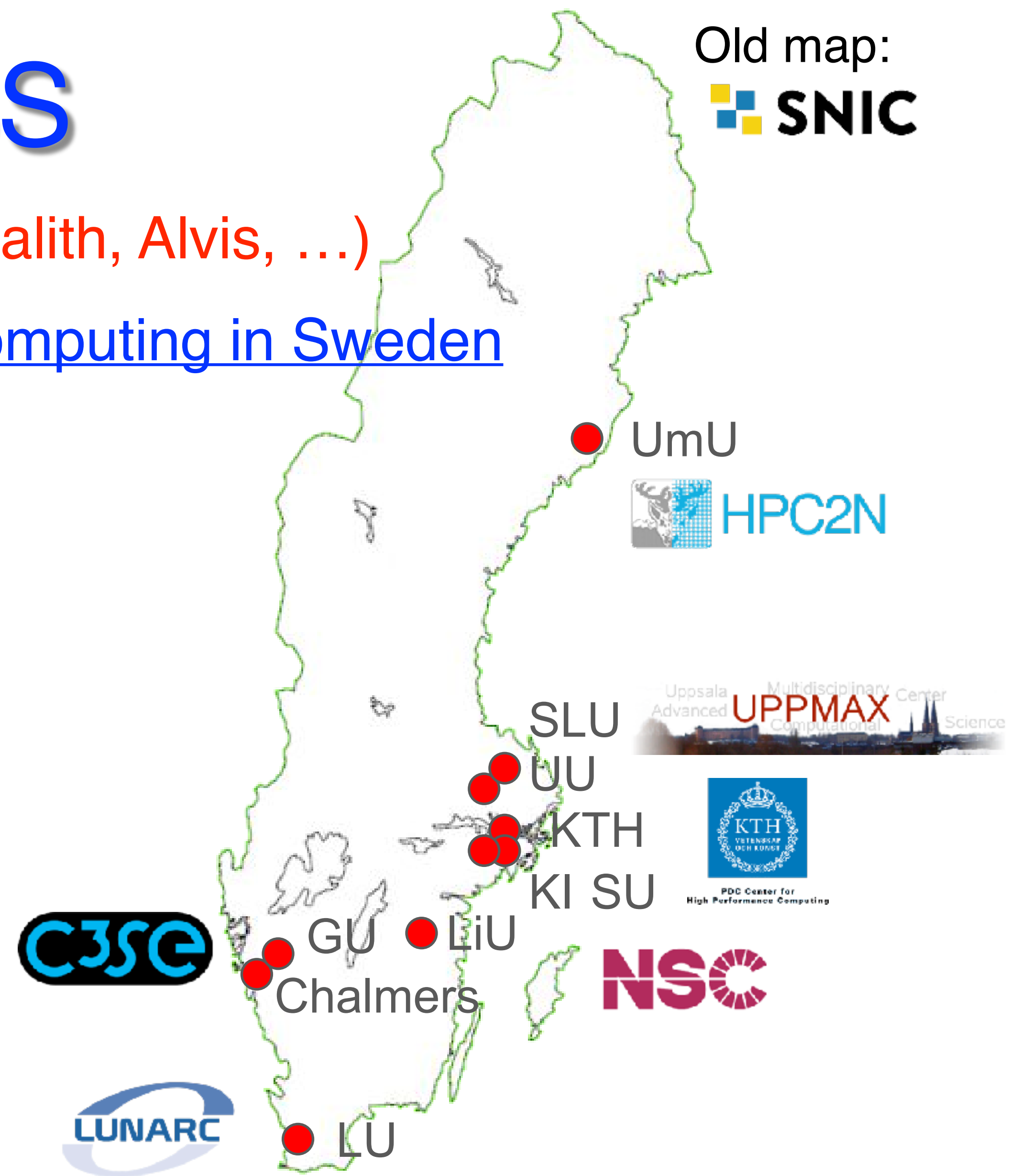
Old map:
 **SNIC**

- Continues work of SNIC 2023 - (Dardel, Tetralith, Alvis, ...)

National Academic Infrastructure for Supercomputing in Sweden

Branches at universities:

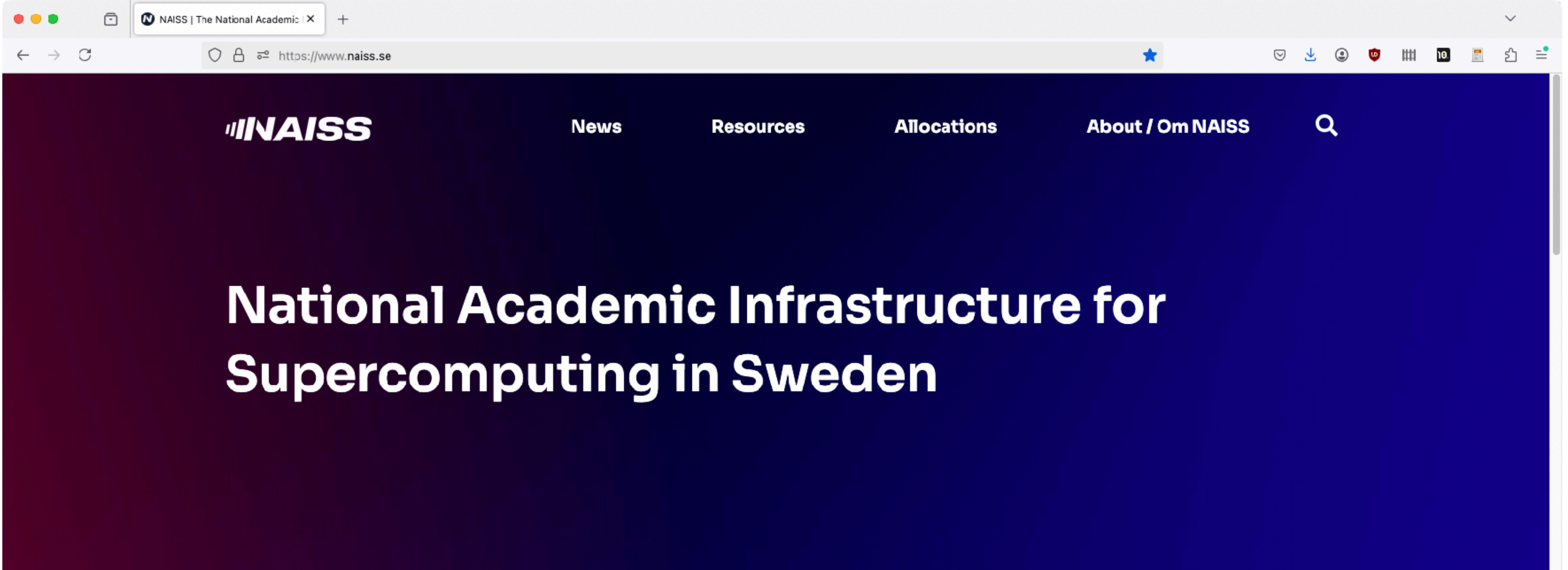
Chalmers	<u>C3SE</u>
Göteborg	
Karolinska	
KTH	<u>PDC</u>
Linköping	<u>NSC</u>
Lund	<u>LUNARC</u>
Stockholm	
Umeå	<u>HPC2N</u>
Uppsala	<u>UPPMAX</u>
+ more: SLU, LTU, LNU	



<https://www.naiss.se/>

 **More info!**

Funding: branches + Vetenskapsrådet (VR)

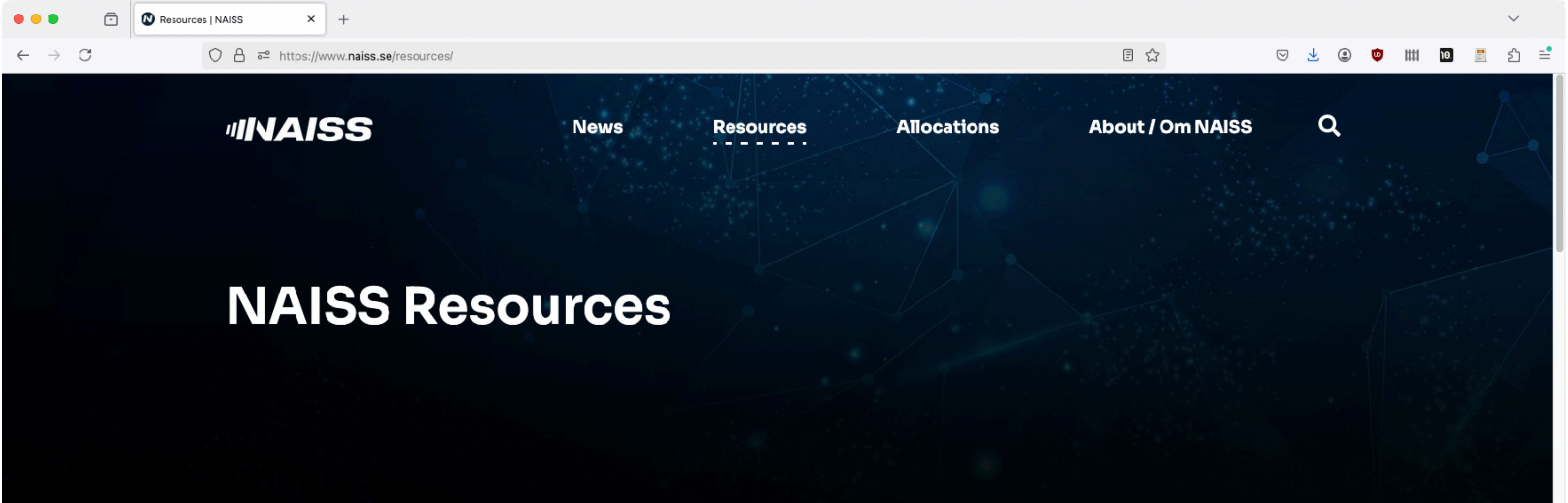


<https://www.naiss.se/>  More info!

NAISS and RISE to set up Swedish AI Factory

EuroHPC JU (Joint Undertaking) has approved a joint application from NAISS and RISE to set up an AI Factory in Sweden. The Factory, which will be called Mimer, combines a new AI-optimised supercomputer with comprehensive support for training, research





