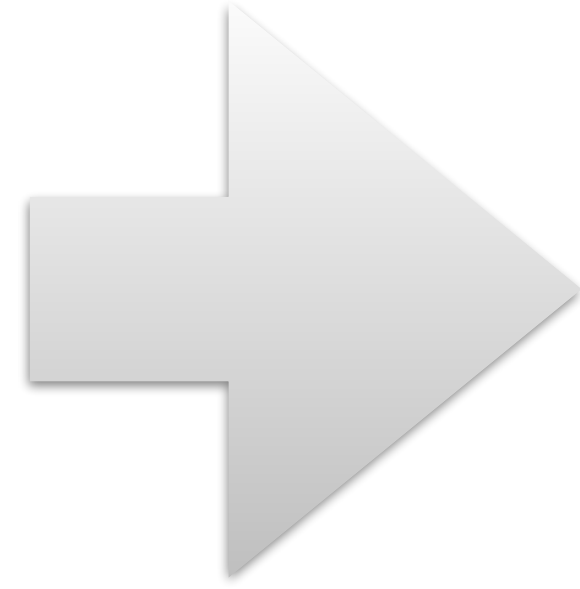


# NSC introduction to Tetralith/Sigma

National Supercomputer Centre (NSC), Linköping University

NAISS training, online @NSC 12<sup>th</sup> Nov 2024, 10:00 - 12:00

# Information / Schedule



[https://www.nsc.liu.se/support/Events/NSC\\_intro\\_Nov2024/](https://www.nsc.liu.se/support/Events/NSC_intro_Nov2024/)

- 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 GPUs (Torben Rasmussen)
- ~11:15** 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



**1989** - NSC first supercomputer centre in Sweden / SAAB partner

**1996** - SMHI partner



**2016** - MET Norway partner



# NAISS

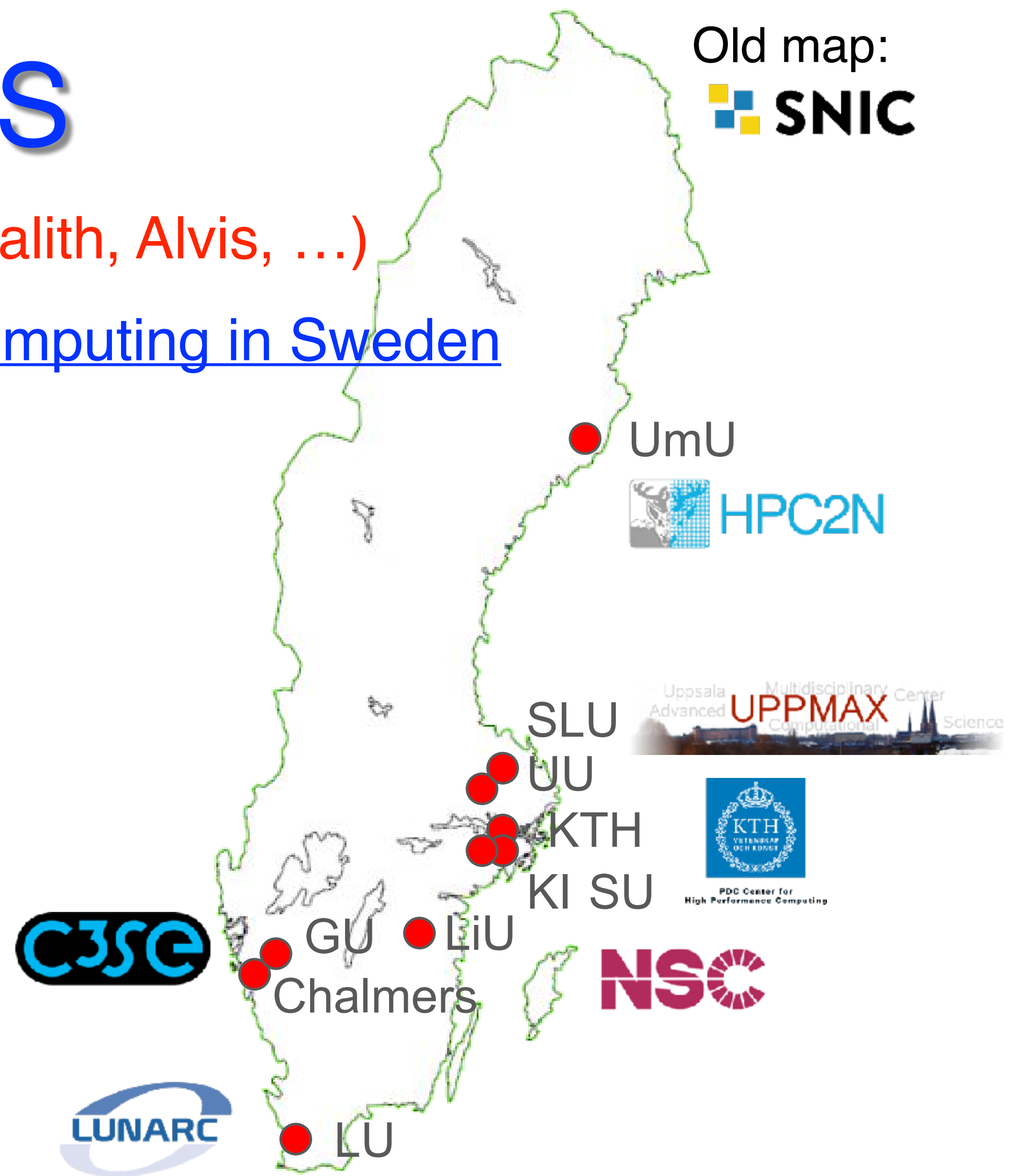
Old map:  
 **SNIC**

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

## National Academic Infrastructure for Supercomputing in Sweden

### Branches at universities (expected):

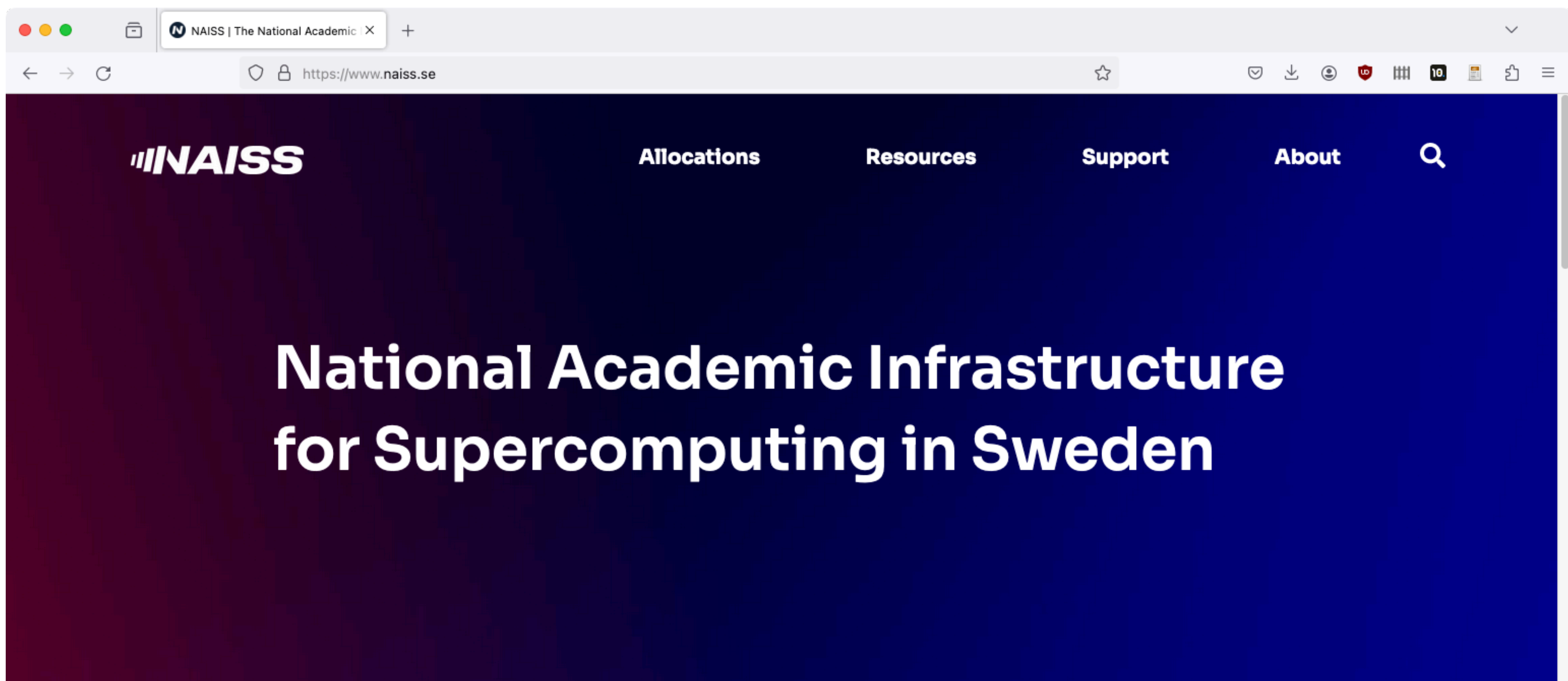
Chalmers	<u>C3SE</u>
Göteborg	
Karolinska	
KTH	<u>PDC</u>
Linköping	<u>NSC</u>
Lund	<u>LUNARC</u>
Stockholm	
Umeå	<u>HPC2N</u>
Uppsala	<u>UPPMAX</u>
+ more? SLU, LTU, MDU	



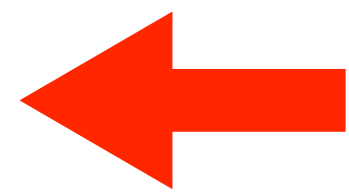
<https://www.naiss.se/>

 **More info!**

*Funding:* branches + Vetenskapsrådet (VR)



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



More info!

