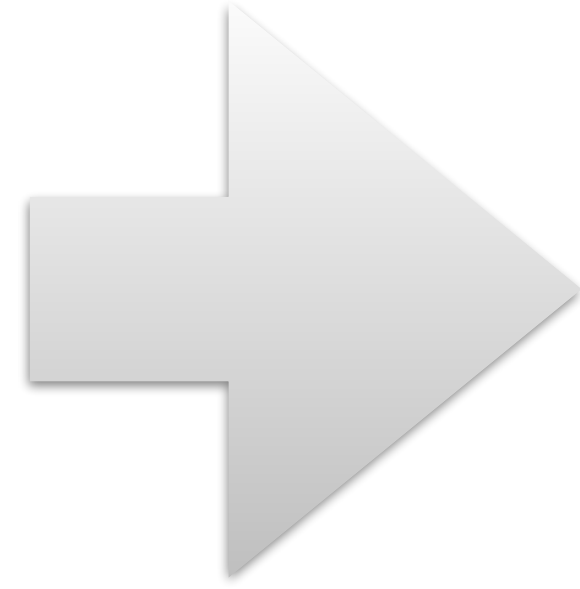


NSC introduction to Tetralith/Sigma

National Supercomputer Centre (NSC), Linköping University

SNIC training, online @NSC 16th Nov 2022, 10:00 - ca. 12:00

Information / Schedule




https://www.nsc.liu.se/support/Events/NSC_intro_Nov2022/

- 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:

-  **SNIC** Swedish National Infrastructure for Computing (10 Univ.)
- **li.u** LINKÖPING UNIVERSITY liu.se