- OVERVIEW
- ALVIS
- BIANCA
- DARDEL
- LUMI SWEDEN
- SWEDISH SCIENCE CLOUD (SSC)
- SWESTORE/DCACHE
- TETRALITH

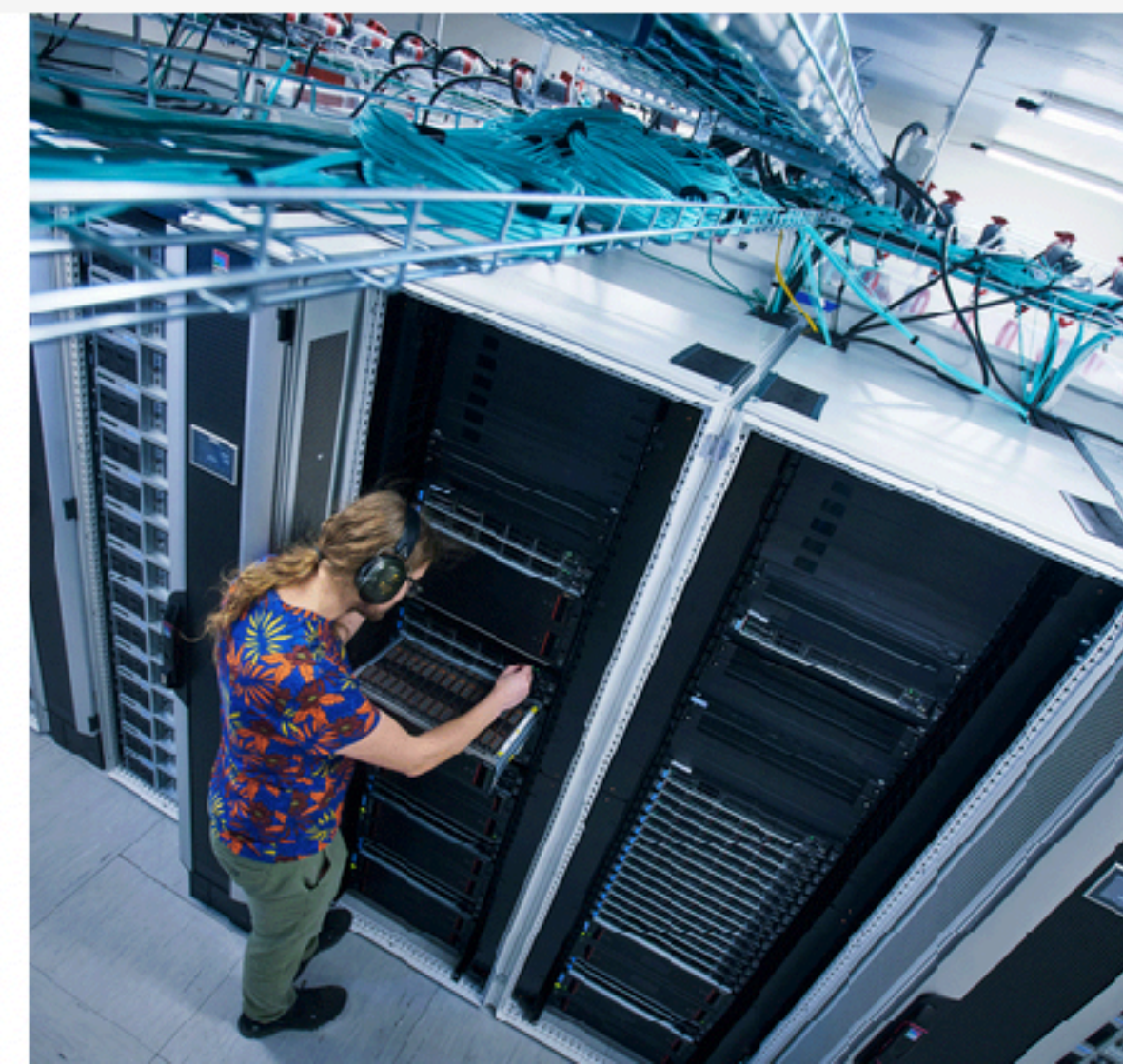
COMPUTE RESOURCE

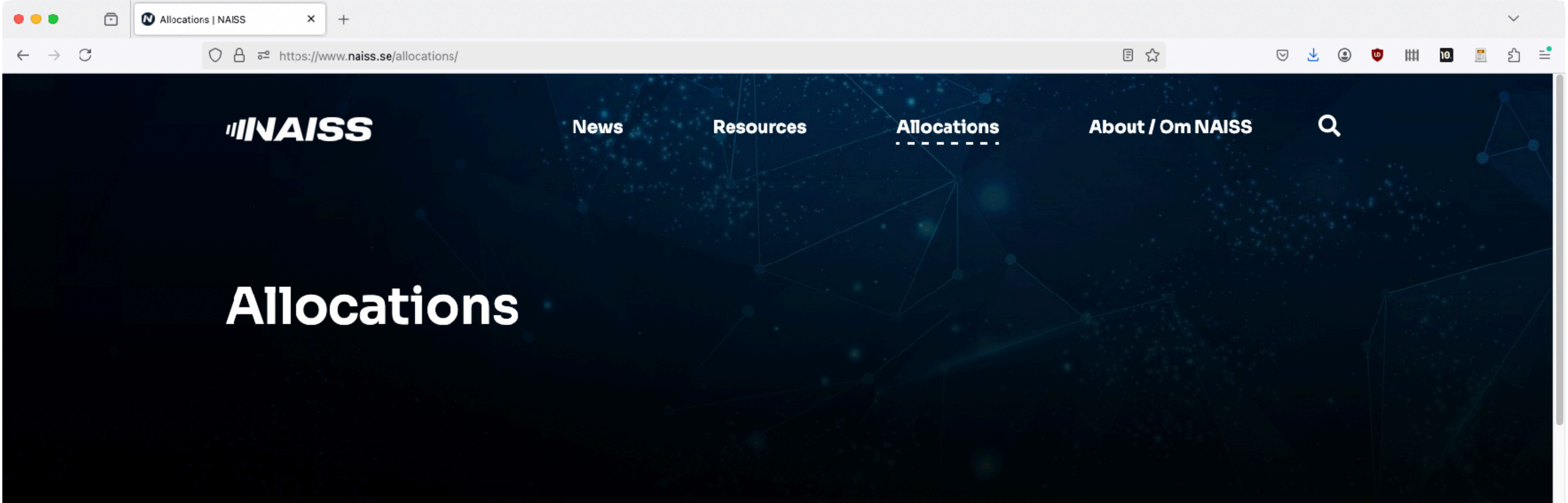
Alvis

Host Data Centre

C3SE, Chalmers University of Technology

Purpose





Allocations

NAISS LARGE COMPUTE SPRING
2025 CALL

NAISS LARGE STORAGE SPRING
2025 CALL

LARGE CALLS 2024



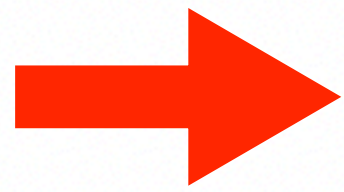
NAISS coordinates and provides large-scale computing and storage capacity to researchers at Swedish universities and other research institutes authorised by the [Swedish Research Council](#) >. Resources are made available through rounds with open application procedures to ensure that the best Swedish research is supported.

Proposals are prepared and submitted via the [Swedish User and Project Repository \(SUPR\)](#) > platform.

Open rounds

NAISS resources are made available through a number of rounds with open application procedures. Computational and storage resources can be applied for as Small, Medium and Large projects.

- STAFF
- STEERING COMMITTEE
- STEERING DOCUMENTS
- ANNUAL REPORTS
- NEWSLETTER
- NEWS
- EVENTS
- TRAINING
- CONTACT



About us

(För information om NAISS på svenska [se denna sida >.](#))

The National Academic Infrastructure for Supercomputing in Sweden (NAISS) maintains advanced computing, artificial intelligence, and data services that support research ranging from fundamental research in mathematics or physics to climate modelling, the green transition, life science and economics. NAISS is hosted by [Linköping University >](#), with funding provided by the [Swedish Research Council \(Vetenskapsrådet\) >](#) for the years 2023–2026 under contract 2022-06725.

NAISS is the largest and most widely used research infrastructure in Sweden, involving more than 7,600 users at some 30 universities and research institutes (statistics from 2023). We also maintain special dedicated resources for infrastructures, agencies, and external users.

We aim to evolve with our users and their needs. NAISS should be your partner from the first time you open an account on a cluster and need Linux training to the point where you manage a team running a state-of-the-art simulation or AI training on 10,000 GPUs.

A diverse portfolio of computing infrastructure

The main resources provided by NAISS and collaborating organisations include

- High-performance computing clusters/supercomputers consisting of nodes with high-end CPUs or GPUs and large amounts of memory, where thousands of such nodes are connected by very fast networks.

Training

NAISS offers a wide range of courses, workshops and seminars that are free to all users. Training is provided by staff from the NAISS branches distributed across Sweden.

This list is updated weekly.

For more information and registration, please click the titles below to go to the hosting branch event pages.

Date	Event	Where
15 April	NSC introduction to Tetralith/Sigma	Online
24-25 April, 28-29 April	Using Python in an HPC environment	Online
5-9 May	Programming Formalisms	Online
8 May	NAISS Zoom-in - a virtual open-house	Online
16 May	Transferring Files to/from HPC Clusters	Online
21 May	Introduction seminar for Alvis users	Online
	- Improve Your Handling of	Online
27 May	Cluster architecture and job submission	Online
2-3 June	Intermediate Bash and Linux	Online
10-11 June	Introduction to Pandas for data science	Online
12 June	NAISS Zoom-in - a virtual open-house	Online

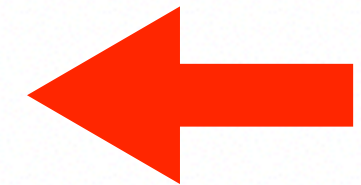
- NAISS training info, also see training newsletter!

<https://www.naiss.se/training>

- STAFF
- STEERING COMMITTEE
- STEERING DOCUMENTS
- ANNUAL REPORTS
- NEWSLETTER
- NEWS
- EVENTS
- TRAINING
- CONTACT

Access and support

All NAISS resource allocations are based on proposals. Getting started with a small allocation only requires a brief description of your needs in the [SUPR user portal >](#), and we will typically get back to you within days. Medium and large-scale proposals undergo more extensive review, as described under [Allocations >](#), where you can also find information about the National Allocation Committee (NAC). Computing and storage resources are typically scarce, and the prioritisation is based on scientific excellence and the expected impact.



Thanks to additional funding by our partner universities, NAISS is providing nationwide support through local staff at branches across Sweden, ensuring access to a range of different competences. Open house events will be organised at all these sites. In cases where the competence you need is not available locally, NAISS support staff will connect you with suitable experts at other sites. In some cases, local NAISS staff is physically co-located at a local computing center.

Governance

Major decisions in NAISS are taken by the Steering Committee, which is appointed by Linköping University Vice-Chancellor Jan-Ingvar Jönsson. Professor Jan-Eric Sundgren. The main executive officer of NAISS is the Director, Erik Lindahl, joined by Anna Jänis as head of administration and a management team including associate directors as described on the [Staff >](#) page.



- For access and support:

<https://supr.naiss.se/>

New NAISS cluster: Arrhenius

- Carl Axel Arrhenius (1757-1824), ytterbium discovery
- **EuroHPC “mid-range”**, ca. 6-700 MSEK
- Installation & start **HT 2025** (CPU first, GPU later)
- “Tetralith replacement”
- Users: academic (EuroHPC/NAISS), industry

NSC: Quick Overview

Part of LiU and NAISS (Director: Erik Lindahl)

~ **40** people (not all full-time)

Mostly **system experts** and **application experts**

- Provide computational resources
- Software installation (global / local)
- Troubleshooting / advice
- Training (NAISS, local and other)

NSC Academic Clusters

32 cores/node

Tetralith (2018 -) 1908 x 2 x 16 cores, Intel Xeon Gold 6130

NAISS

(2020 -) 170 x T4 GPU-nodes

Top500 no. 359 (74)

Sigma (2018 -) 110 x 2 x 16 cores, Intel Xeon Gold 6130 “same” as Tetralith

(2020 -) 2 x V100 GPU-nodes



BerzeLiUs (2021 -) Nvidia DGX SuperPOD, (60 + 34) x 8 A100 **GPUs**



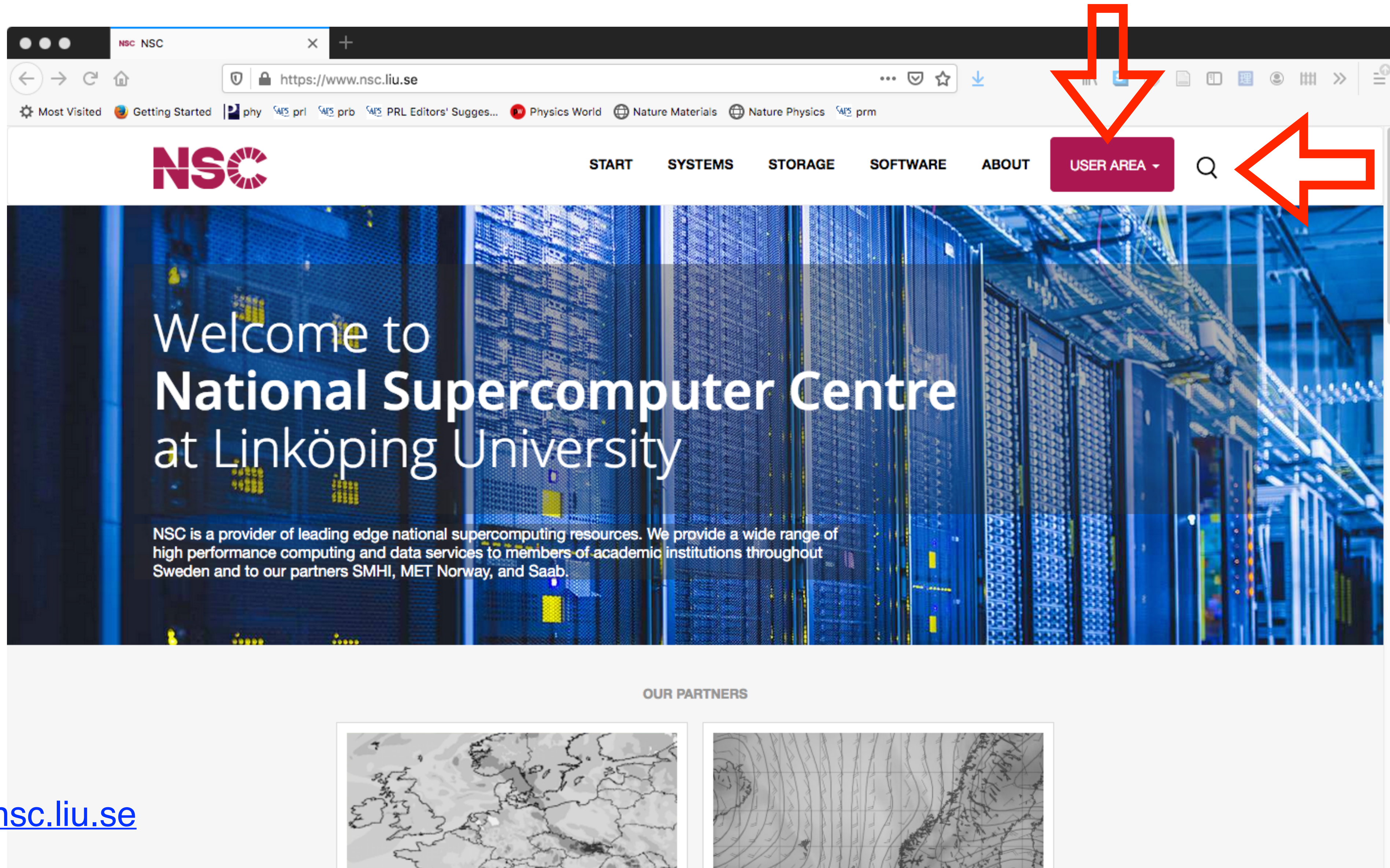
*Knut and Alice
Wallenberg
Foundation*

AI/ML, for all researchers in Sweden



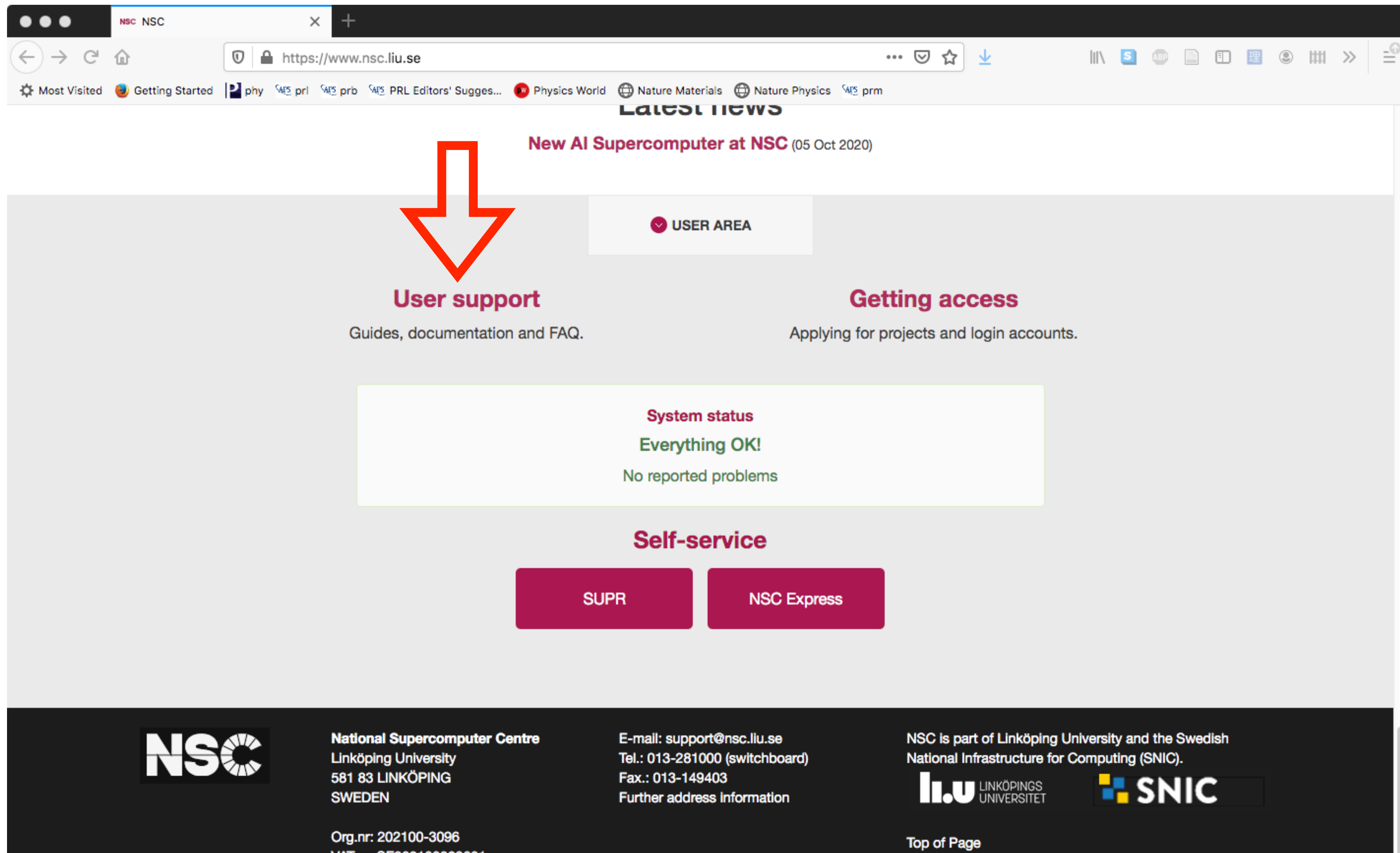
**Top500 no. 204
& 237 (83)**

Where to find Information?