The National Academic Infrastructure for Supercomputing in Sweden (NAISS) is the new infrastructure organisation for high-performance computing, storage, and data services for academic users in Sweden. NAISS is hosted by Linköping University but acts independently with a national



## Events

**15 Apr**

INTERNAL MEETING

Radisson Blu Waterfront Hotel Stockholm

**NAISS User Support Kick-off**

**16-18 Apr**

TRAINING

Online

**VASP/EMTO Best Practices Workshop**

**16 Apr**

TRAINING

Online

**TTT4HPC Episode 1: HPC Resources: RAM, CPUs/ GPUs, I/O**

**19 Apr**

TRAINING

Online

**Introduction to Bianca: Handling Sensitive Research Data**

**22-26 Apr**

TRAINING

Online

**Programming Formalisms**

**23 Apr**

TRAINING

Online

**Introduction to**

# NAISS Resources

OVERVIEW

ALVIS

BIANCA

DARDEL

LUMI SWEDEN

RACKHAM

SWEDISH SCIENCE CLOUD (SSC)

SWESTORE/DCACHE

TETRALITH

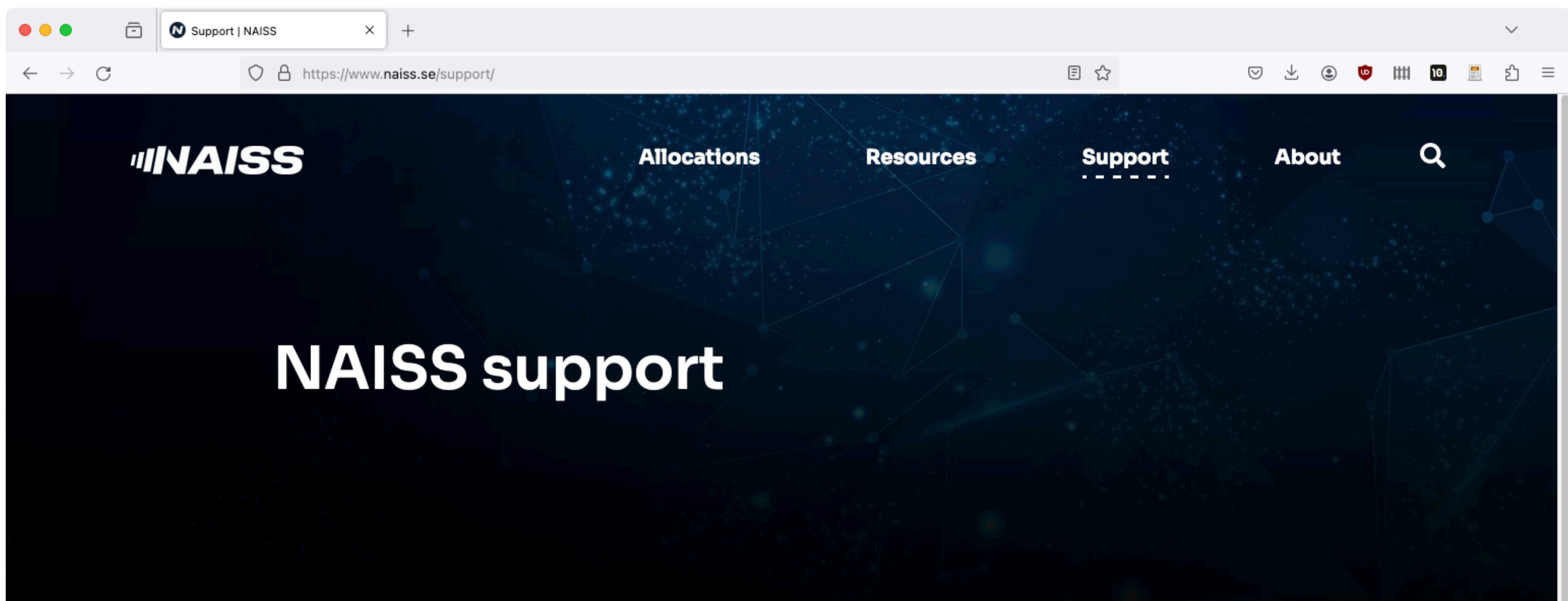
COMPUTE RESOURCE

## Alvis

### Host Data Centre

C3SE, Chalmers University of Technology





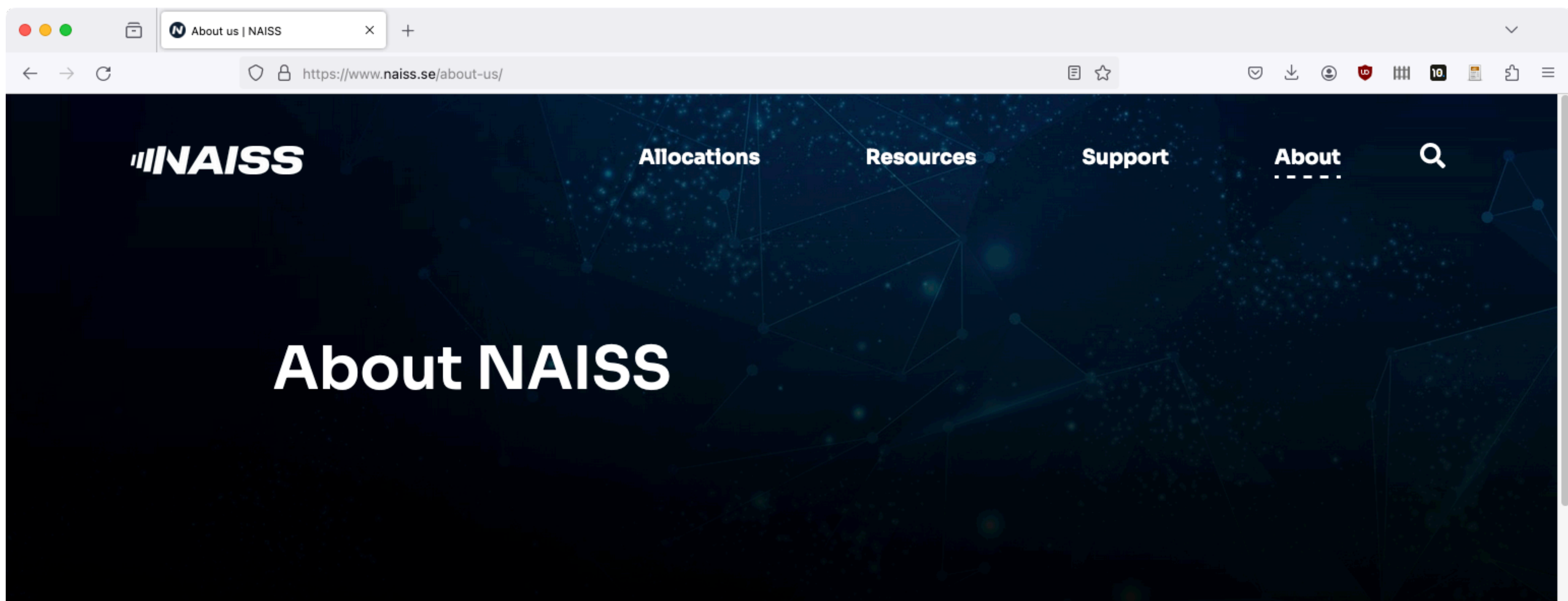
Support is available to all projects using NAISS resources.

Some examples of the support available include:

- Advise regarding proposals and suitable resources
- Using the SUPR web-system for submitting proposals
- Accessing and using allocated resources
- Installing required software
- Troubleshooting problematic jobs
- Utilizing resources efficiently

Help with scientific software development or other long-term commitment is, in general, out of scope. For this we refer to application experts or research software engineers at your





[CONTACT](#)

[STAFF](#)

[STEERING COMMITTEE MINUTES](#)

[NEWS & NEWSLETTERS](#)

[EVENTS](#)

The National Academic Infrastructure for Supercomputing in Sweden (NAISS) is the new infrastructure organization for high-performance computing, storage, and data services for academic users in Sweden. NAISS is hosted by Linköping University but acts independently with a national perspective and responsibility. NAISS main funding is provided by the Swedish Research council (VR) while the user support, organized in a decentralized branch structure, is built up in partnership with several Swedish universities.

From a user perspective, there will initially only be minimal differences between the previous SNIC and NAISS regimes. The allocation process of our resources will continue in the same way as previously.

NAISS has taken over the financing of the existing systems Dardel, Tetralith, Alvis, Bianca and

# New NAISS cluster: Arrhenius

- Carl Axel Arrhenius (1757-1824), ytterbium discovery
- **EuroHPC “mid-range”**, ca. 6-700 MSEK
- **2024**: procurement, **2025**: installation & start
- “Tetralith replacement”
- Users: academic (EuroHPC/NAISS), industry

# NSC: Quick Overview

Current Director: Björn Alling, Nov 2021 -

~ 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. 318 (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 x 8 A100 GPUs



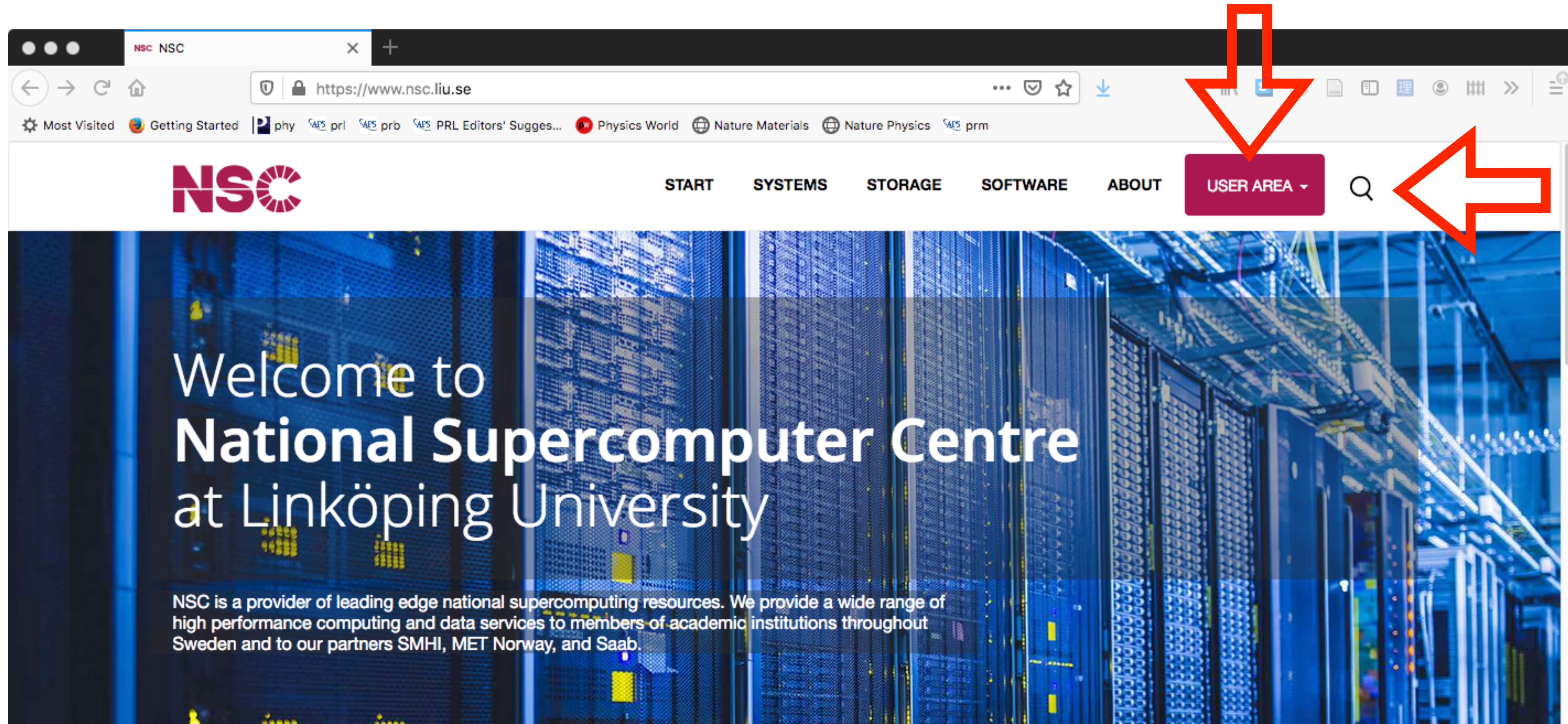
*Knut and Alice  
Wallenberg  
Foundation*