1983 - SAAB buys Cray1

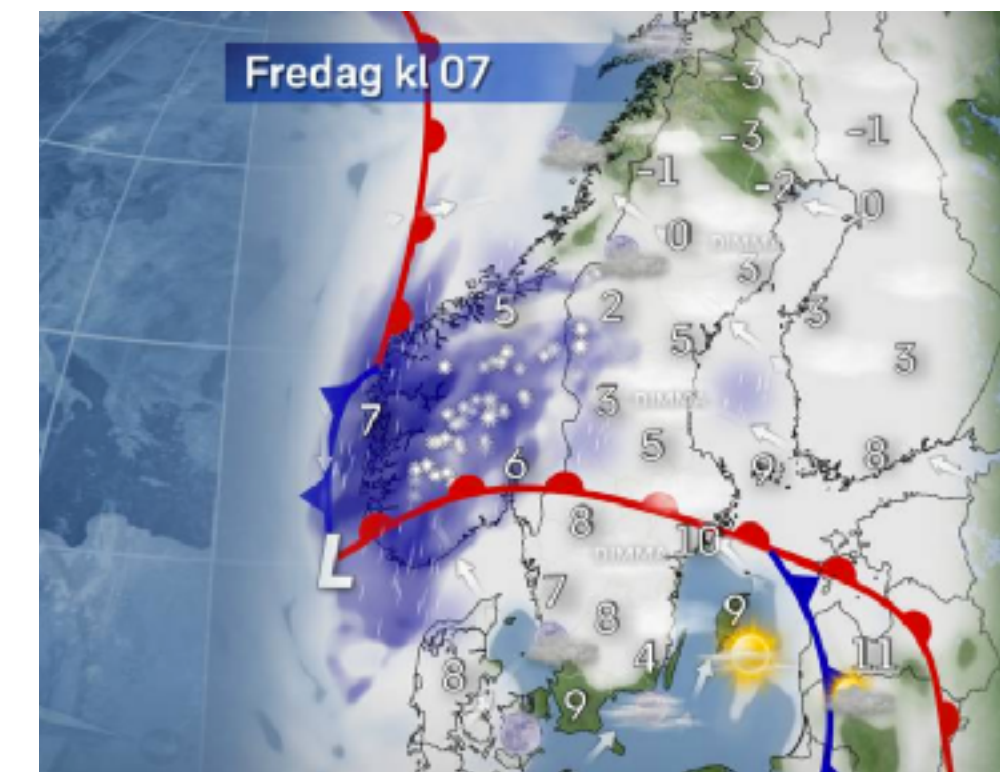


1989 - NSC first supercomputer centre in Sweden / SAAB partner

1996 - SMHI partner



2016 - MET Norway partner



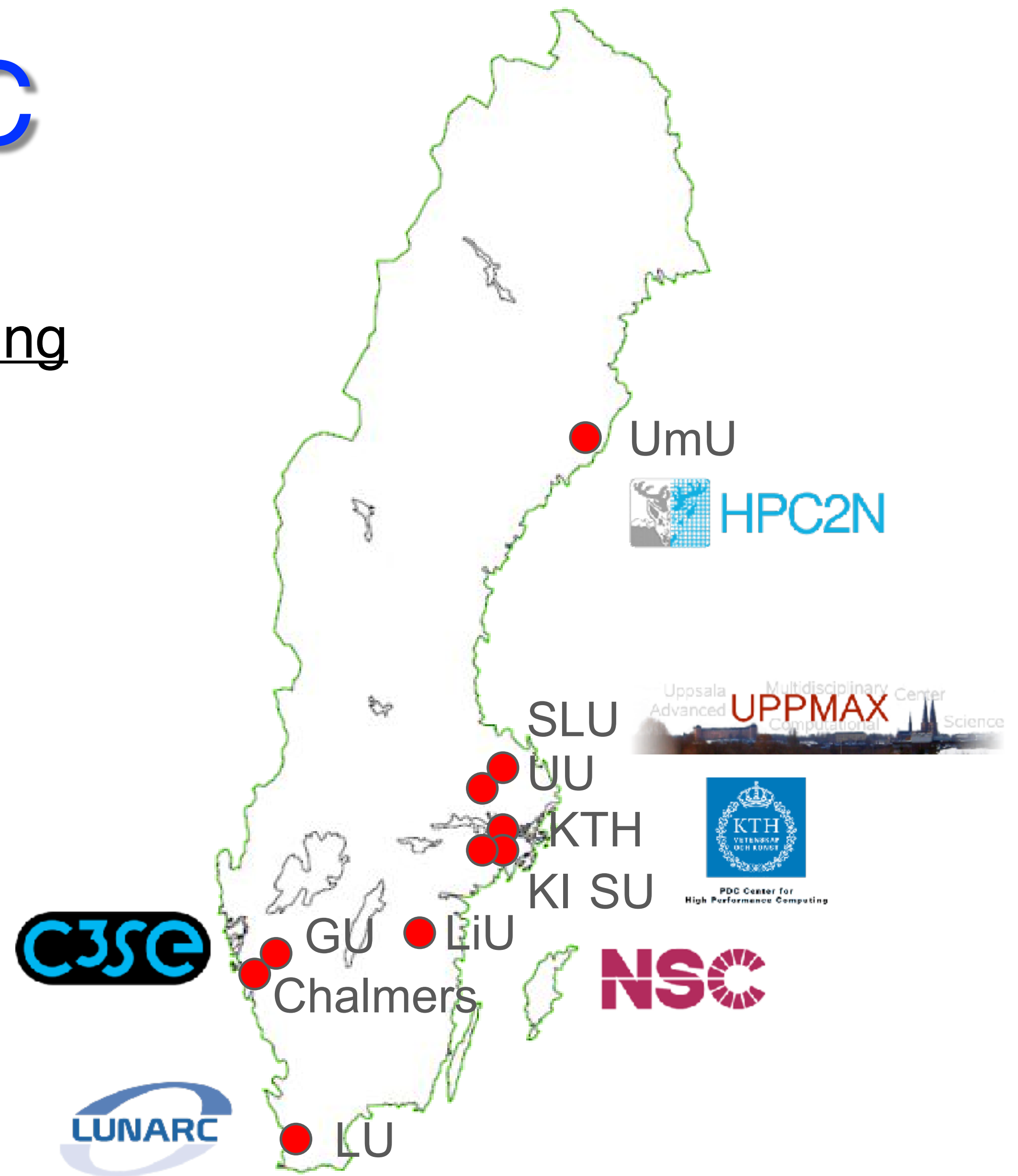


SNIC

Swedish National Infrastructure for Computing

10 universities & 6 HPC centers:

- Chalmers [C3SE](#)
- Göteborg
- Karolinska
- KTH [PDC](#)
- Linköping [NSC](#)
- Lund [LUNARC](#)
- SLU
- Stockholm
- Umeå [HPC2N](#)
- Uppsala [UPPMAX](#)