<https://www.nsc.liu.se>

Where to find Information?



The screenshot shows a web browser window with the URL <https://www.nsc.liu.se>. The page features a navigation bar with links to 'Most Visited', 'Getting Started', and various research groups. A large red arrow points to the 'User support' section, which includes links to 'Guides, documentation and FAQ.' and 'Getting access' (Applying for projects and login accounts.). Below this is a 'System status' box indicating 'Everything OK!' and 'No reported problems'. At the bottom, there is a 'Self-service' section with buttons for 'SUPR' and 'NSC Express'. The footer contains contact information for the National Supercomputer Centre, including email, phone, fax, and address, as well as logos for Linköping University and SNIC.

NSC NSC

[←](#) [→](#) [↻](#) [🏠](#) [🔒](#) [https://www.nsc.liu.se](#) [⋮](#) [🛡️](#) [★](#) [↓](#) [📖](#) [📄](#) [📅](#) [🔍](#) [👤](#) [⌵](#) [⌵](#) [⌵](#)

[⚙️ Most Visited](#) [🌐 Getting Started](#) [📄 phy](#) [📄 SPS prl](#) [📄 SPS prb](#) [📄 SPS PRL Editors' Sugges...](#) [📄 Physics World](#) [📄 Nature Materials](#) [📄 Nature Physics](#) [📄 SPS prm](#)

Latest news

New AI Supercomputer at NSC (05 Oct 2020)

USER AREA

User support
Guides, documentation and FAQ.

Getting access
Applying for projects and login accounts.

System status
Everything OK!
No reported problems

Self-service

SUPR **NSC Express**

NSC

National Supercomputer Centre
Linköping University
581 83 LINKÖPING
SWEDEN

E-mail: support@nsc.liu.se
Tel.: 013-281000 (switchboard)
Fax.: 013-149403
Further address information

NSC is part of Linköping University and the Swedish National Infrastructure for Computing (SNIC).

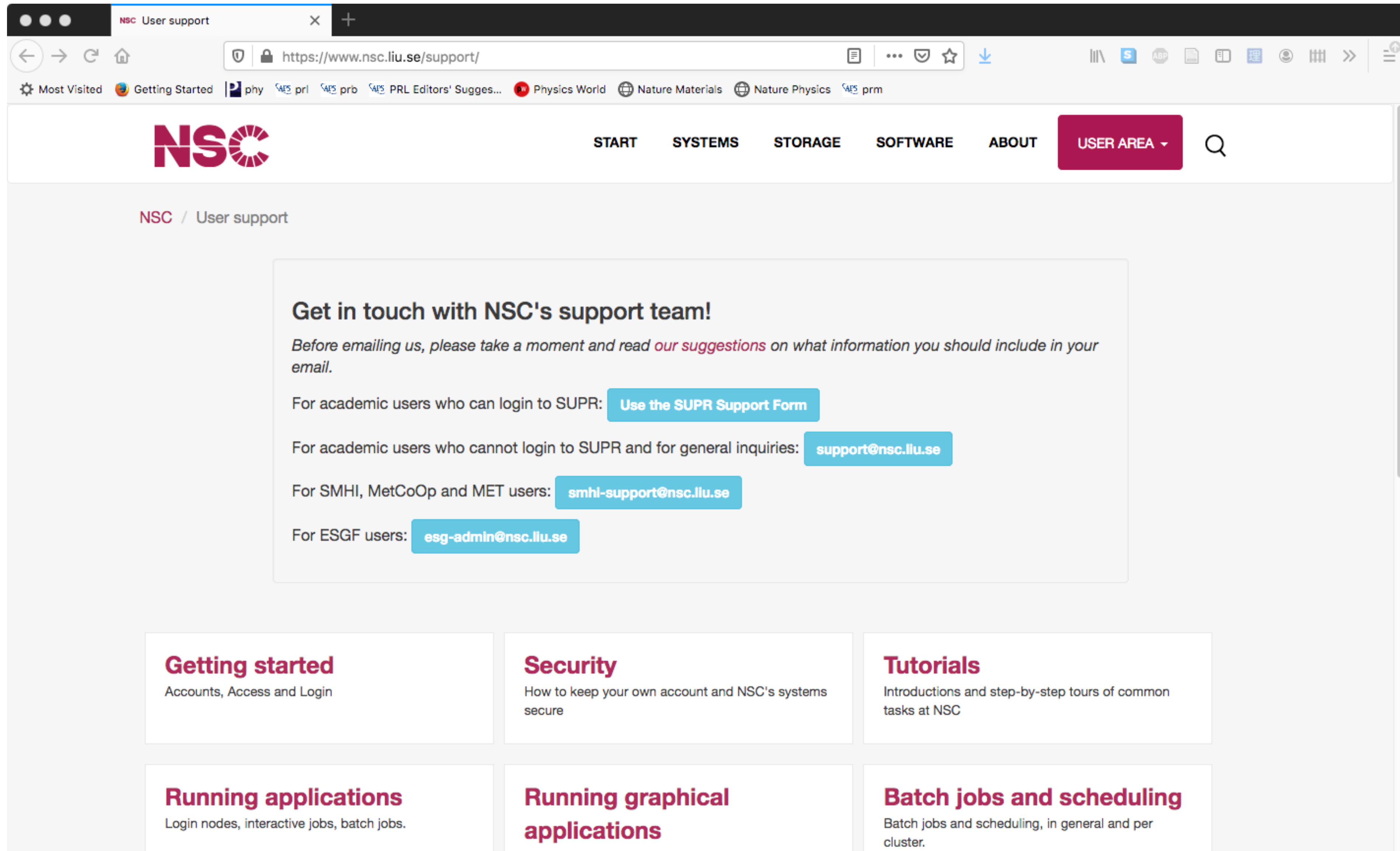
li.u LINKÖPING
UNIVERSITET

SNIC

Org.nr: 202100-3096
VAT: SE5823100000001

Top of Page

Where to find Information?



The screenshot shows a web browser window with the address bar displaying `https://www.nsc.liu.se/support/`. The browser's address bar includes navigation icons (back, forward, refresh, home) and a search icon. Below the address bar, there is a bookmark bar with several links: 'Most Visited', 'Getting Started', 'phy', 'SAPS prl', 'SAPS prb', 'SAPS PRL Editors' Sugges...', 'Physics World', 'Nature Materials', 'Nature Physics', and 'SAPS prm'. The main content area of the browser shows the NSC website. The header of the website features the NSC logo on the left and a navigation menu on the right with links: 'START', 'SYSTEMS', 'STORAGE', 'SOFTWARE', 'ABOUT', 'USER AREA' (with a dropdown arrow), and a search icon. Below the header, the breadcrumb 'NSC / User support' is visible. The main content area is titled 'Get in touch with NSC's support team!' and includes a paragraph: 'Before emailing us, please take a moment and read *our suggestions* on what information you should include in your email.' Below this, there are four rows of contact information, each with a text label and a blue button containing an email address: 'For academic users who can login to SUPR: Use the SUPR Support Form', 'For academic users who cannot login to SUPR and for general inquiries: support@nsc.liu.se', 'For SMHI, MetCoOp and MET users: smhi-support@nsc.liu.se', and 'For ESGF users: esg-admin@nsc.liu.se'. At the bottom of the page, there is a grid of six cards, each with a title and a brief description: 'Getting started' (Accounts, Access and Login), 'Security' (How to keep your own account and NSC's systems secure), 'Tutorials' (Introductions and step-by-step tours of common tasks at NSC), 'Running applications' (Login nodes, interactive jobs, batch jobs), 'Running graphical applications', and 'Batch jobs and scheduling' (Batch jobs and scheduling, in general and per cluster).

NSC User support

https://www.nsc.liu.se/support/

Most Visited Getting Started phy SAPS prl SAPS prb SAPS PRL Editors' Sugges... Physics World Nature Materials Nature Physics SAPS prm

NSC

START SYSTEMS STORAGE SOFTWARE ABOUT USER AREA

NSC / User support

Get in touch with NSC's support team!

Before emailing us, please take a moment and read *our suggestions* on what information you should include in your email.

For academic users who can login to SUPR: [Use the SUPR Support Form](#)

For academic users who cannot login to SUPR and for general inquiries: support@nsc.liu.se

For SMHI, MetCoOp and MET users: smhi-support@nsc.liu.se

For ESGF users: esg-admin@nsc.liu.se

Getting started

Accounts, Access and Login

Security

How to keep your own account and NSC's systems secure

Tutorials

Introductions and step-by-step tours of common tasks at NSC

Running applications

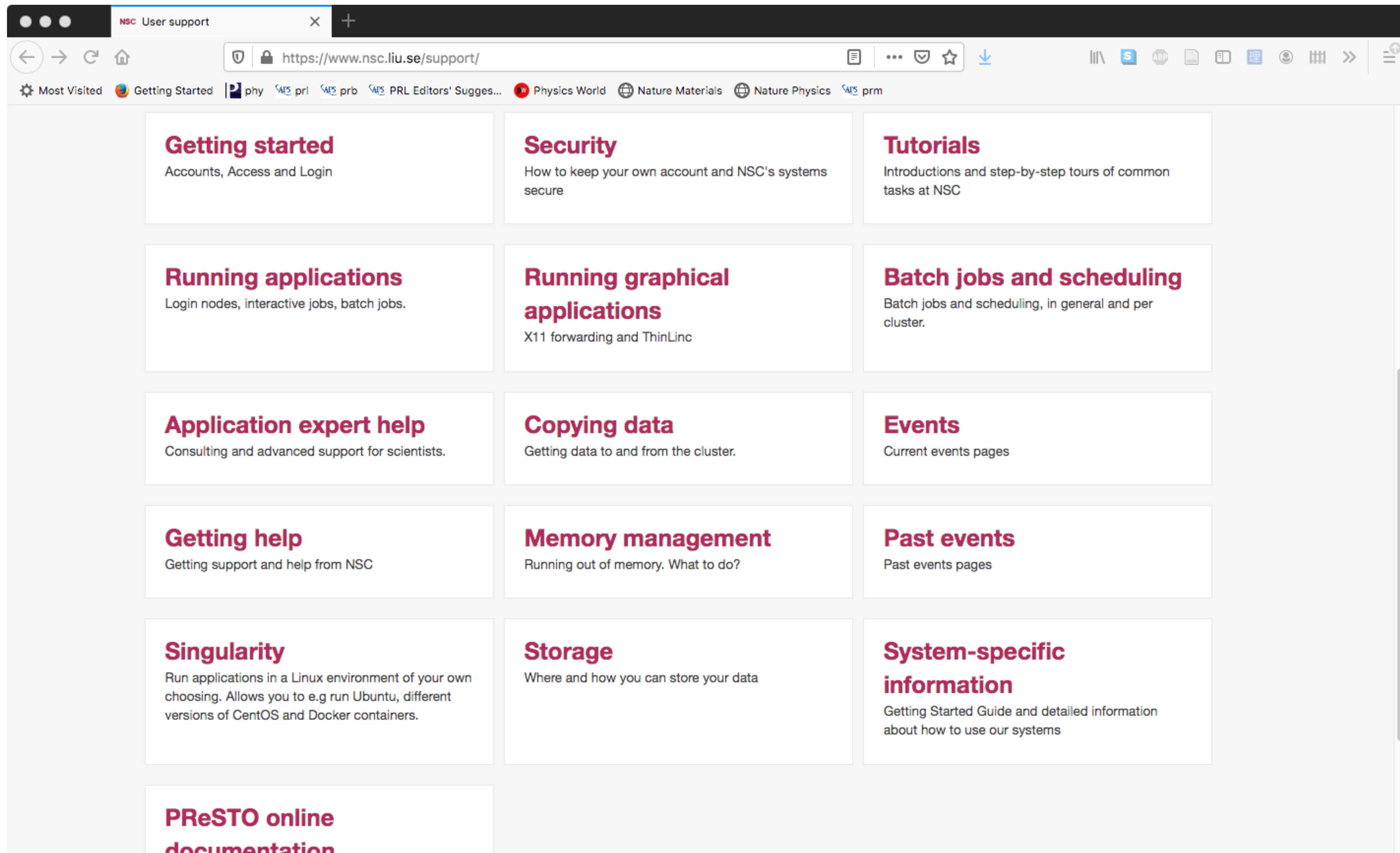
Login nodes, interactive jobs, batch jobs.