*AI/ML, for all researchers in Sweden*



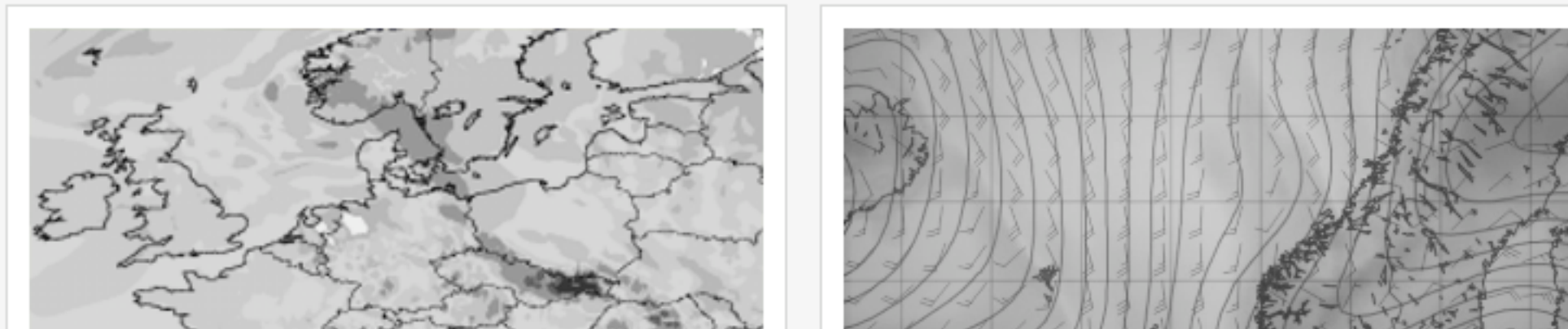
**Top500 no. 171  
& 201 (83)**

# Where to find Information?



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

## OUR PARTNERS



# Where to find Information?

The screenshot shows a web browser window with the URL <https://www.nsc.liu.se>. The page features a navigation menu with a dropdown arrow pointing to "USER AREA". Below this, there are four main sections: "User support" (Guides, documentation and FAQ.), "Getting access" (Applying for projects and login accounts.), "System status" (Everything OK! No reported problems), and "Self-service" (with buttons for SUPR and NSC Express).

**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  
Org.nr: 202100-3096

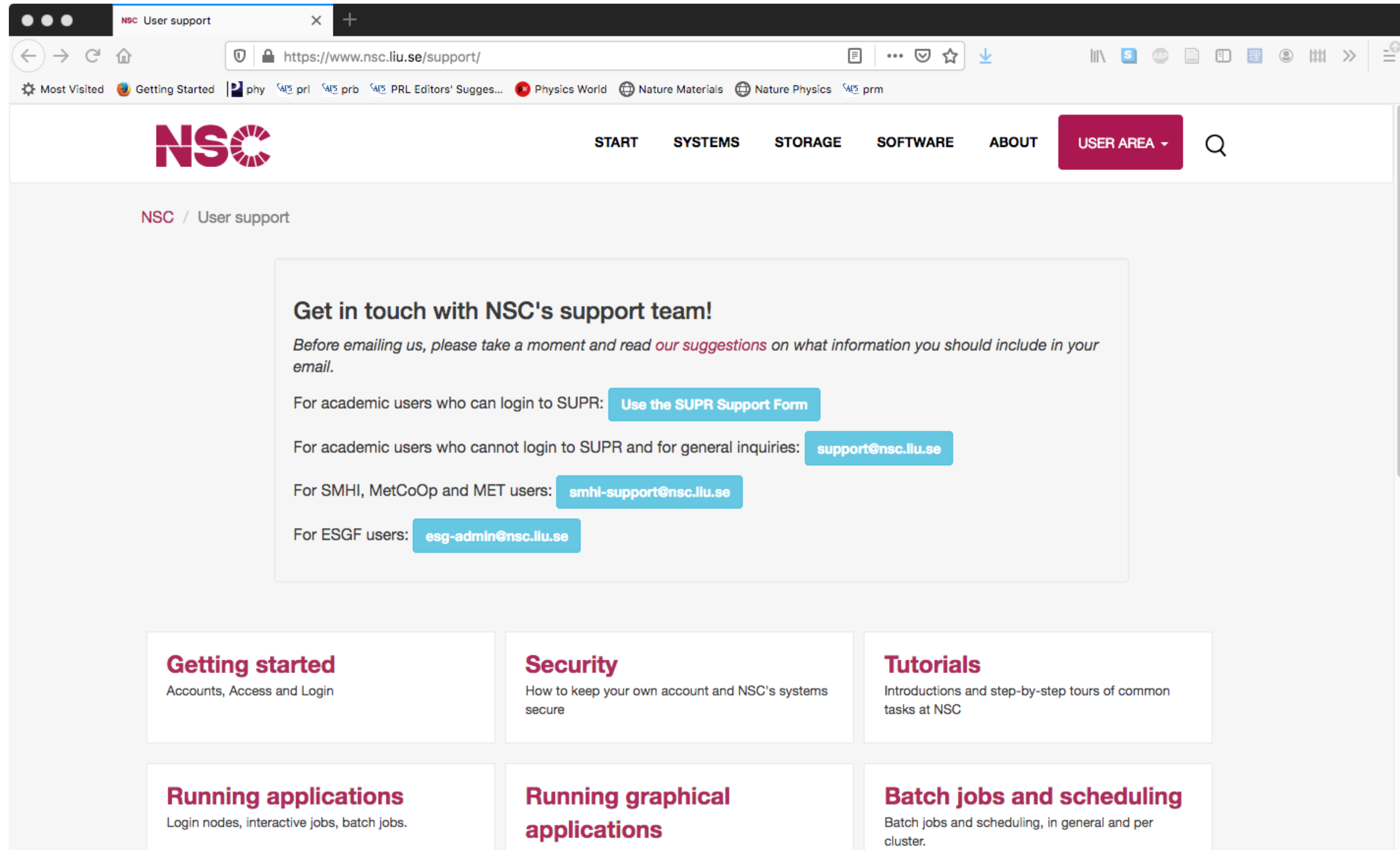
E-mail: support@nsc.liu.se  
Tel.: 013-281000 (switchboard)  
Fax.: 013-149403  
Further address information

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

li.u LINKÖPINGS UNIVERSITET    SNIC

Top of Page

# Where to find Information?



The image shows a browser window displaying the NSC User support page. The browser's address bar shows the URL <https://www.nsc.liu.se/support/>. The page features a navigation menu with links for START, SYSTEMS, STORAGE, SOFTWARE, ABOUT, and a highlighted USER AREA. The main content area is titled "NSC / User support" and contains a central box with the heading "Get in touch with NSC's support team!". Below this heading, there is a paragraph of text and four lines of contact information, each with a corresponding email address in a blue button: "Use the SUPR Support Form", "support@nsc.liu.se", "smhi-support@nsc.liu.se", and "esg-admin@nsc.liu.se". At the bottom of the page, there are six white boxes with red headings and black text, providing links to various support topics: "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/>

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](mailto:support@nsc.liu.se)

For SMHI, MetCoOp and MET users: [smhi-support@nsc.liu.se](mailto:smhi-support@nsc.liu.se)

For ESGF users: [esg-admin@nsc.liu.se](mailto: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

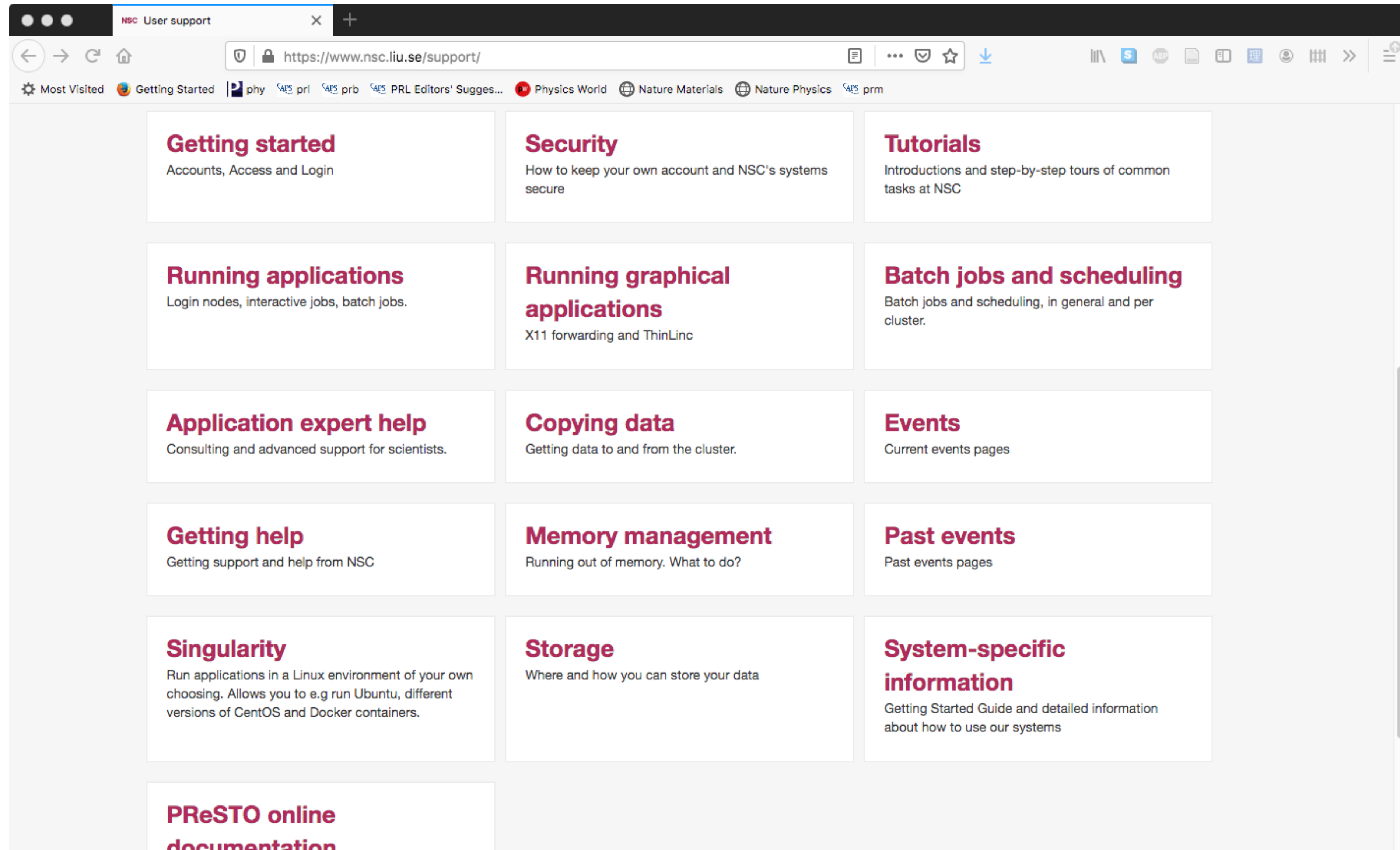
Login nodes, interactive jobs, batch jobs.