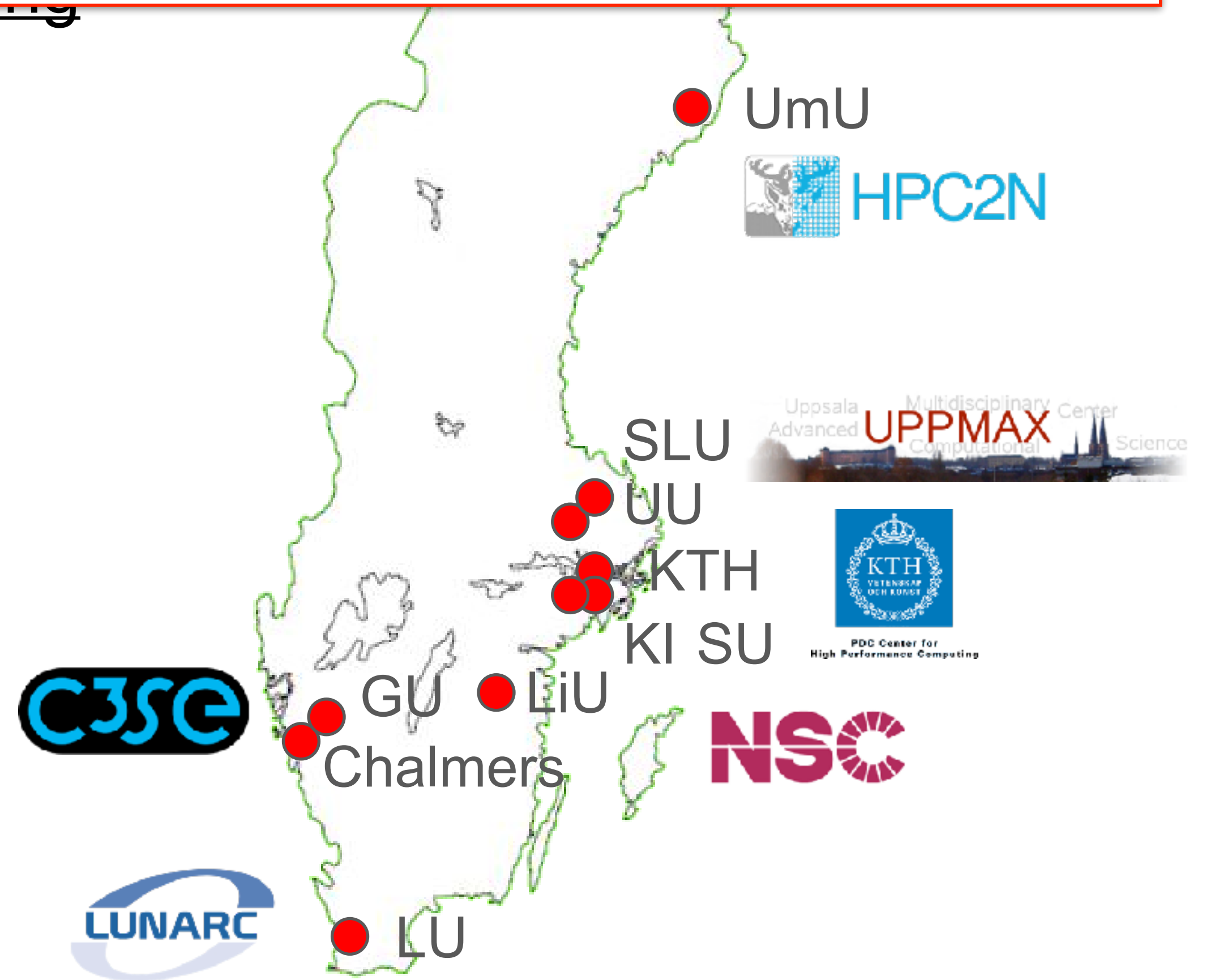
New organization 2023-01-01:

National Academic Infrastructure for Supercomputing in Sweden (NAISS)

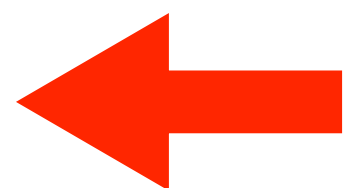
- Continues work of SNIC, <https://www.naiss.se/>