Running graphical applications

Batch jobs and scheduling

Batch jobs and scheduling, in general and per cluster.

Where to find Information?



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Getting started Accounts, Access and Login	Security How to keep your own account and NSC's systems secure	Tutorials Introductions and step-by-step tours of common tasks at NSC
Running applications Login nodes, interactive jobs, batch jobs.	Running graphical applications X11 forwarding and ThinLinc	Batch jobs and scheduling Batch jobs and scheduling, in general and per cluster.
Application expert help Consulting and advanced support for scientists.	Copying data Getting data to and from the cluster.	Events Current events pages
Getting help Getting support and help from NSC	Memory management Running out of memory. What to do?	Past events Past events pages
Singularity Run applications in a Linux environment of your own choosing. Allows you to e.g run Ubuntu, different versions of CentOS and Docker containers.	Storage Where and how you can store your data	System-specific information Getting Started Guide and detailed information about how to use our systems
PReSTO online documentation		

Getting Access to HPC - SUPR

NAISS SUPR

[Start](#)
[Support](#)
[Login](#)

Your are not logged in.

[Start](#)

SUPR - Swedish User and Project Repository

NAISS takes over from SNIC
From 1 January 2023, NAISS takes over the role previously held by SNIC. Read more at the [NAISS site](#).

SUPR is the NAISS database used to keep track of persons, projects, project proposals and more. To use most SUPR functions you need to be logged in.

[Login using SWAMID](#) [Login using Email and Password](#) [Login using Client Certificate](#)

If You Cannot Login

[Request Password for Existing Person](#) [Resend Confirmation Email](#) [Register New Person](#)

Proposals Rounds

You can [view information about proposal rounds](#) without logging in.

List of Current NAISS/SNIC Projects

You can view a [list of current NAISS/SNIC projects](#) without logging in.

Current NAISS User Agreement

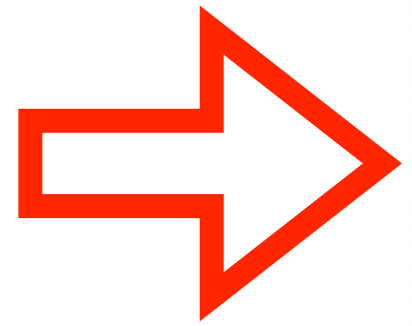
You can view the [current NAISS User Agreement](#) without logging in.

Information Regarding Personal Data Processing

You can view [information regarding personal data processing](#) at the NAISS website without logging in.

<https://supr.naiss.se/>

Getting Access to HPC - SUPR



NAISS SUPR
Start
Support
Login
You are not logged in.

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<https://supr.naiss.se/>

Support via SUPR

NAISS
SUPR

Admin

User

Start

Reviews

Declared Competence

Projects

NAISS 2023/6-41

(multicentre)

LiU-2019-26 (NSC)

SNIC 2022/1-6

(multicentre)

SNIC 2022/1-24

(multicentre)

SNIC 2022/6-189

(multicentre)

LiU-compute-2022-10

(NSC)

NAISS 2023/22-205 (NSC)

Accounts

Proposals

NAISS 2023/22-205 (NSC)

NAISS 2023/1-33

(multicentre)

Rounds

Groups

application-experts

nsc-staff

SNIC-application-mgmt

SNIC-training-coordination

Vasp-5.4.4 VA210132

Personal Information

Support

Logout

Logged in as:
Weine Olovsson
(weine.lovsson@liu.se)
Turn on warning colour.

Start

SUPR - Weine Olovsson

NAISS takes over from SNIC

From 1 January 2023, NAISS takes over the role previously held by SNIC. Read more at the [NAISS site](#).

Get a Two-Factor Authentication Recovery Code

You use two-factor authentication when logging in. If you get a two-factor recovery code, you will be able to use it in the future to reset your two-factor secret, for example if you lose access to the device where you installed the two-factor app.

Get Recovery Code

Not Now, Remind Me Later

NAISS Activity Report Wanted

The Swedish Research Council requires NAISS to provide reporting of results from all NAISS projects. As a consequence, NAISS requires you to provide activity reports within three months after the end of your NAISS projects and before submitting continuation proposals. You are the PI or proxy for the following recent project that does not yet have an activity report submitted:

Project	Project Title	Project Type	End Date
NAISS 2023/22-205	VASP workshop at NSC 4-5th Apr 2023	NAISS Small Compute	2023-05-01

Projects

You belong to the following active projects:

Project	PI	Project Title	Project Type	Centre	Start Date	End Date	Your Role
NAISS 2023/6-41	Rickard Armiento	Storage for theoretical physics environm...	NAISS Medium Storage	(multiple)	2023-03-07	2024-04-01	extended member
LiU-2019-26	Igor Abrikosov	Electronic structure theory for material...	Centre Local Compute	NSC	2019-06-25	2023-07-01	member

A large red arrow pointing to the right, highlighting the 'Support' link in the left sidebar of the SUPR interface.

Support via SUPR

Support

Support

https://supr.naiss.se/support/

110%

NAISS
SUPR

Admin User

Start

Reviews

Declared Competence

Projects

NAISS 2023/6-41

(multicentre)

LiU-2019-26 (NSC)

SNIC 2022/1-6

(multicentre)

SNIC 2022/1-24

(multicentre)

SNIC 2022/6-189

(multicentre)

LiU-compute-2022-10

(NSC)

NAISS 2023/22-205 (NSC)

Accounts

Proposals

NAISS 2023/22-205 (NSC)

NAISS 2023/1-33

(multicentre)

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nsc-staff

SNIC-application-mgmt

SNIC-training-coordination

Vasp-5.4.4 VA210132

Personal Information

Support

Logout

Logged in as:
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(weine.clovsson@liu.se)
Turn on warning colour.

Start / Support

Support

Use this form to request support for NAISS systems and services (including the SUPR portal itself). If you have multiple issues that are not related, please use the form multiple times, once for each issue.

Replies will be sent to your registered email address weine.clovsson@liu.se. If it is wrong, please [change it](#) (and confirm it using the email you get) before submitting a support request here.

Problem Type

Select the problem type that best describes what you want support for. If no other type is appropriate, select **Other issues**.

(select problem type)

Centre and Resource

If your problem is related to a specific resource at a centre, select that. If your problem is related to multiple resources at a centre (or no resource listed here at all), select the centre and mention the resources in the problem description below.

(select centre or resource)

Project

If your problem is related to a specific project, select that.

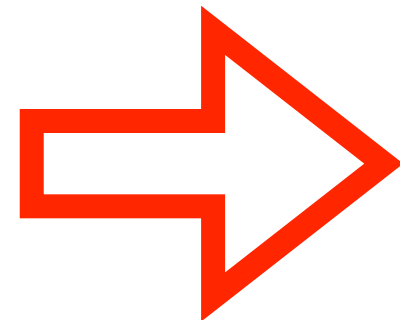
(select project if appropriate)

Summary

Provide a concise one-line summary of your problem. It will be used as the subject line in emails about this problem. A good summary makes it easier for the issue to reach the correct persons.

Do not use only generic phrases like "Help", "Problem", "Question", etc.

Projects in SUPR



Support

https://supr.naiss.se/support/

110%

NAISS
SUPR

Admin User

Start

Reviews

Declared Competence

Projects

NAISS 2023/6-41

(multicentre)

LiU-2019-26 (NSC)

SNIC 2022/1-6

(multicentre)

SNIC 2022/1-24

(multicentre)

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(select project if appropriate)

Summary

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Do not use only generic phrases like "Help", "Problem", "Question", etc.

Projects in SUPR

Electronic theory of materials p...X

← → ↺ https://supr.naiss.se/project/22940/ 110% ☆

📧 ⬇️ 🔒 📄 10. 📄 📄 ☰

The Principal Investigator and the proxy can add and remove members in SUPR. Membership in this project can also be requested using the [Request Membership in Project](#) function. The Principal Investigator and the proxy will then get an email with a link in it, that is used to approve or deny the membership request.

Leave Project

Leave Project

Storage projects linked to this compute project

Members of this compute project become extended members of the linked storage project and can access its storage.

Storage Project	Title	PI
SNIC 2022/6-10	Storage for theoretical physics environm...	Rickard Armiento
NAISS 2023/6-41	Storage for theoretical physics environm...	Rickard Armiento

Resources

Allocation shows the current allocation.

Compute

Total Allocation during the whole project is shown with a **Percentage** field to the right, that compares **Total Usage** with the total allocation. The **Allocation until Today** field shows the allocation until today, also with a **Percentage** comparison.

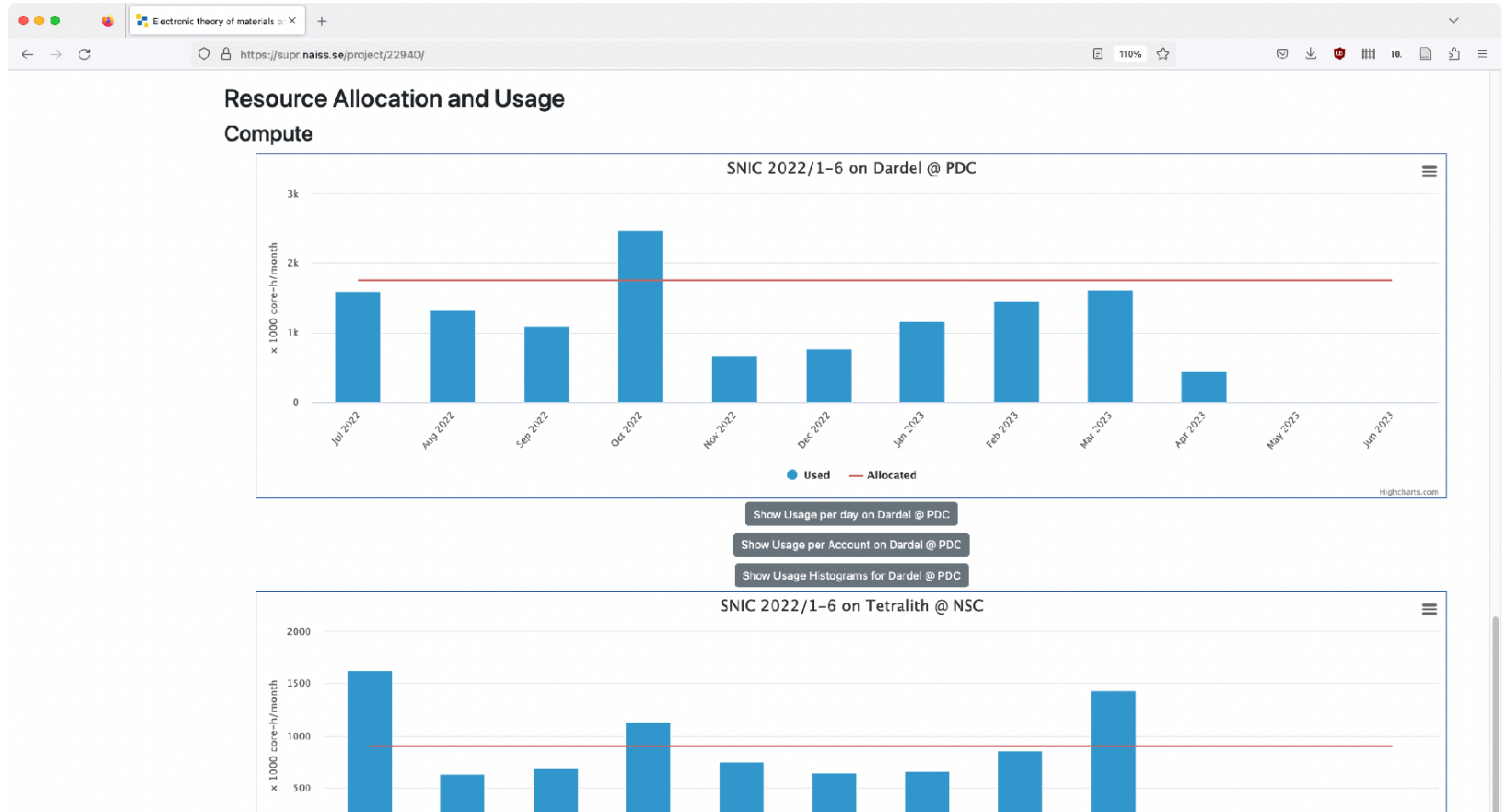
Resource	Allocation Unit	Allocation			Total	
		Total Usage	until Today	Percentage	Allocation	Percentage
Dardel @ PDC	1750 x 1000 core-h/month	12 646.8	16 450.0	76.9 %	21000.0	60.2 %
Tetralith @ NSC	900 x 1000 core-h/month	8 652.5	8 460.0	102.3 %	10800.0	80.1 %

Resource Allocation and Usage

Compute

SNIC 2022/6-10	Dardel @ PDC
--------------------------------	--------------

Projects in SUPR

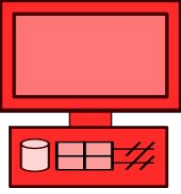


When & Why to use HPC?