### Running graphical applications

### Batch jobs and scheduling

Batch jobs and scheduling, in general and per cluster.

# Where to find Information?

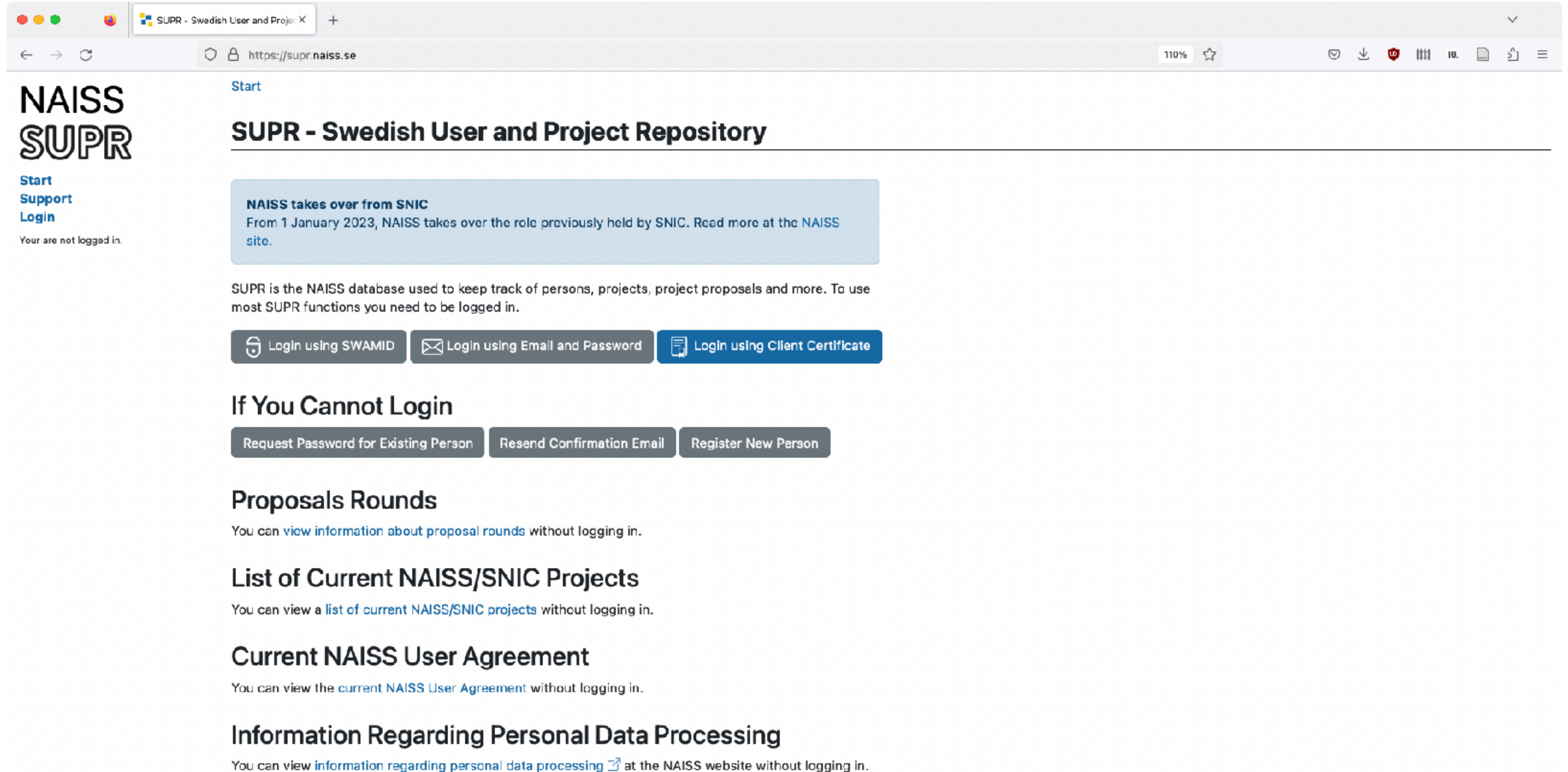


The screenshot shows a web browser window with the URL <https://www.nsc.liu.se/support/>. The page features a grid of 15 help topics, each with a title and a brief description. The topics are arranged in a 5x3 grid, with the last cell in the bottom row containing only a title.

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



# Getting Access to HPC - SUPR



The screenshot shows a web browser window with the URL <https://supr.naiss.se>. The page features the NAISS SUPR logo on the left and a main content area with the following sections:

- 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.
- Text: 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.
- Buttons: Login using SWAMID, Login using Email and Password, Login using Client Certificate
- If You Cannot Login**
- Buttons: Request Password for Existing Person, Resend Confirmation Email, Register New Person
- Proposals Rounds**
- Text: You can view information about proposal rounds without logging in.
- List of Current NAISS/SNIC Projects**
- Text: You can view a list of current NAISS/SNIC projects without logging in.
- Current NAISS User Agreement**
- Text: You can view the current NAISS User Agreement without logging in.
- Information Regarding Personal Data Processing**
- Text: You can view information regarding personal data processing at the NAISS website without logging in.

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

# Support via SUPR

The screenshot shows a web browser window with the URL <https://supr.naiss.se>. The page title is "SUPR - Weine Olovsson". The left sidebar contains navigation links: Admin, User, Start, Reviews, Declared Competence, Projects (listing various NAISS and SNIC projects), Accounts, Proposals, Rounds, Groups, Personal Information, Support, and Logout. The main content area has a "Start" section with a "SUPR - Weine Olovsson" header. Below this, there are three informational boxes: 1) "NAISS takes over from SNIC" with a link to read more. 2) "Get a Two-Factor Authentication Recovery Code" with buttons for "Get Recovery Code" and "Not Now, Remind Me Later". 3) "NAISS Activity Report Wanted" with a table of recent projects. At the bottom, a "Projects" section lists active projects with columns for Project, PI, Project Title, Project Type, Centre, Start Date, End Date, and Your Role.

**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.

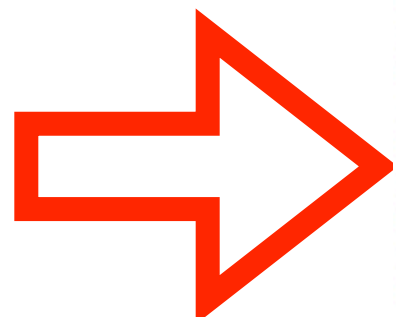
Get Recovery Code Not Now, Remind Me Later

**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



# Support via SUPR

The screenshot shows a web browser window with the URL <https://supr.naiss.se/support/>. The page features a navigation menu on the left with categories like Start, Reviews, Projects, Accounts, and Proposals. The main content area is titled 'Support' and includes instructions on how to use the form, a 'Problem Type' dropdown menu, a 'Centre and Resource' dropdown menu, a 'Project' dropdown menu, and a 'Summary' section. The user is logged in as 'Weine Olovsson'.

**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.olvsson@liu.se](mailto:weine.olvsson@liu.se))  
Turn on warning colour.

**Start / Support**

## Support

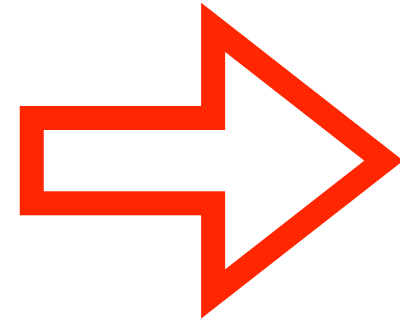
Use this form to request support for NAISS systems and services (including the SUPR portal itself). If you have multiple issues that are not related, please use the form multiple times, once for each issue.

Replies will be sent to your registered email address [weine.olvsson@liu.se](mailto:weine.olvsson@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**.

# Projects in SUPR



Support

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.olvsson@liu.se](mailto:weine.olvsson@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**.

### 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.

### Project

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

### 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.

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

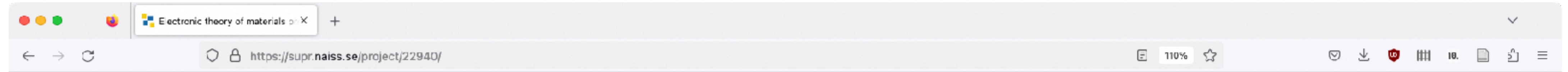
Logged in as:

Weine Olovsson

[[weine.olvsson@liu.se](mailto:weine.olvsson@liu.se)]

Turn on warning colour.

# Projects in SUPR



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
<a href="#">SNIC 2022/6-10</a>	Storage for theoretical physics environm...	Rickard Armiento
<a href="#">NAISS 2023/6-41</a>	Storage for theoretical physics environm...	Rickard Armiento

## Resources

**Allocation** shows the current allocation.

## Compute

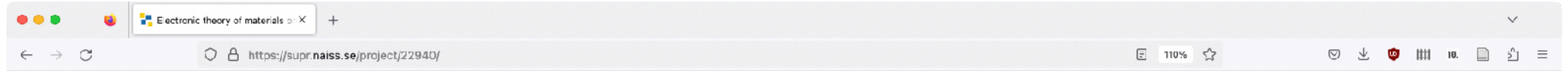
**Total Allocation** during the whole project is shown with a **Percentage** field to the right, that compares **Total Usage** with the total allocation. The **Allocation until Today** field shows the allocation until today, also with a **Percentage** comparison.