HPC = High Performance Computing

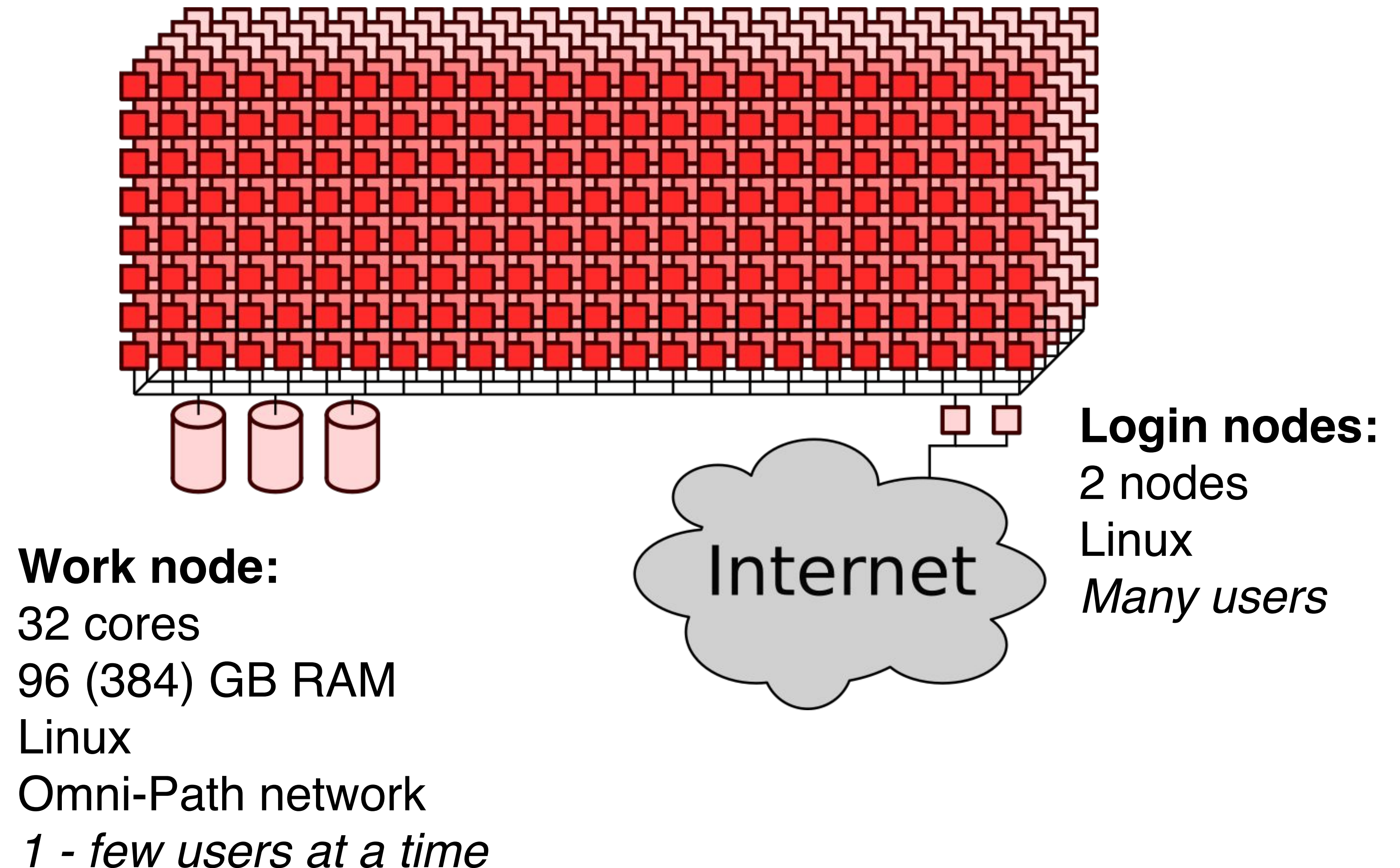
- **High number** of simulation or data analysis jobs
- The jobs are **too large** for a desktop/laptop
- Used in most research fields today
 - Numerical weather prediction
 - Climate simulations
 - Flow simulations
 - Materials science
 - Many disciplines within Chemistry, Physics, Biology
 - ...

Desktop PC vs HPC



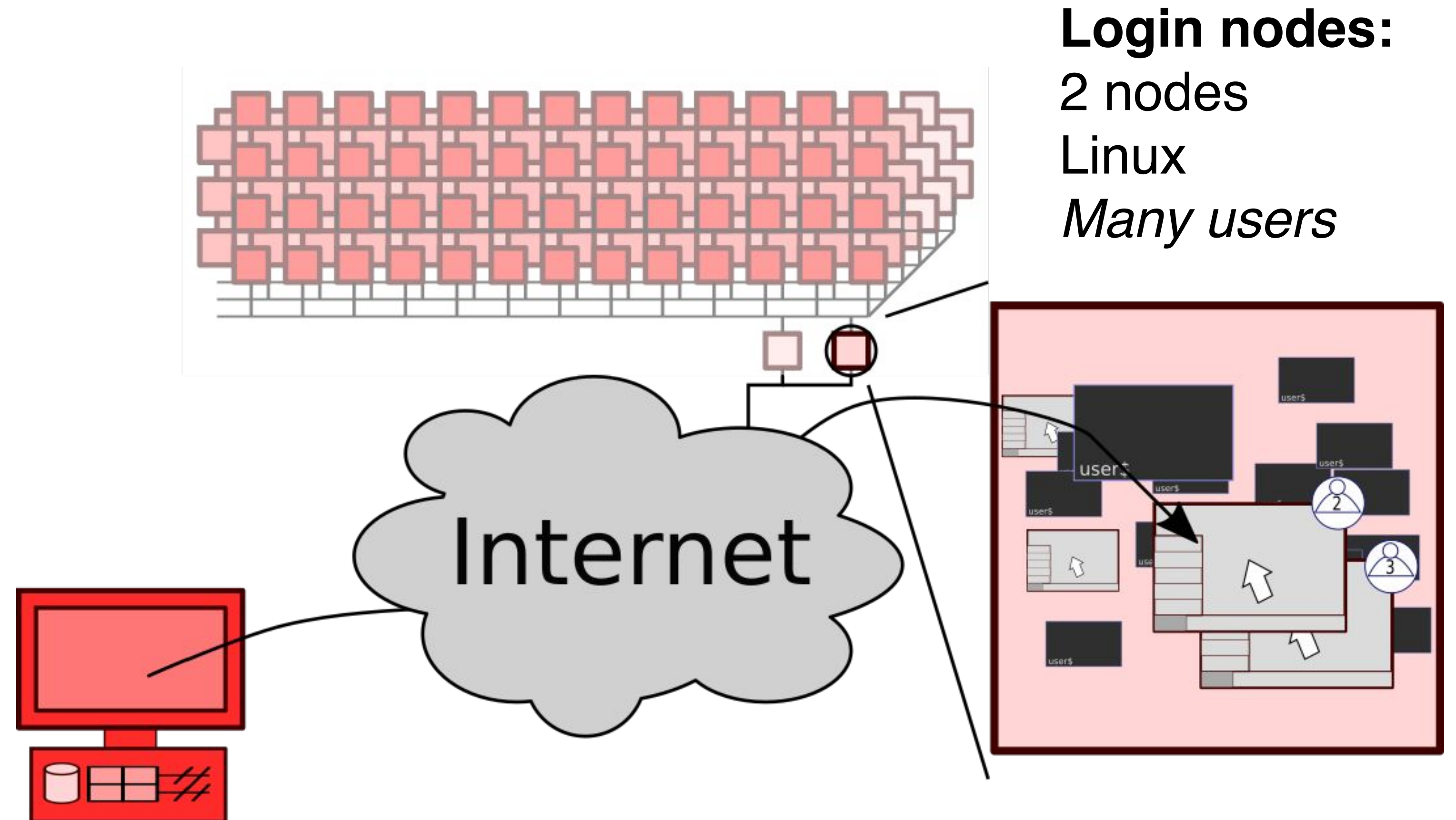
Desktop/laptop:
8 cores
16 GB RAM
Windows, MacOS (Unix), Linux
1 user

Tetralith: 1908 nodes, **Sigma:** 110 nodes



Access to Tetralith

- Typical access: using ssh
- For graphics, use ThinLinc
- Many users share login node
- Be mindful of login node usage
- Work node access via queue system (Slurm)



Access to Tetralith: ssh

ssh: the common, classical way, to login

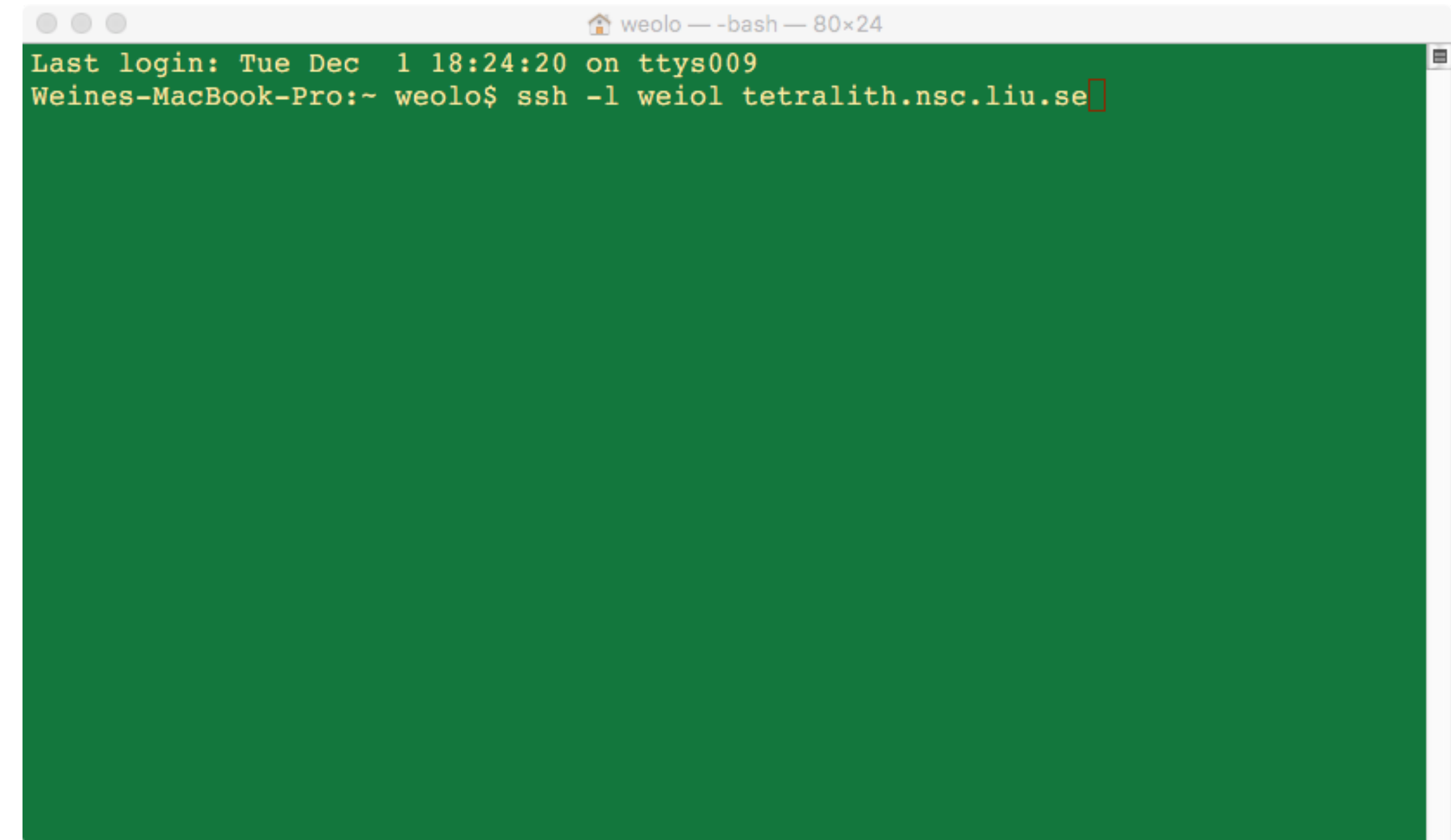
Typical login via terminal from Linux / Mac:

```
ssh username@tetralith.nsc.liu.se
```

- Windows: can use PuTTY

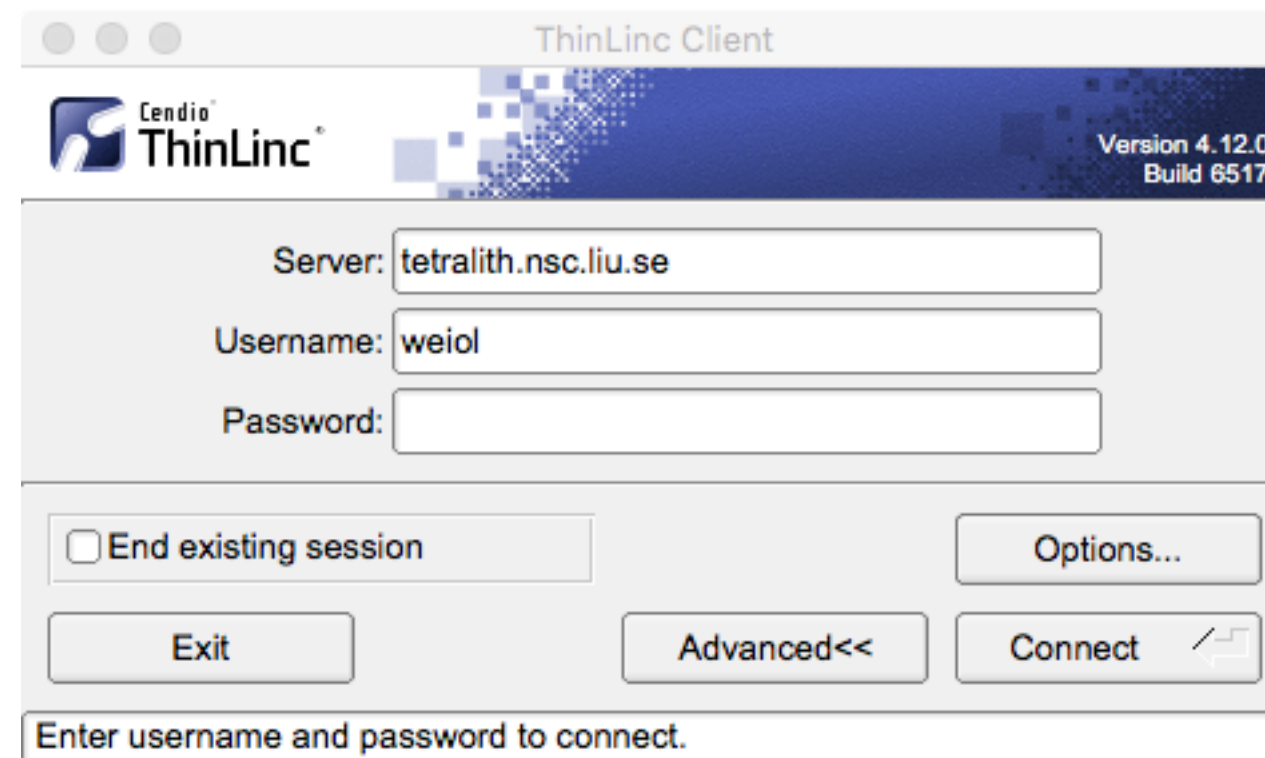
Note: to end up on a specific login node use:

```
tetralith1.nsc.liu.se  
tetralith2.nsc.liu.se
```

A screenshot of a terminal window on a Mac. The window title is 'weolo — -bash — 80x24'. The terminal shows the output of a previous login: 'Last login: Tue Dec 1 18:24:20 on ttys009' and 'Weines-MacBook-Pro:~ weolo\$'. The current command being entered is 'ssh -l weiol tetralith.nsc.liu.se'. The terminal background is green.

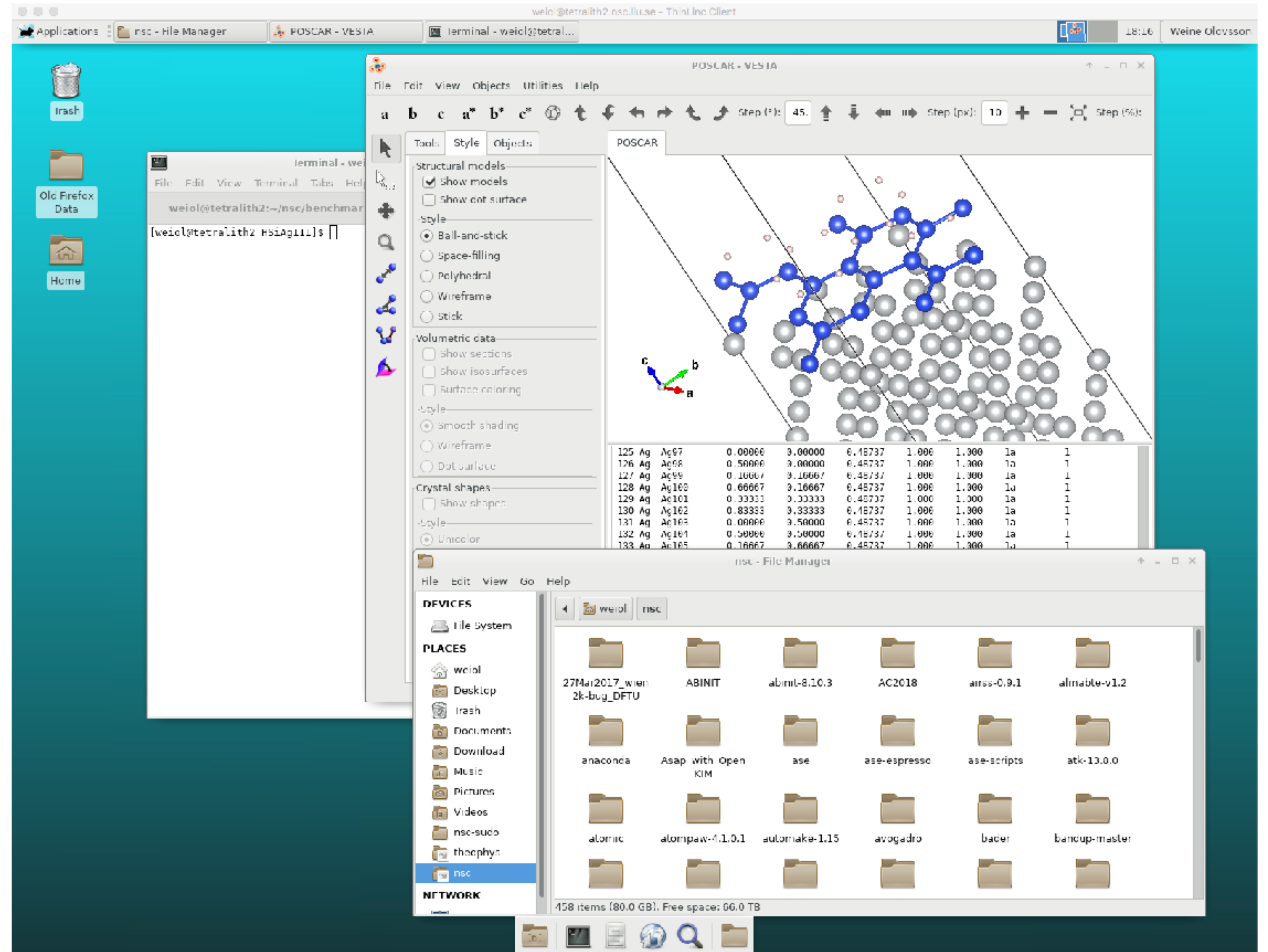
```
weolo — -bash — 80x24  
Last login: Tue Dec 1 18:24:20 on ttys009  
Weines-MacBook-Pro:~ weolo$ ssh -l weiol tetralith.nsc.liu.se
```


Access to Tetralith: ThinLinc

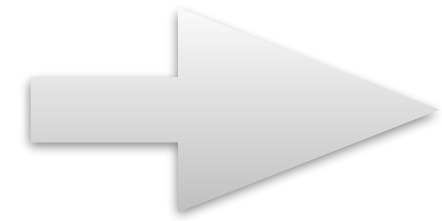


- ThinLinc - *virtual desktop*
- Persistent sessions (compare screen, tmux)
- Recommended for graphics
- Hardware acc. graphics (vglrun) in some cases

<https://www.nsc.liu.se/support/graphics/>



Some Basics



- **Linux**, see e.g. guide and forum
 - ▶ Basic commands: `cd`, `pwd`, `ls`, `mkdir`, `mv`, `grep`, `less`, `cat`, ...
- Common tools
 - ▶ Text editors: `vi`, `gedit`, `emacs`, `nano`, ...
 - ▶ Plotting graphs: `gnuplot`, `grace`, ...
 - ▶ Analysis (basic/complex): `python`, `R`, `Matlab`, ...
- Useful things
 - ▶ Persistent terminal session: `screen`, `tmux`
 - ▶ Check compute usage: `projinfo`
 - ▶ Check disk usage: `nscquota`

Files & Storage

Recover deleted files?

Three types of storage areas available:

1. Personal home directory, e.g. /home/x_user
2. Project storage, owned by PI, e.g. /proj/ourstuff
3. Work node local disk (during runs)

Backup?

yes!

no!

no!

Snapshot?

yes!

yes!

no!

Some notes:

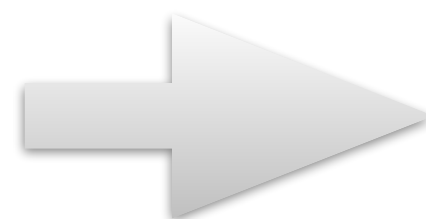
- Use `nscquota` to check available disk space
- Project storage is linked to specific project allocation and life time
- Good idea to have your own backup
- Data is never 100% safe, there's always some risk

<https://www.nsc.liu.se/support/storage/snic-centrestorage/recover-deleted-files/>

<https://www.nsc.liu.se/support/storage/index.html>

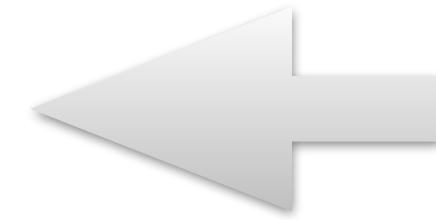
Basic Security

- Unique password (non-trivial but not overly complicated)
- Suspicion that your account is compromised -> contact NSC
- Don't hesitate to contact us!
- Sharing accounts is not allowed (accounts are personal)
Share files e.g. by managing project memberships and use /proj



Software: How do I get Code X?

1. Check installed software webpage
2. Check module system (module avail)
3. Ask NSC support
4. Build and install yourself



Special wrappers/rec. e.g.: Gaussian

NSC software installation policy:

- Users encouraged to install in /home or /proj
- NSC can help to install on request



Testing,
benchmarking,
optimization

Global installation: wide or not usage, license?

<https://www.nsc.liu.se/software/installed/>

<https://www.nsc.liu.se/software/installation-policy/>

Software: Installation Webpage

The screenshot shows a web browser window with the address bar displaying `https://www.nsc.liu.se/software/installed/`. The browser tab is titled "NSC Installed software". The webpage features a navigation bar with the NSC logo on the left and links for START, SYSTEMS, STORAGE, SOFTWARE, ABOUT, and a USER AREA dropdown on the right. A red arrow points to the SOFTWARE link in the navigation bar. Below the navigation bar, there is a secondary menu with links for Software documentation, Software installation policy, Software licensing, Compilers, NSC build environment, and Modules. A red arrow points to the "Installed software" link in this secondary menu. The main content area has a breadcrumb trail "NSC / Software / Installed software" and a heading "Installed software". Below this heading, a paragraph states: "NSC has a large number of software installations available, often in multiple versions to suit the needs of various user communities. For a list of installed software, please see the corresponding resource page below. If you need software that is presently not installed, please see our [software installation policy](#)." A red arrow points to the "Software portfolios by cluster" section, which contains a bulleted list: "• [Tetralith & Sigma Software List](#)." and "• For Freja and Nebula, please look at the list above (software present there that is not already on Freja/Nebula can be requested).". Below this is the "Module system" section, which says: "You can also query the [module system](#) for available software and recommendations on what versions to use, e.g:". A code block contains the commands: `module avail` and `module add vasp/recommendation`. The "SNIC knowledge base" section follows, with text: "Information on software and availability for all of SNIC is also available in the [SNIC knowledge base software section](#)." and "There is specific information for these NSC resources:". A red arrow points to the URL `https://www.nsc.liu.se/software/installed/` at the bottom right of the page.

NSC Installed software

`https://www.nsc.liu.se/software/installed/`

NSC

START SYSTEMS STORAGE SOFTWARE ABOUT USER AREA

Software documentation Software installation policy Software licensing Compilers NSC build environment Modules

MPI libraries Math libraries Python at NSC Anaconda at NSC Installed software

NSC / Software / Installed software

Installed software

NSC has a large number of software installations available, often in multiple versions to suit the needs of various user communities. For a list of installed software, please see the corresponding resource page below. If you need software that is presently not installed, please see our [software installation policy](#).

Software portfolios by cluster

- [Tetralith & Sigma Software List](#).
- For Freja and Nebula, please look at the list above (software present there that is not already on Freja/Nebula can be requested).

Module system

You can also query the [module system](#) for available software and recommendations on what versions to use, e.g:

```
module avail
module add vasp/recommendation
```

SNIC knowledge base

Information on software and availability for all of SNIC is also available in the [SNIC knowledge base software section](#).
There is specific information for these NSC resources:

<https://www.nsc.liu.se/software/installed/>

Software: Installation Webpage

NSC Installed Software | Tetralith Sof X

← → ↺ https://www.nsc.liu.se/software/catalogue/tetralith/ ☆ 📧 ⬇ 👤 🛡 📊 10. 📄 📌 ☰

NSC Software Installations

Tetralith Sigma Nebula Bi Berzelius

Software on Tetralith and Sigma

The scientific applications listed in the table below have been installed centrally under `/software/sse2/`. Each software installation is categorized into one of three [software support tiers](#), depending on the level of help we can provide for that particular software.

Some useful software and tools, such as a few editors are installed as part of the operating system and are not listed here.

This list was last updated on: 2025-04-14

All

Chem

Phys

Bio

CAE

Geo

Math

Devel

Data

Tools

Vis

Misc

Search:

Software	Description	Support
ABAQUS	The Abaqus FEA software suite offers various tools for stress analysis, heat transfer, fluid mechanics etc.	tier3
ABINIT	ABINIT calculates the total energy and properties of materials and molecules using, primarily, DFT.	tier2
AlphaFold	Implementation of the inference pipeline of AlphaFold v2.	tier3
Amber	Amber is a suite of biomolecular simulation programs.	tier3
Anaconda	The Anaconda Python distribution platform for Python and R scientific computing.	tier2
ANSYS	Software suite for computational fluid dynamics, stress analysis and many more CAE tasks.	tier2
ANSYS-EM	Software suite for Electromagnetics simulations.	tier3
arm-DDT	ARM/Allinea DDT is a debugging tool for scalar, multi-threaded and large-scale parallel applications.	tier2

A large red outline arrow pointing horizontally to the left, positioned to the right of the search bar and pointing towards it.

<https://www.nsc.liu.se/software/catalogue/tetralith/>

Software: Installation Webpage

NSC Installed Software | Tetralith Sof X

← → ↻ https://www.nsc.liu.se/software/catalogue/tetralith/ ☆ 10.

NSC Software Installations

Tetralith Sigma Nebula Bi Berzelius

Software on Tetralith and Sigma

The scientific applications listed in the table below have been installed centrally under `/software/sse2/`. Each software installation is categorized into one of three [software support tiers](#), depending on the level of help we can provide for that particular software.

Some useful software and tools, such as a few editors are installed as part of the operating system and are not listed here.