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 %

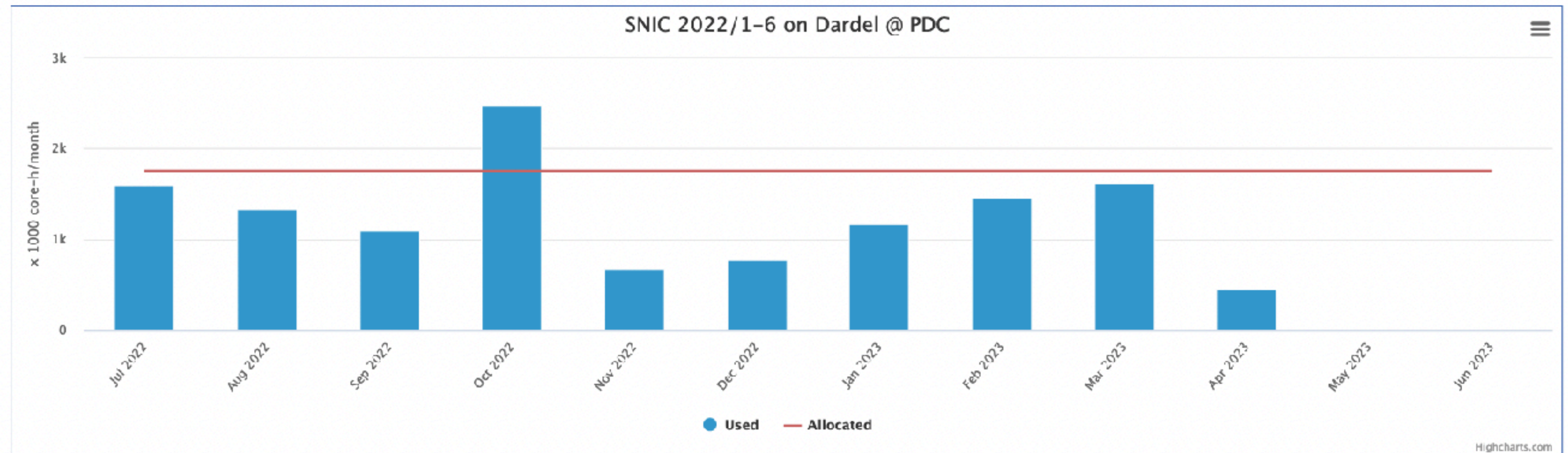
## Resource Allocation and Usage

### Compute

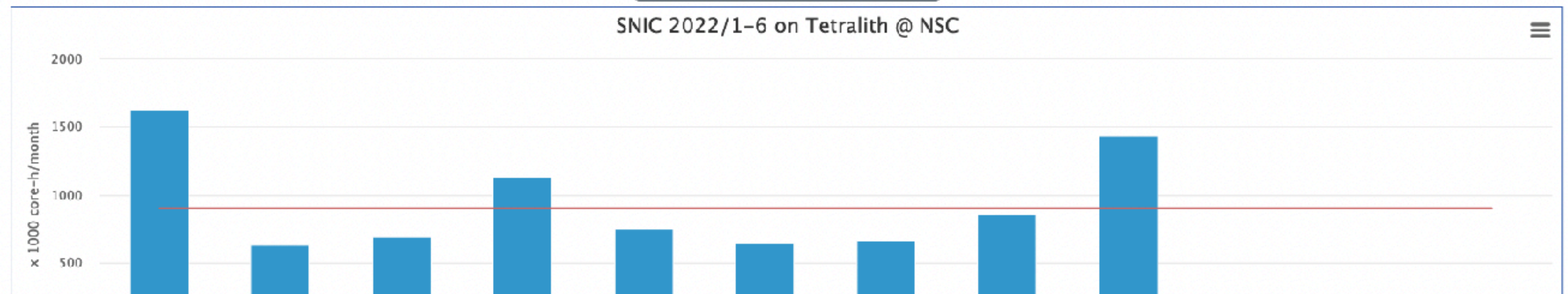
# Projects in SUPR



## Resource Allocation and Usage Compute



- Show Usage per day on Dardel @ PDC
- Show Usage per Account on Dardel @ PDC
- Show Usage Histograms for Dardel @ PDC



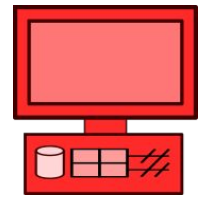
# When & Why to use HPC?

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

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



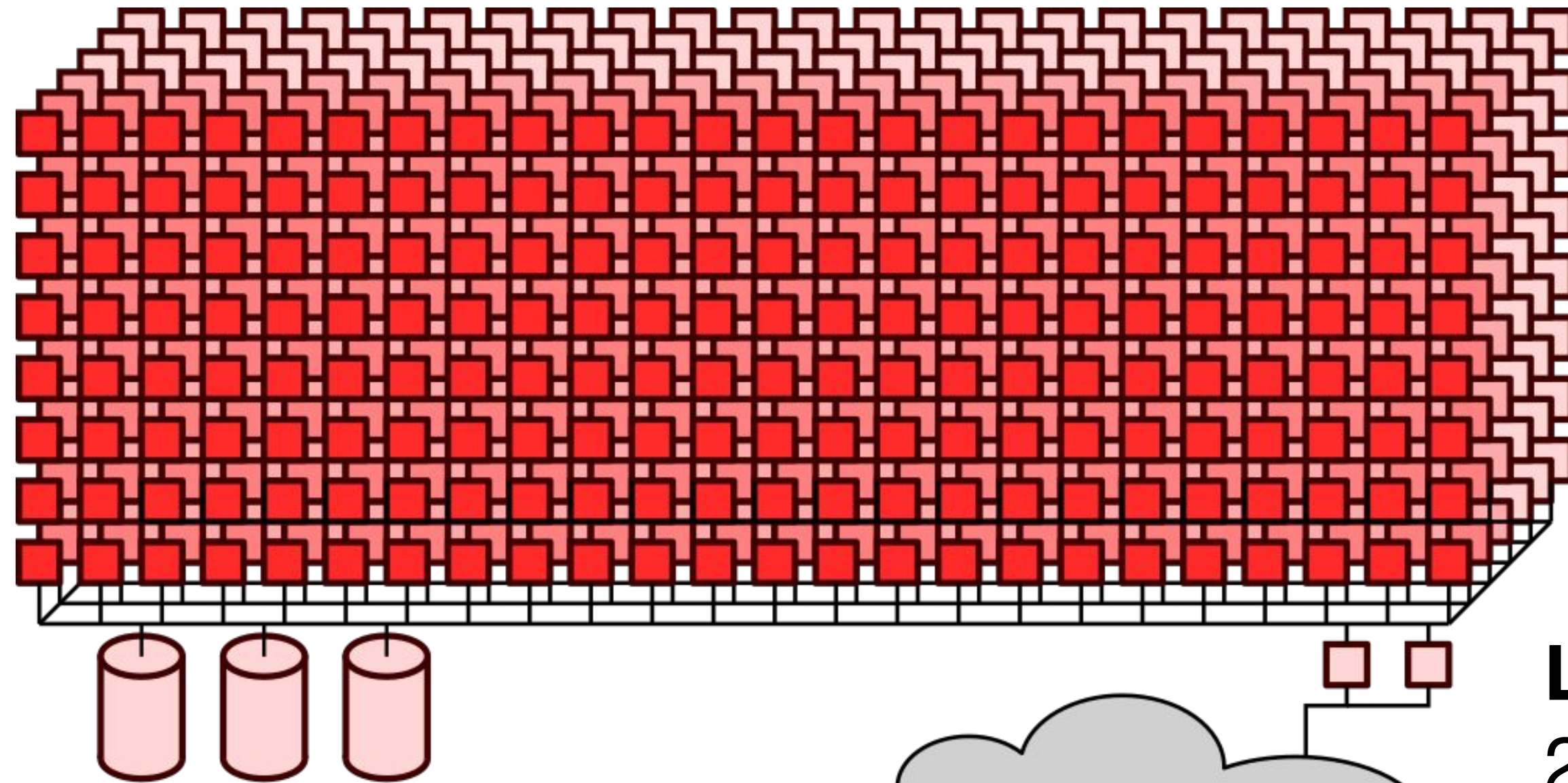
## Desktop/laptop:

8 cores

16 GB RAM

Windows, MacOS (Unix), Linux

*1 user*



## Work node:

32 cores

96 (384) GB RAM

Linux

Omni-Path network

*1 - few users at a time*

## Login nodes:

2 nodes

Linux

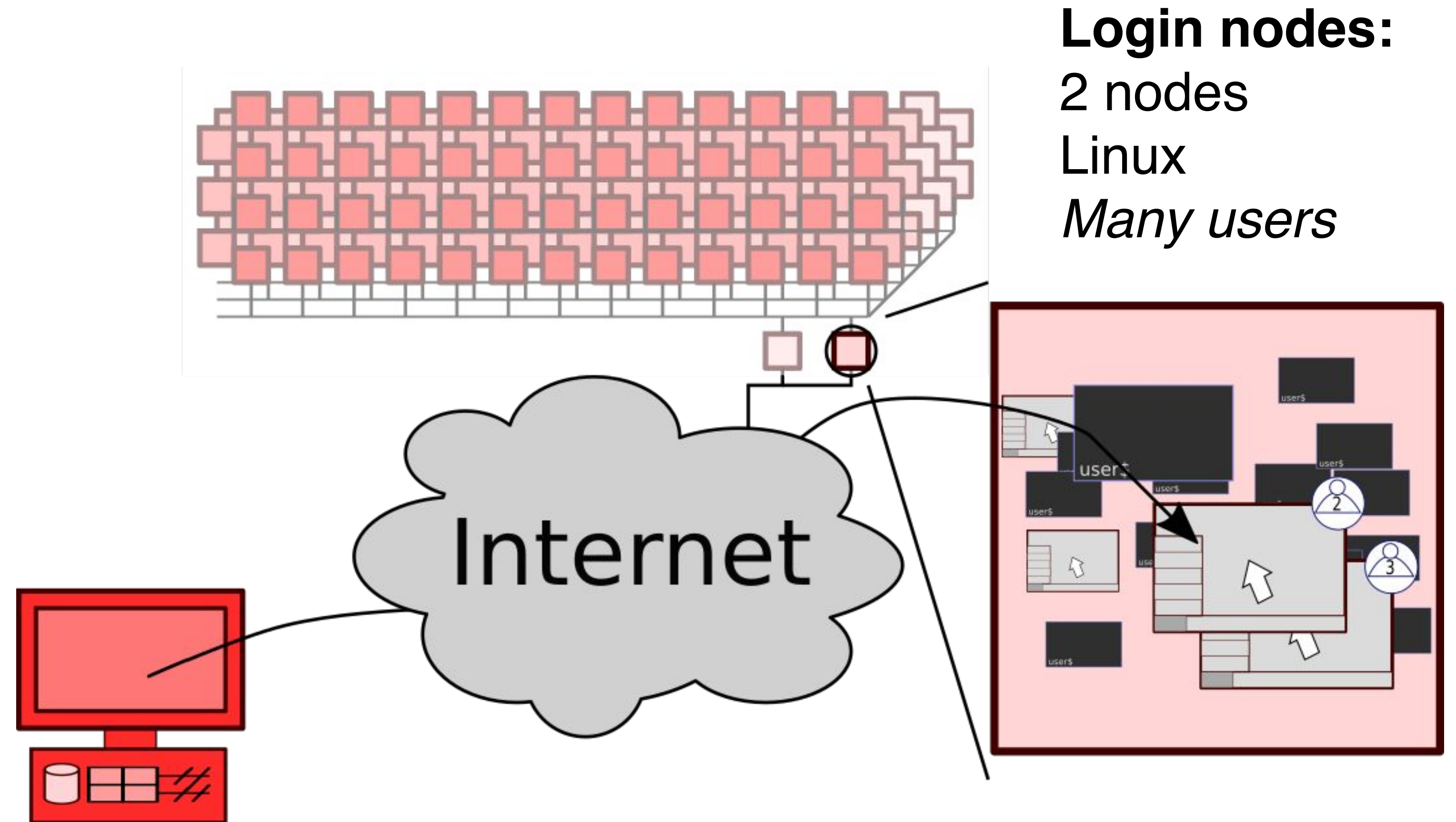
*Many users*

Internet



# 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

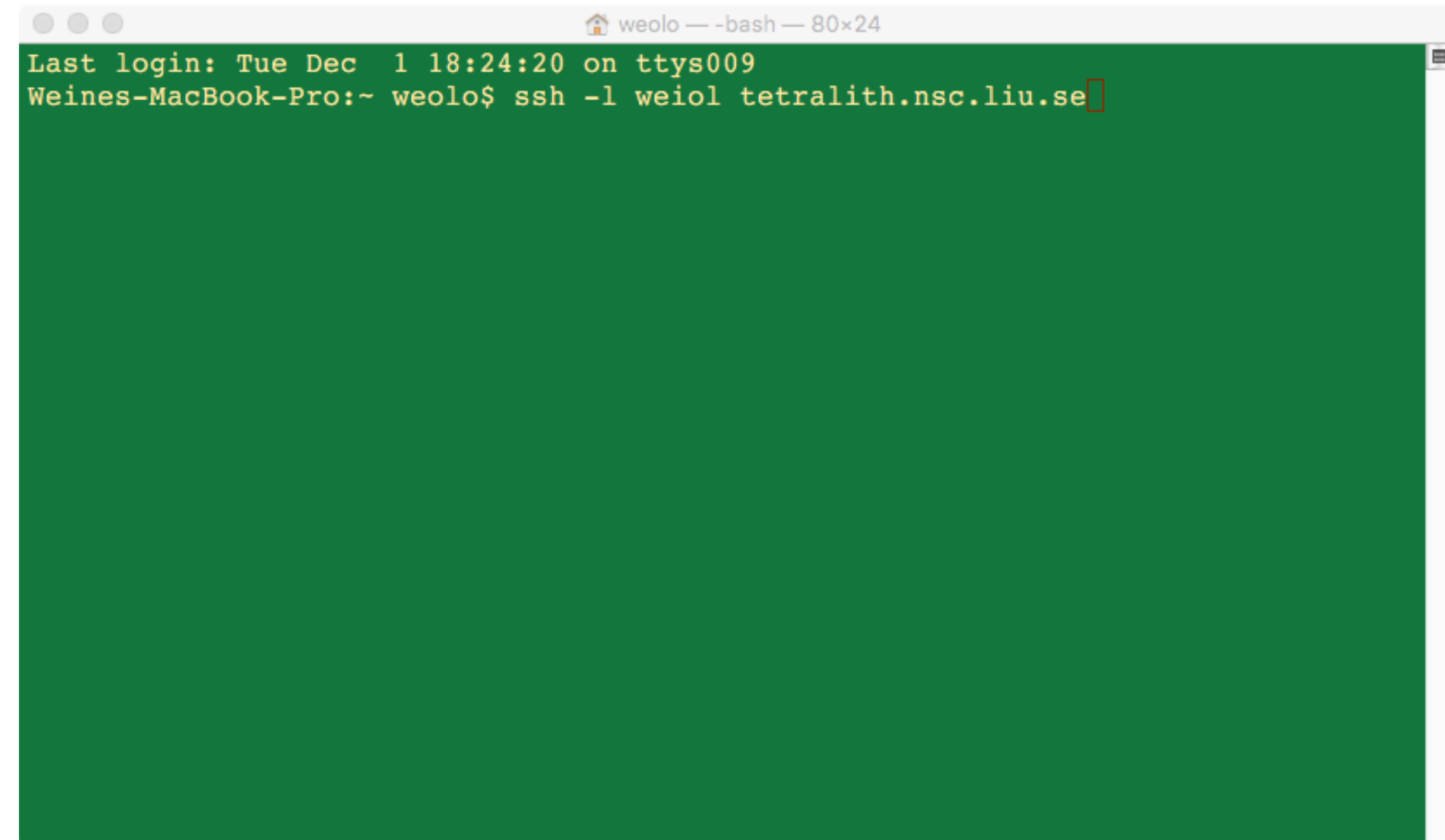
Typical login via terminal from Linux / Mac:

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

- Windows: can use PuTTY

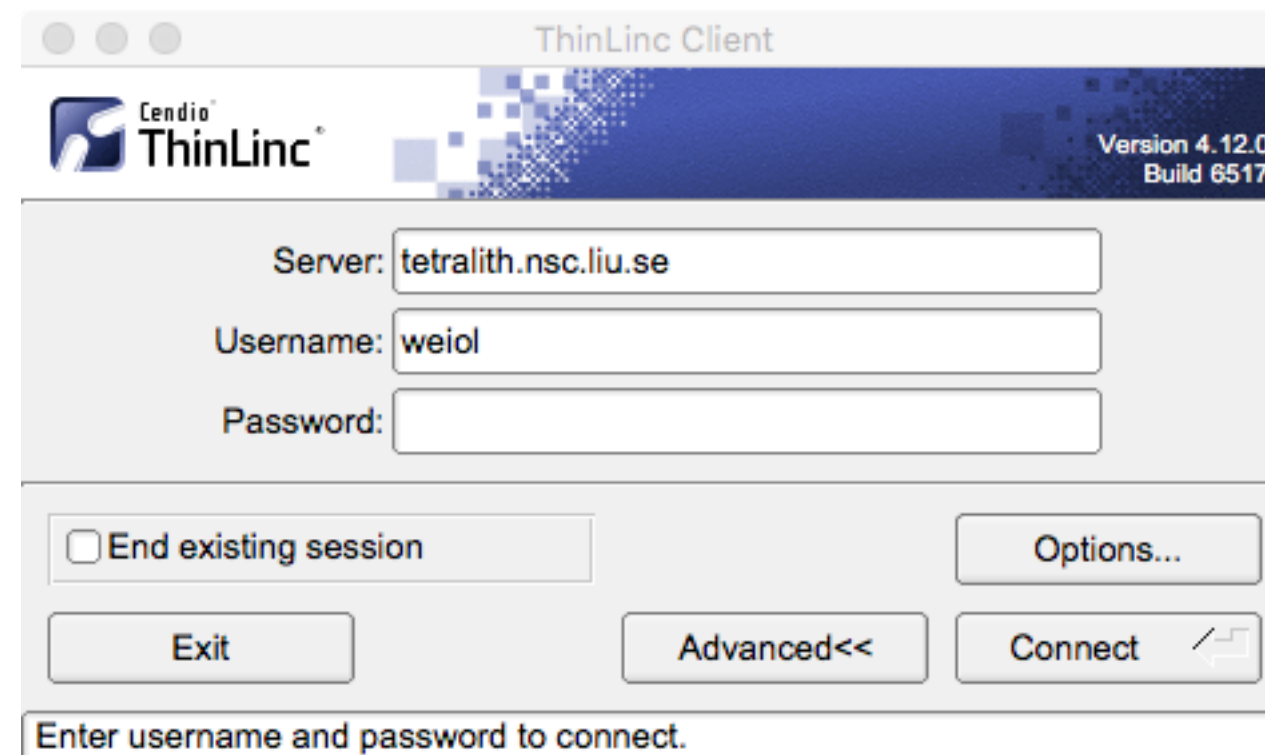
Note: to end up on a specific login node use:

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

A terminal window with a green background and white text. The window title is "weolo — -bash — 80x24". The terminal output shows "Last login: Tue Dec 1 18:24:20 on ttys009" followed by the prompt "Weines-MacBook-Pro:~ weolo\$". The user has entered the command "ssh -l weiol tetralith.nsc.liu.se" and the cursor is at the end of the line.

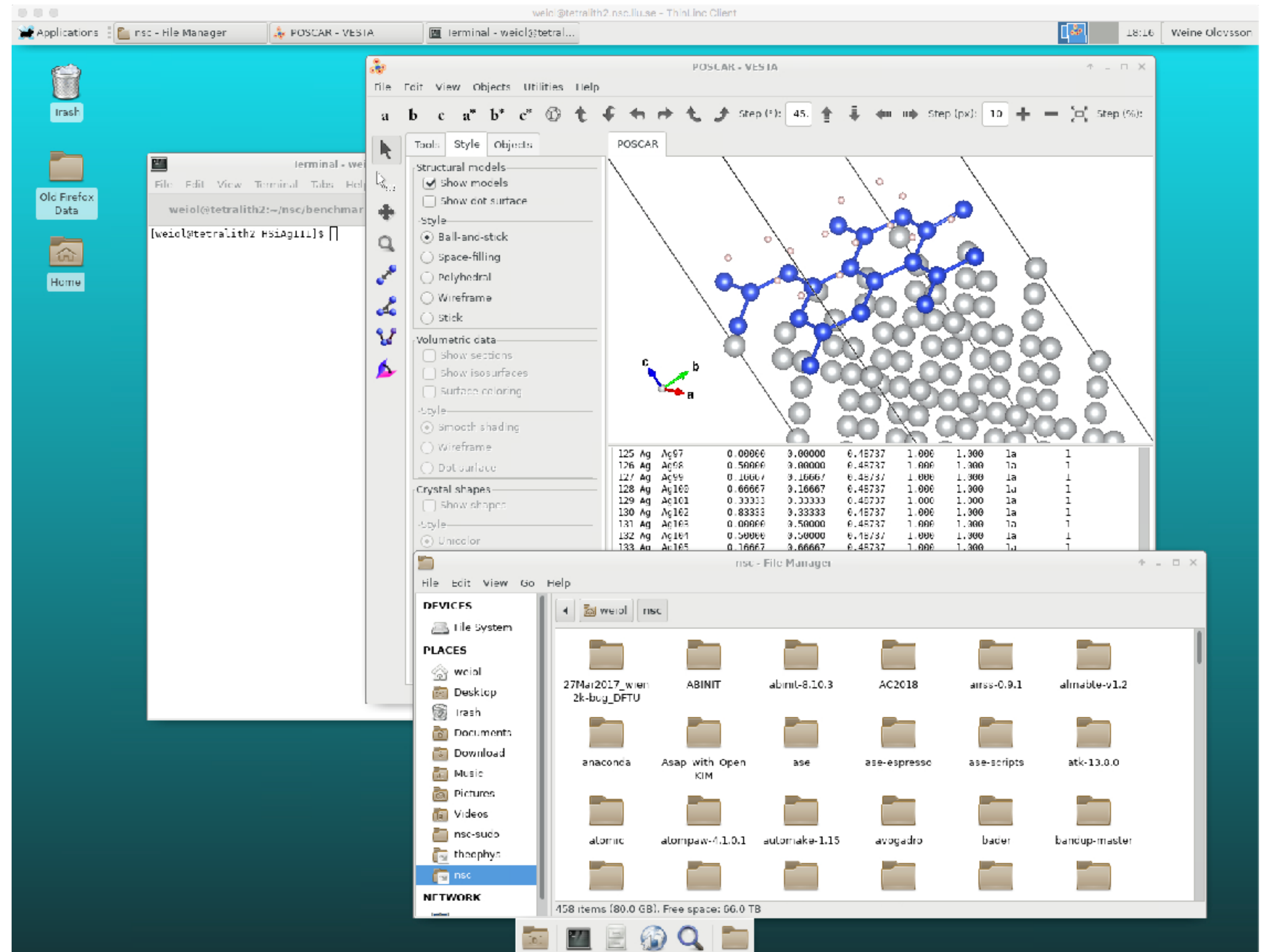
```
weolo — -bash — 80x24  
Last login: Tue Dec 1 18:24:20 on ttys009  
Weines-MacBook-Pro:~ weolo$ ssh -l weiol tetralith.nsc.liu.se
```