This list was last updated on: 2025-04-14

All Chem Phys Bio CAE Geo Math Devel Data Tools Vis Misc

Search: vasp

Software	Description	Support
p4vasp	p4vasp is a popular tool for VASP visualization.	tier3
py4vasp	A python interface to extract data from VASP calculations	tier3
VASP	Electronic structure calculations using PAW-method DFT	tier1
VASP-OMC	Modified VASP for occupation matrix control	tier3
VASP-VTST	Utility version of VASP including: VTST 3.2, VASPsol, BEEF	tier3

Showing 5 entries (filtered from 115 total entries)

NSC

National Supercomputer Centre
Linköping University
581 83 LINKÖPING
SWEDEN

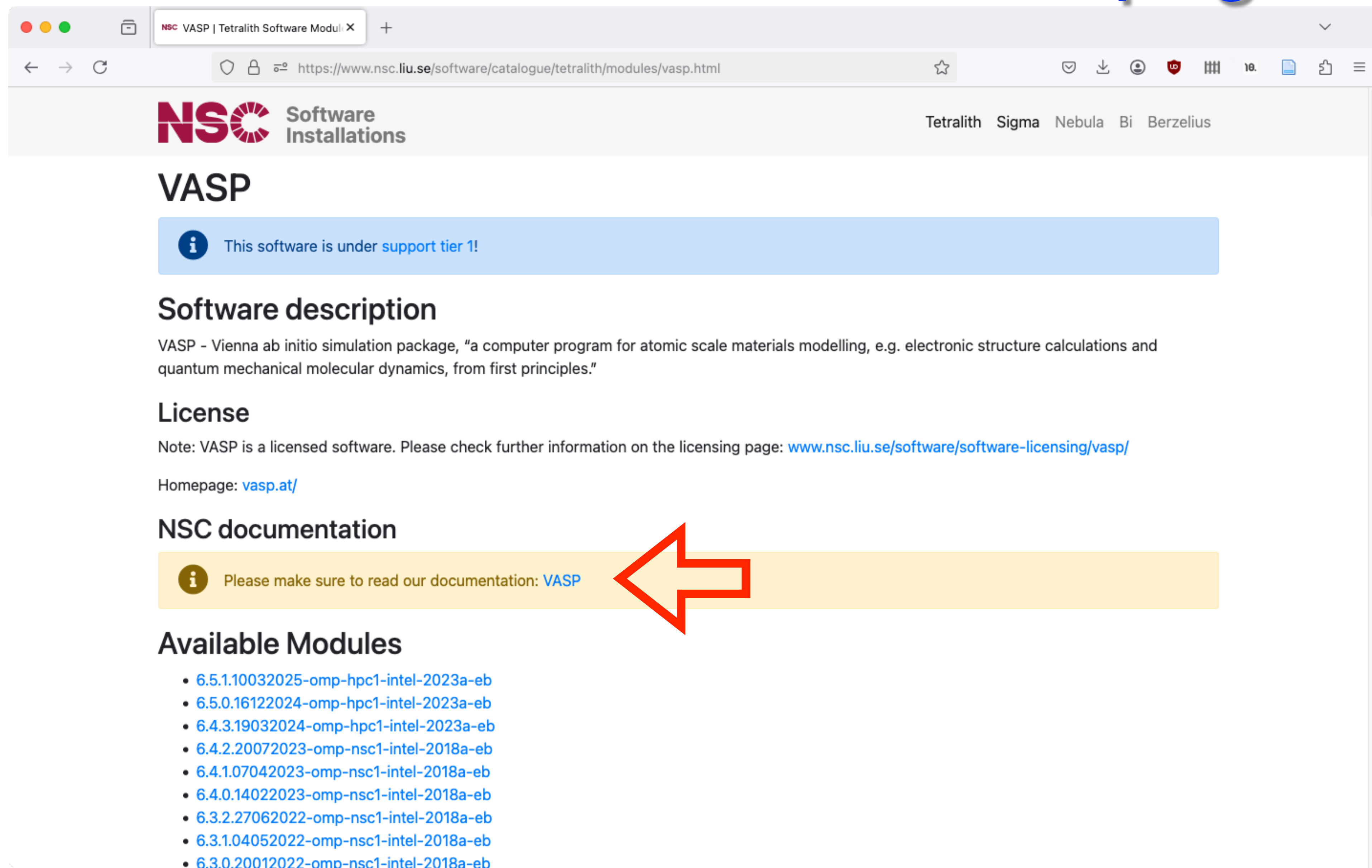
E-mail: support@nsc.liu.se
Tel.: 013-281000 (switchboard)
Fax.: 013-149403
Further address information

NSC is part of Linköping University and a branch in the
National Academic Infrastructure for Supercomputing in Sweden.

LINKÖPING

NAISS

Software: Installation Webpage



The screenshot shows a web browser window with the address bar displaying <https://www.nsc.liu.se/software/catalogue/tetralith/modules/vasp.html>. The page header features the NSC Software Installations logo and navigation links for Tetralith, Sigma, Nebula, Bi, and Berzelius. The main heading is "VASP". A blue information bar states: "This software is under [support tier 1!](#)". The "Software description" section defines VASP as a Vienna ab initio simulation package for atomic scale materials modelling. The "License" section notes that VASP is licensed software and provides a link to the licensing page: www.nsc.liu.se/software/software-licensing/vasp/. The "NSC documentation" section includes a yellow information bar with the text: "Please make sure to read our documentation: [VASP](#)". A large red arrow points from this bar to the "Available Modules" section. The "Available Modules" section lists several module identifiers, including 6.5.1.10032025-omp-hpc1-intel-2023a-eb, 6.5.0.16122024-omp-hpc1-intel-2023a-eb, 6.4.3.19032024-omp-hpc1-intel-2023a-eb, 6.4.2.20072023-omp-nsc1-intel-2018a-eb, 6.4.1.07042023-omp-nsc1-intel-2018a-eb, 6.4.0.14022023-omp-nsc1-intel-2018a-eb, 6.3.2.27062022-omp-nsc1-intel-2018a-eb, 6.3.1.04052022-omp-nsc1-intel-2018a-eb, and 6.3.0.20012022-omp-nsc1-intel-2018a-eb.

NSC Software Installations

Tetralith Sigma Nebula Bi Berzelius

VASP

i This software is under [support tier 1!](#)

Software description

VASP - Vienna ab initio simulation package, "a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum mechanical molecular dynamics, from first principles."

License

Note: VASP is a licensed software. Please check further information on the licensing page: www.nsc.liu.se/software/software-licensing/vasp/

Homepage: vasp.at/

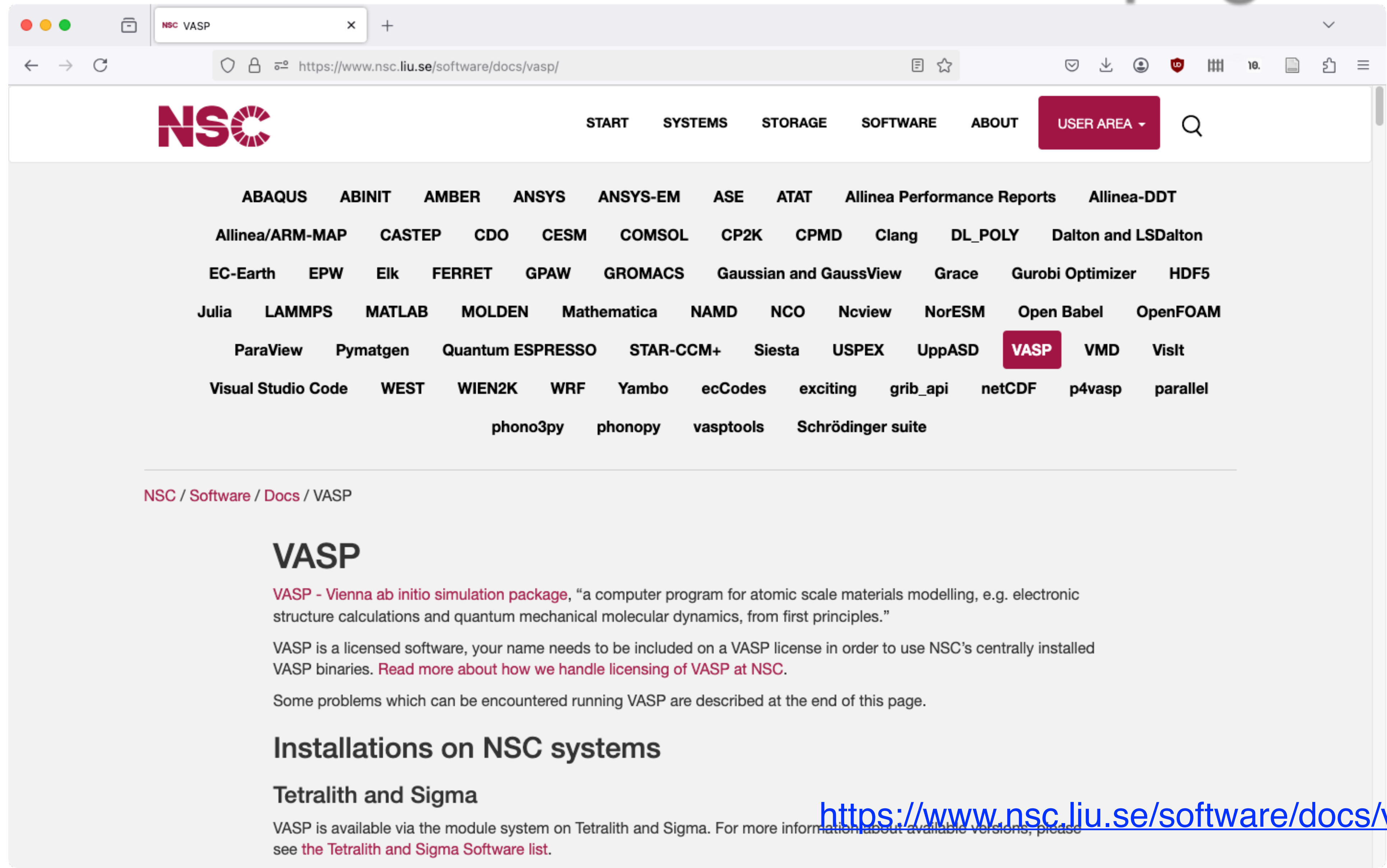
NSC documentation

i Please make sure to read our documentation: [VASP](#)

Available Modules

- [6.5.1.10032025-omp-hpc1-intel-2023a-eb](#)
- [6.5.0.16122024-omp-hpc1-intel-2023a-eb](#)
- [6.4.3.19032024-omp-hpc1-intel-2023a-eb](#)
- [6.4.2.20072023-omp-nsc1-intel-2018a-eb](#)
- [6.4.1.07042023-omp-nsc1-intel-2018a-eb](#)
- [6.4.0.14022023-omp-nsc1-intel-2018a-eb](#)
- [6.3.2.27062022-omp-nsc1-intel-2018a-eb](#)
- [6.3.1.04052022-omp-nsc1-intel-2018a-eb](#)
- [6.3.0.20012022-omp-nsc1-intel-2018a-eb](#)

Software: Installation Webpage



The screenshot shows a web browser window with the address bar displaying <https://www.nsc.liu.se/software/docs/vasp/>. The page features the NSC logo and a navigation menu with links to START, SYSTEMS, STORAGE, SOFTWARE, and ABOUT. A prominent red button labeled 'USER AREA' is located in the top right corner. Below the navigation menu, a grid of software names is displayed, with 'VASP' highlighted in a red box. The grid includes software such as ABAQUS, ABINIT, AMBER, ANSYS, ANSYS-EM, ASE, ATAT, Allinea Performance Reports, Allinea-DDT, Allinea/ARM-MAP, CASTEP, CDO, CESSM, COMSOL, CP2K, CPMD, Clang, DL_POLY, Dalton and LSDalton, EC-Earth, EPW, Elk, FERRET, GPAW, GROMACS, Gaussian and GaussView, Grace, Gurobi Optimizer, HDF5, Julia, LAMMPS, MATLAB, MOLDEN, Mathematica, NAMD, NCO, Ncview, NorESM, Open Babel, OpenFOAM, ParaView, Pymatgen, Quantum ESPRESSO, STAR-CCM+, Siesta, USPEX, UppASD, VASP, VMD, VisIt, Visual Studio Code, WEST, WIEN2K, WRF, Yambo, ecCodes, exciting, grib_api, netCDF, p4vasp, parallel, phono3py, phonopy, vaspools, and Schrödinger suite.

NSC / Software / Docs / VASP

VASP

VASP - Vienna **ab initio** simulation package, “a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum mechanical molecular dynamics, from first principles.”

VASP is a licensed software, your name needs to be included on a VASP license in order to use NSC’s centrally installed VASP binaries. [Read more about how we handle licensing of VASP at NSC.](#)

Some problems which can be encountered running VASP are described at the end of this page.

Installations on NSC systems

Tetralith and Sigma

VASP is available via the module system on Tetralith and Sigma. For more information about available versions, please see [the Tetralith and Sigma Software list](#).

<https://www.nsc.liu.se/software/docs/vasp/>

Software: Module System

module help ...	Show information for module ...
module avail	List available modules
module avail ...	Search after module containing ... in its name
module add ...	Add a module (same as module load ...)
module list	List your loaded modules
module rm ...	Remove the ... module
module purge	Remove all loaded modules (useful to start “clean”)

Software: Module System

NSC module usage:

- Only load specific software module (not dependencies)
at many other centers, must load all dependencies
- Only load build environment when building
gives access to specific build time modules

Software: Module System

```
[weiol@tetralith2 ~]$ module avail vasp
```

```
----- /software/sse/modules -----
p4vasp/recommendation (D) VASP-VTST/3.2-sol-5.4.4.16052018-vanilla-nsc1-intel-2018a-eb
VASP/5.4.4.16052018-wannier90-nsc1-intel-2018a-eb VASP/6.3.0.20012022-omp-nsc1-intel-2018a-eb
p4vasp/tmp1 VASP-VTST/4.2-6.3.0.20012022-nsc1-intel-2018a-eb
VASP/5.4.4.16052018-wannier90-nsc2-intel-2018a-eb VASP/6.3.1.04052022-omp-nsc1-intel-2018a-eb
p4vasp/0.3.30-nsc1 VASP/recommendation (D)
VASP/6.1.0.28012020-nsc1-intel-2018a-eb VASP/6.3.2.27062022-omp-nsc1-intel-2018a-eb
VASP-OMC/recommendation (D) VASP/5.4.4.16052018-nsc1-intel-2018a-eb
VASP/6.1.2.25082020-nsc1-intel-2018a-eb vasptools/0.3
VASP-OMC/5.4.4.16052018-nsc1-intel-2018a-eb VASP/5.4.4.16052018-nsc1-intel-2018b-eb
VASP/6.1.2.25082020-omp-nsc1-intel-2018a-eb. VASP-VTST/recommendation (D)
VASP/5.4.4.16052018-nsc2-intel-2018a-eb VASP/6.2.0.14012021-omp-nsc1-intel-2018a-eb
VASP-VTST/3.2-sol-5.4.4.16052018-nsc2-intel-2018a-eb VASP/5.4.4.16052018-vanilla-nsc1-intel-2018a-eb
VASP/6.2.1.29042021-omp-nsc1-intel-2018a-eb
```

Where:

D: Default Module

Use "module spider" to find all possible modules.

Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".

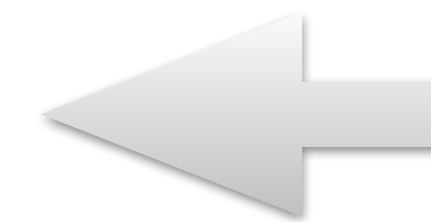
```
[weiol@tetralith2 ~]$
```

<https://www.nsc.liu.se/software/modules/>

Software: Compilers and Libraries

NSC recommendation: to compile your own software, load a **build environment**

- Compilers
 - Intel: icc, ifort
 - Gcc: gcc, gfortran
- MPI libraries
 - Intel (impi), OpenMPI
- Math libraries
 - e.g. MKL
- Build environments
 - e.g. buildenv-intel/2023a-eb



Software: Build Environment

```
[weiol@tetralith1 ~]$ module avail buildenv
```

```
----- /software/sse/modules -----  
buildenv-gcc/recommendation (D)      buildenv-gcc/2016b-eb      buildenv-gcccuda/11.4-9.3.0-bare  
buildenv-intel/2015.1.133-impi-2018.1.163-eb  buildenv-intel/2018b-eb  buildenv-nvhpc/recommendation (D)  
buildenv-gcc/7.3.0-bare              buildenv-gcc/2018a-eb      buildenv-mpi-gcc/recommendation (D)  
buildenv-intel/2016b-eb              buildenv-intel/2018.u1-bare  buildenv-gcc/9.3.0-bare  
buildenv-gcccuda/recommendation (D)      buildenv-mpi-gcc/2018a-eb  buildenv-intel/2017.u7-bare  
buildenv-intel/2021.3.0-oneapi         buildenv-gcc/11.3.0-bare   buildenv-gcccuda/10.2-7.3.0-bare  
buildenv-intel/recommendation (D)        buildenv-intel/2018a-eb    buildenv-nvhpc/cu11.4-22.1-bare
```

Where:

D: Default Module

Use "module spider" to find all possible modules.

Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".

```
[weiol@tetralith1 ~]$
```


Software: Build Environment

```
[weiol@tetralith1 ~]$ module add buildenv-intel/2018a-eb
```

```
*****
```

```
You have loaded an intel buildenv module
```

```
*****
```

```
The buldenv-intel module makes available:
```

- Compilers: icc, ifort, etc.
- Mpi library with mpi-wrapped compilers: intel mpi with mpiicc, mpiifort, etc.
- Numerical libraries: intel MKL

It also makes a set of dependency library modules available via the regular module command. Just do:

```
module avail
to see what is available.
```

NOTE: You should never load build environments inside submitted jobs.
(with the single exception of when using supercomputer time to compile code.)

```
[weiol@tetralith1 ~]$ module list
```

Currently Loaded Modules:

1) mpprun/4.1.3	5) buildtool-easybuild/4.3.0-nscde3532a	9) ifort/.2018.1.163-GCC-6.4.0-2.28 (H) 13)
buildenv-intel/2018a-eb		
2) nsc/.1.1 (H, S)	6) GCCcore/6.4.0	10) impi/.2018.1.163 (H)
3) EasyBuild/4.3.0-nscde3532a	7) binutils/.2.28 (H)	11) imkl/.2018.1.163 (H)
4) nsc-eb-scripts/1.2	8) icc/.2018.1.163-GCC-6.4.0-2.28 (H)	12) intel/2018a

Where:

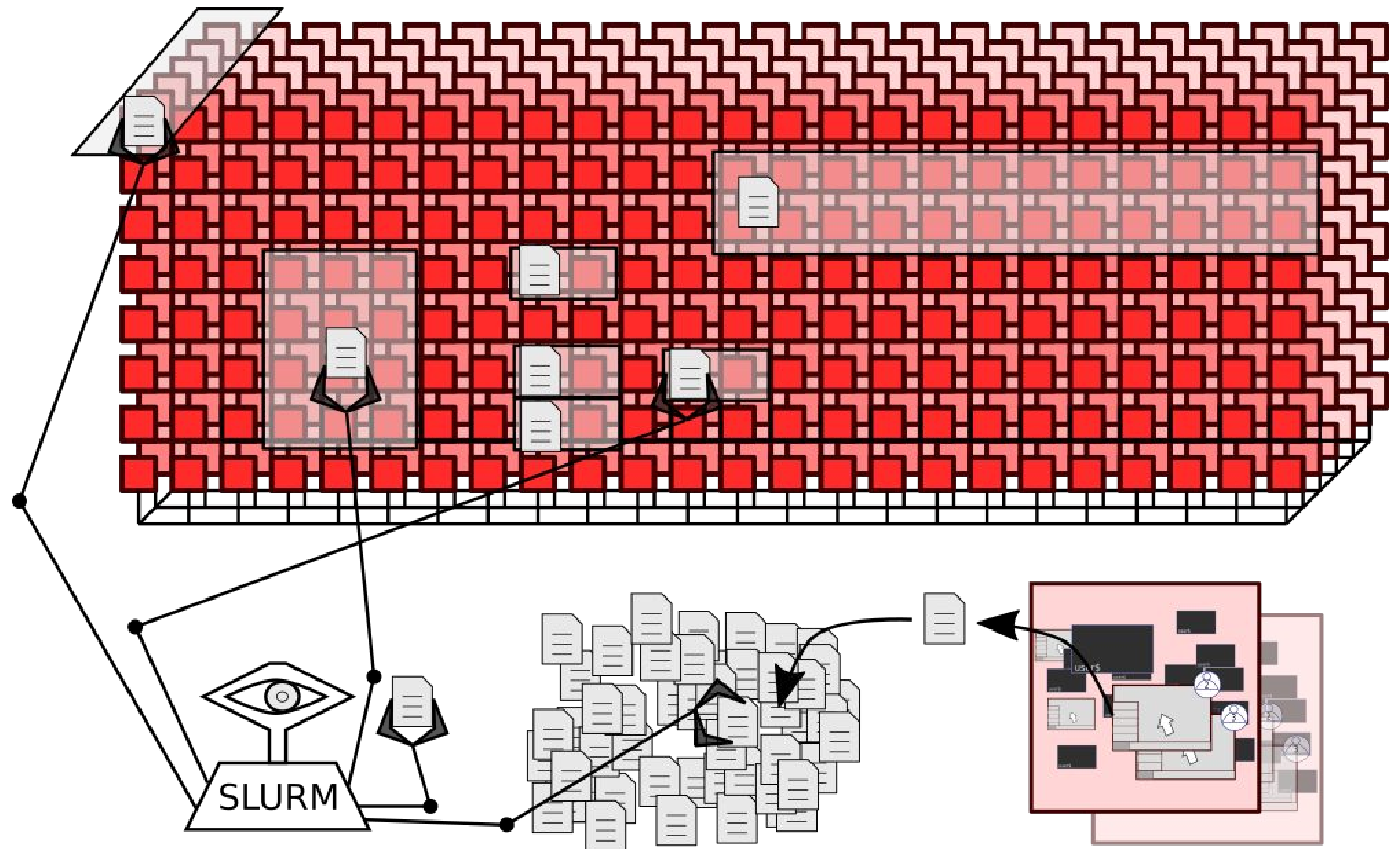
S: Module is Sticky, requires --force to unload or purge

H: Hidden Module

```
[weiol@tetralith1 ~]$
```


Queue System: Slurm

- Many jobs & users
- Resource access via Slurm
- Several methods:
 - sbatch
 - interactive
- Run as much possible, based on prior usage
- Fairshare scheduling with backfill
- 168 hours (7d) walltime limit
- Avoid short time wide jobs, “flat jobs”
- Priority boosting available



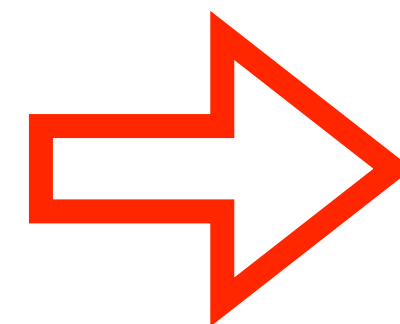
Slurm: Running Batch Job

- Regular production runs
- Output to files

`slurm-JOBID.out`

project
time
MPI ranks
job name

NSC MPI job
launching tool



Example: a job script called “run.sh”

```
#!/bin/bash
#SBATCH -A naiss2024-00-00
#SBATCH -t 1:00:00
#SBATCH -n 32
#SBATCH -J vaspstst

module load VASP/6.4.3.19032024-omp-hpc1-intel-2023a-eb
mpprun vasp_std
```

Submit job:

`sbatch run.sh`

Check queue:

`squeue -u USERNAME`

Checking jobs:

`jobload JOBID`

`jobsh NODE`

`seff JOBID`

`lastjobs`

login to node, run “top”

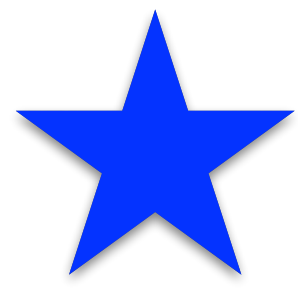
Slurm: Interactive Job

- Testing, debugging
- Hands-on, direct node access

Example: similar settings as for the job script

```
[weiol@tetralith1 ~]$interactive -A naiss2020-13-76 -n 32 -t 1:00:00
salloc: Pending job allocation 11193334
salloc: job 11193334 queued and waiting for resources
salloc: job 11193334 has been allocated resources
salloc: Granted job allocation 11193334
srun: Step created for job 11193334
[weiol@n405 ~]$
```

- Special queue for brief testing, max 1h, max 1 node (also with job script)
 - reservation=now @Tetralith
 - reservation=devel @Sigma



mpprun (update)

- **NSC** MPI job launching tool
- Extra features available, check with:

```
[weiol@tetralith1 ~]$ mpprun --help
usage: mpprun [-h] [--version] [-n NRANKS] [--launcher LAUNCHER] [--handler HANDLER] [--no-smt] [-C]
[--pass EXTRA_LAUNCH_ARGS] [--no-modules] [-c CPUS_PER_TASK] [-d] [-v] [-q] [-i] [--allinfo]
executable ...
```

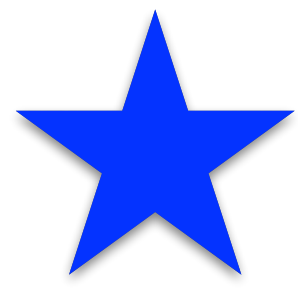
This is a helper program to figure out what MPI launcher to use, with which arguments, in what environment (including which HPC modules to load) when launching a binary or script that uses MPI.

positional arguments:


executable	The binary or script to execute.
arguments	Arguments to pass to the executable.

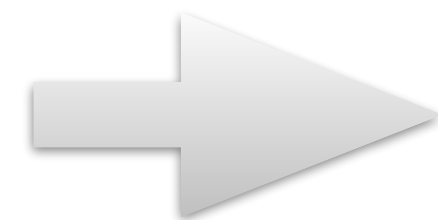
...

+ more lines of detailed description



Tetralith/Sigma OS upgrade

- CentOS 7 (E17) -> Rocky Linux 9 (**E19**)  Security updates
- Disk space (/home, /proj) not affected
- Dec'23 - Jan'24 (finished), **mpprun** was updated
- Might need to **modify scripts**, **use different modules**, **reinstall software** etc.
- Modules missing, software not working, other questions?



<https://supr.naiss.se/support>

<https://www.nsc.liu.se/support/systems/tetralith-os-upgrade/>

<https://www.nsc.liu.se/support/systems/sigma-os-upgrade/>

Best Practices & Suggestions

In general:

- Be careful how you use Tetralith/Sigma login nodes
- Use SUPR to follow project usage
- Use the NSC documentation  **contact us if problems!
we try to describe everything...**
- Be careful about what you put in .bashrc (keep as simple as possible)
- Don't hesitate to contact us for help/questions!

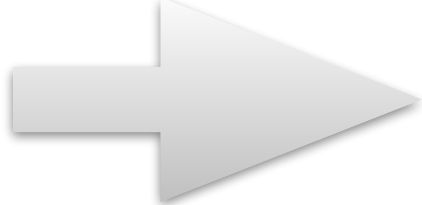
<https://supr.naiss.se/support>

support@nsc.liu.se

Best Practices & Suggestions

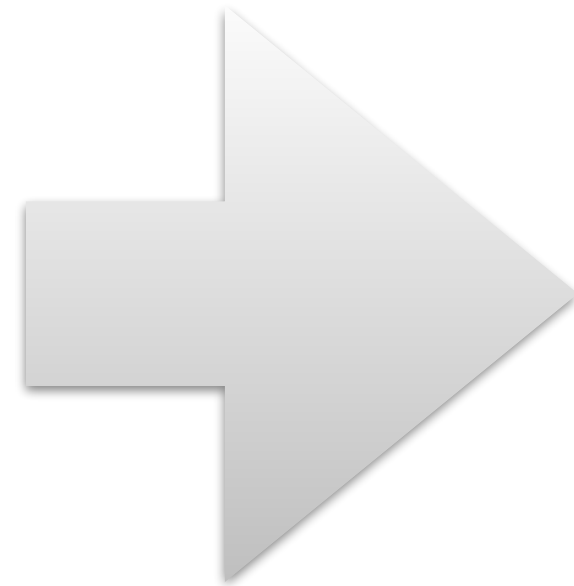
Common problems:

- My job **failed/crashed**. What now?
 - First, try to understand the cause
 - Fill in support form <https://supr.naiss.se/support>

 provide details! username, system, jobid, job path, ...
- Odd problems (lots of things set in .bashrc?)
- Don't run heavy stuff / production work on the login node
 - For brief testing e.g. run interactively --reservation=now @Tetralith
 --reservation=devel @Sigma

Further Resources

- Working effectively on Tetralith / Sigma 2018
- Working with Python on Tetralith 2019
- NSC introduction day 2017 [More details, e.g. running calcs.](#)



[Check links for presentations \(.pdf\)](#)

- **Presentations available at webpage!**

- Working effectively with HPC systems