# Access to Tetralith: ThinLinc

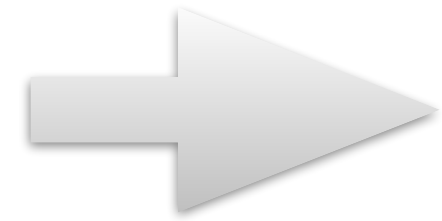


- ThinLinc - *virtual desktop*
- Persistent sessions (compare screen, tmux)
- Recommended for graphics
- Hardware acc. graphics (vglrun) in some cases

<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:

	Backup?	Snapshot?
1. Personal home directory, e.g. /home/x_user	yes!	yes!
2. Project storage, owned by PI, e.g. /proj/ourstuff	no!	yes!
3. Work node local disk (during runs)	no!	no!

### Some notes:

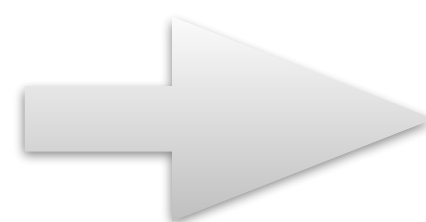
- Use `nscquota` to check available disk space
- Project storage is linked to specific project allocation and life time
- Good idea to have your own backup
- **Data is never 100% safe, there's always some risk**

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

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

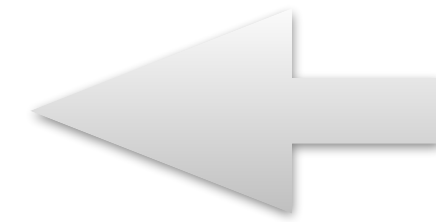
# Basic Security

- 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



Special wrappers/rec. e.g.: Gaussian

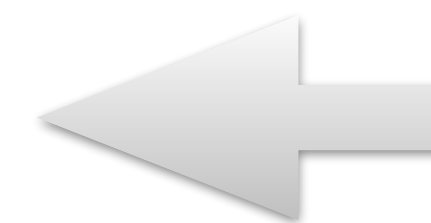
2. Check module system (module avail)

3. Ask NSC support

4. Build and install yourself

## 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

NSC Installed software

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

NSC

START SYSTEMS STORAGE SOFTWARE ABOUT USER AREA

Installed software Software installation policy Software licensing Compilers NSC build environment Modules

MPI libraries Math libraries Python at NSC

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 Bi and Nebula, please look at the list above (software present there that is not already on Bi/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](#).

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



# Software: Installation Webpage

The screenshot shows a web browser window with the URL <https://www.nsc.liu.se/software/catalogue/tetralith/>. The page header includes the NSC logo and navigation links for Tetralith, Sigma, Nebula, Bi, and Berzelius. The main heading is "Software on Tetralith and Sigma". Below this, there is explanatory text about software support tiers and a list of categories: All, Chem, Phys, Bio, CAE, Geo, Math, Devel, Data, Tools, Vis, Misc. A search bar is present with a red arrow pointing to it. A table lists various software packages with their descriptions and support tiers.

**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/sse/>. 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: 2022-10-26

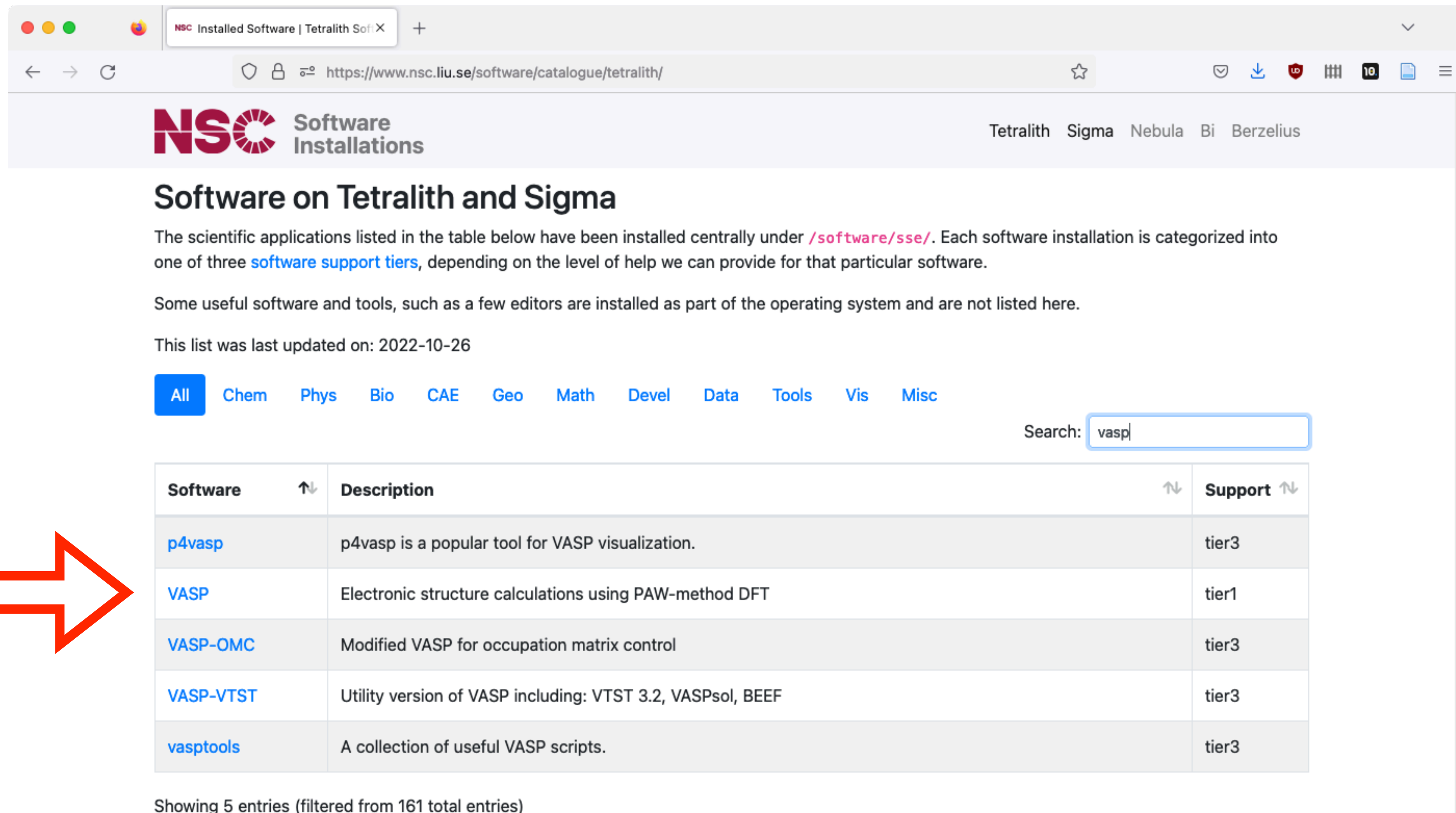
[All](#) [Chem](#) [Phys](#) [Bio](#) [CAE](#) [Geo](#) [Math](#) [Devel](#) [Data](#) [Tools](#) [Vis](#) [Misc](#)

Search:

Software	Description	Support
<a href="#">ABAQUS</a>	The Abaqus FEA software suite offers various tools for stress analysis, heat transfer, fluid mechanics <i>etc.</i>	tier3
<a href="#">ABINIT</a>	ABINIT calculates the total energy and properties of materials and molecules using, primarily, DFT.	tier2
<a href="#">allinea-DDT</a>	ARM/Allinea DDT is a debugging tool for scalar, multi-threaded and large-scale parallel applications.	tier2
<a href="#">allinea-forge</a>	ARM/Allinea DDT is a debugging tool for scalar, multi-threaded and large-scale parallel applications.	tier2
<a href="#">allinea-MAP</a>	ARM/Allinea MAP is a profiler for scalar, multi-threaded and large-scale parallel applications.	tier2
<a href="#">AlphaFold</a>	Implementation of the inference pipeline of AlphaFold v2.0.	tier3
<a href="#">Amber</a>	Amber is a suite of biomolecular simulation programs.	tier3
<a href="#">Anaconda</a>	The Anaconda Python distribution platform for Python and R scientific computing.	tier2

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

# Software: Installation Webpage



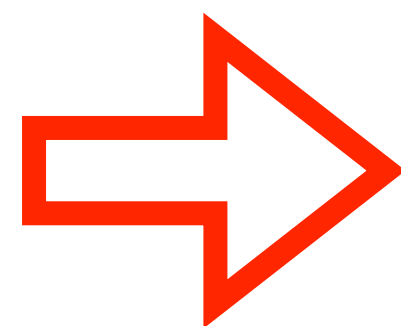
The screenshot shows a web browser window with the URL <https://www.nsc.liu.se/software/catalogue/tetralith/>. The page title is "NSC Software Installations". The navigation menu includes "Tetralith", "Sigma", "Nebula", "Bi", and "Berzelius". The main heading is "Software on Tetralith and Sigma".

The text explains that scientific applications are installed centrally under </software/sse/> and are categorized into three software support tiers. A note states that some useful software and tools are installed as part of the operating system and are not listed here. The list was last updated on 2022-10-26.

Navigation tabs include: All, Chem, Phys, Bio, CAE, Geo, Math, Devel, Data, Tools, Vis, Misc. A search bar contains the text "vasp".

Software	Description	Support
<a href="#">p4vasp</a>	p4vasp is a popular tool for VASP visualization.	tier3
<a href="#">VASP</a>	Electronic structure calculations using PAW-method DFT	tier1
<a href="#">VASP-OMC</a>	Modified VASP for occupation matrix control	tier3
<a href="#">VASP-VTST</a>	Utility version of VASP including: VTST 3.2, VASPsol, BEEF	tier3
<a href="#">vasptools</a>	A collection of useful VASP scripts.	tier3

Showing 5 entries (filtered from 161 total entries)



# Software: Installation Webpage

The screenshot shows a web browser window with the URL <https://www.nsc.liu.se/software/catalogue/tetralith/modules/vasp.html>. The page header includes the NSC logo and the text "Software Installations". Navigation links for "Tetralith", "Sigma", "Nebula", "Bi", and "Berzelius" are visible. The main content area is titled "VASP" and features a blue information banner stating "This software is under support tier 1!". Below this is a "Software description" section, followed by a "License" section with a note and a link to the licensing page. The "NSC documentation" section contains a yellow information banner with a red arrow pointing to the text "Please make sure to read our documentation: [VASP](#)". At the bottom, the "Available Modules" section lists several version identifiers.

**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/](http://www.nsc.liu.se/software/software-licensing/vasp/)

Homepage: [vasp.at/](http://vasp.at/)

### NSC documentation

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

### Available Modules

- [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](#)
- [6.2.1.29042021-omp-nsc1-intel-2018a-eb](#)
- [6.2.0.14012021-omp-nsc1-intel-2018a-eb](#)
- [6.1.2.25082020-omp-nsc1-intel-2018a-eb](#)
- [6.1.2.25082020-nsc1-intel-2018a-eb](#)
- [6.1.0.28012020-nsc1-intel-2018a-eb](#)

# Software: Installation Webpage

NSC VASP

https://www.nsc.liu.se/software/installed/tetralith/vasp/

NSC

START SYSTEMS STORAGE SOFTWARE ABOUT USER AREA

ABAQUS ABINIT AMBER ANSYS ANSYS-EM ASE ATAT Allinea Performance Reports Allinea-DDT  
Allinea/ARM-MAP CASTEP CDO CESM COMSOL CP2K CPMD DL\_POLY Dalton/LSDalton EC-Earth  
EPW Eik FERRET GPAW GROMACS 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 VMD VisIt WEST WIEN2K Yambo ecCodes  
exciting grib\_api netCDF p4vasp parallel phono3py phonopy vasptools Schrödinger suite **VASP**  
Clang Gaussian and GaussView

NSC / Software / Installed software / / VASP

## VASP Installations on Tetralith & Sigma

First of all, **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.

### VASP6

VASP6 was released in beginning of 2020. This means e.g. that VASP5 license holders will need to update their license in order to access VASP6 installations at NSC. If you have a VASP 5.4.4 license, you are typically covered for updates of VASP 6.X.X for three years, check your license for the exact details.

### Documentation

# Software: Module System

<b>module help ...</b>	Show information for module ...
<b>module avail</b>	List available modules
<b>module avail ...</b>	Search after module containing ... in its name
<b>module add ...</b>	Add a module (same as module load ...)
<b>module list</b>	List your loaded modules
<b>module rm ...</b>	Remove the ... module
<b>module purge</b>	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".

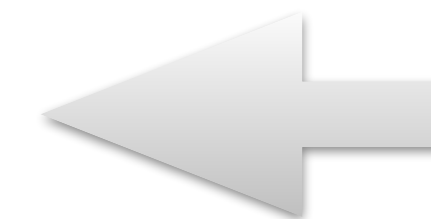
```
[weiol@tetralith2 ~]$
```

<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:

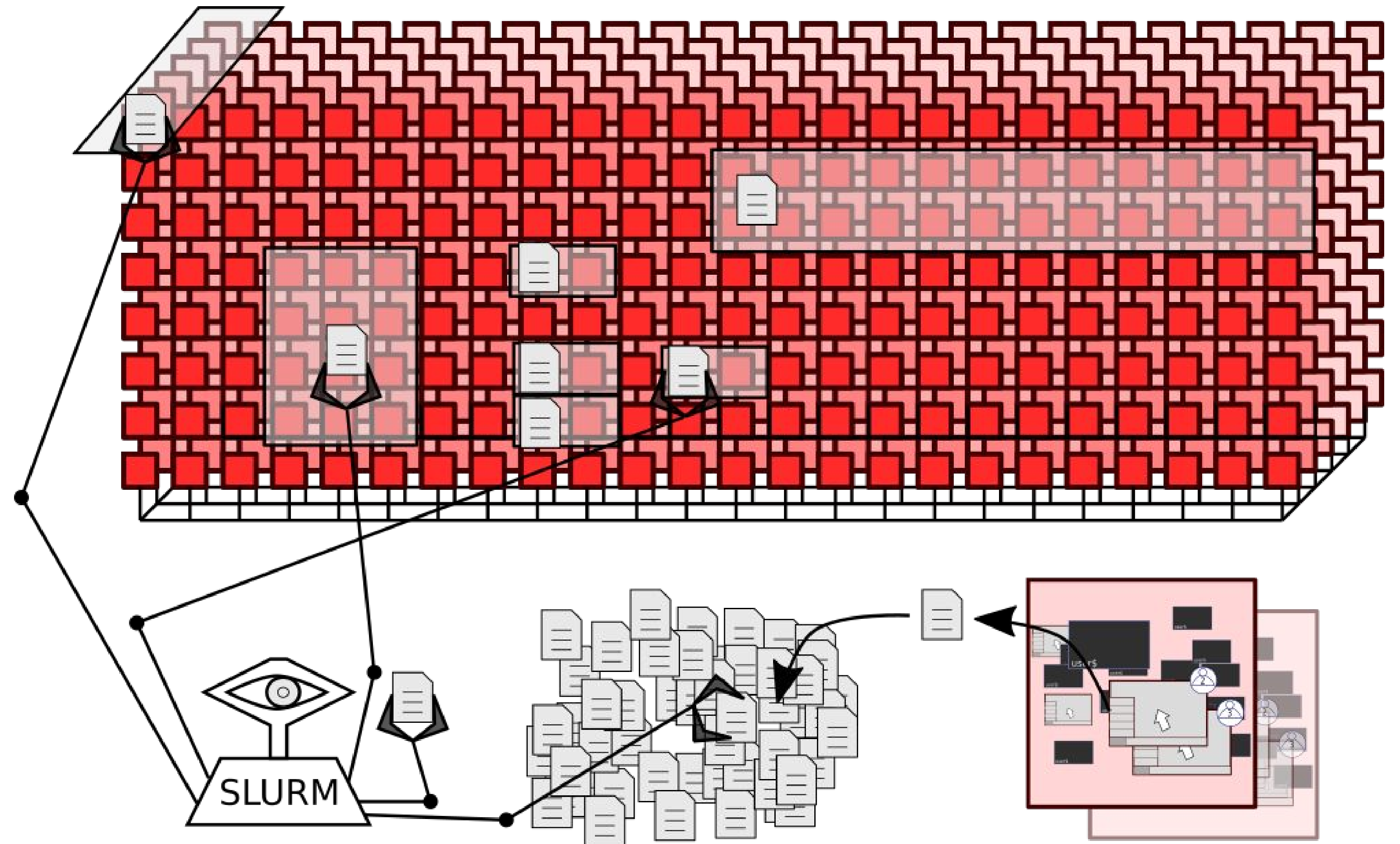
**S:** Module is Sticky, requires `--force` to unload or purge

**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



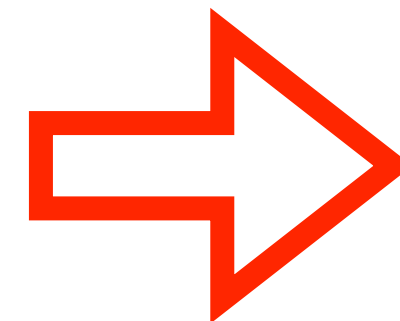
# Slurm: Running Batch Job

- 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 ...
```

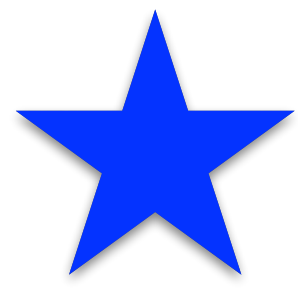
This is a helper program to figure out what MPI launcher to use, with which arguments, in what environment (including which HPC modules to load) when launching a binary or script that uses MPI.

positional arguments:

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

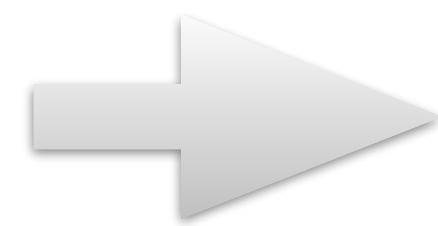
...

+ 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?



[support@nsc.liu.se](mailto:support@nsc.liu.se)

<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 [support@nsc.liu.se](mailto:support@nsc.liu.se) for help/questions



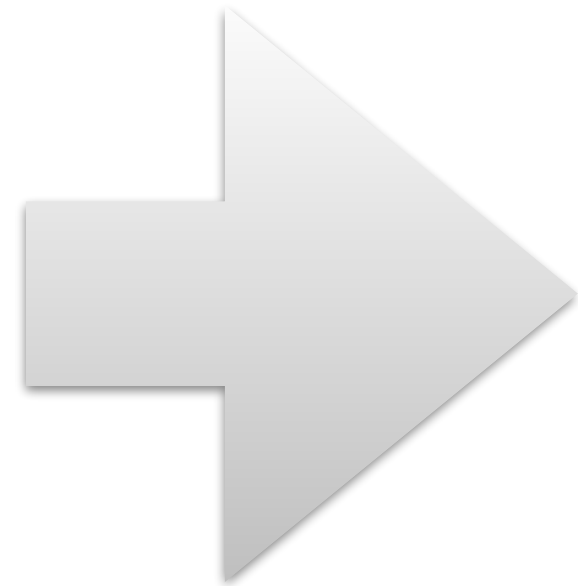
# Best Practices & Suggestions

## Common problems:

- My job **failed/crashed**. What now?
  - First, try to understand the cause
  - Contact [support@nsc.liu.se](mailto:support@nsc.liu.se) / fill in form <https://supr.naiss.se>
    - ➔ [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](#)