10 universities & 6 HPC centers:

Chalmers	C3SE
Göteborg	
Karolinska	
KTH	PDC
Linköping	NSC
Lund	LUNARC
SLU	
Stockholm	
Umeå	HPC2N
Uppsala	UPPMAX



<https://snic.se/>



See SNIC newsletters!

ing: 10 univ. + Vetenskapsrådet (VR)

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 (SNIC, local and other)

NSC Academic Clusters

32 cores/node

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



(2020 -) 170 x T4 GPU-nodes

Top500 no. 183 (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

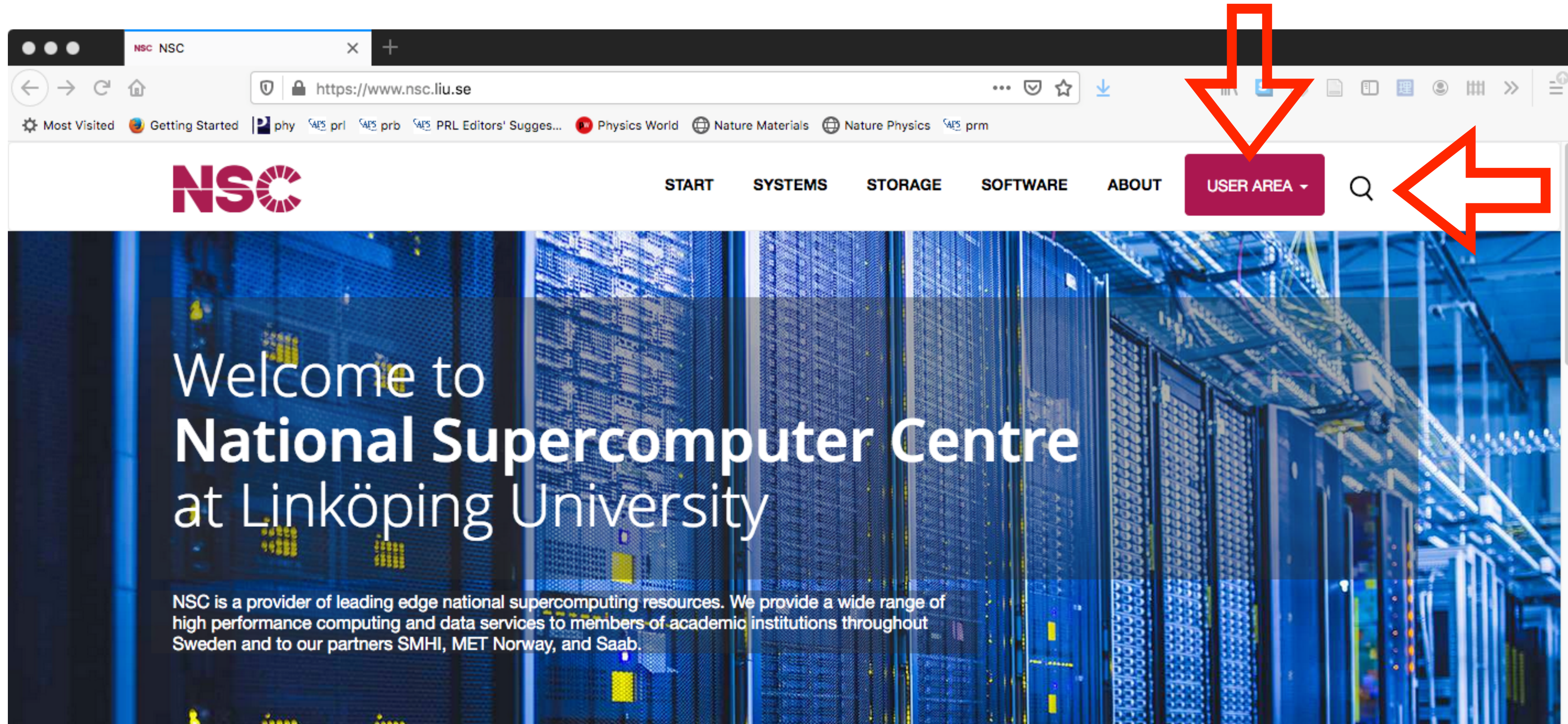


*Knut and Alice
Wallenberg
Foundation*



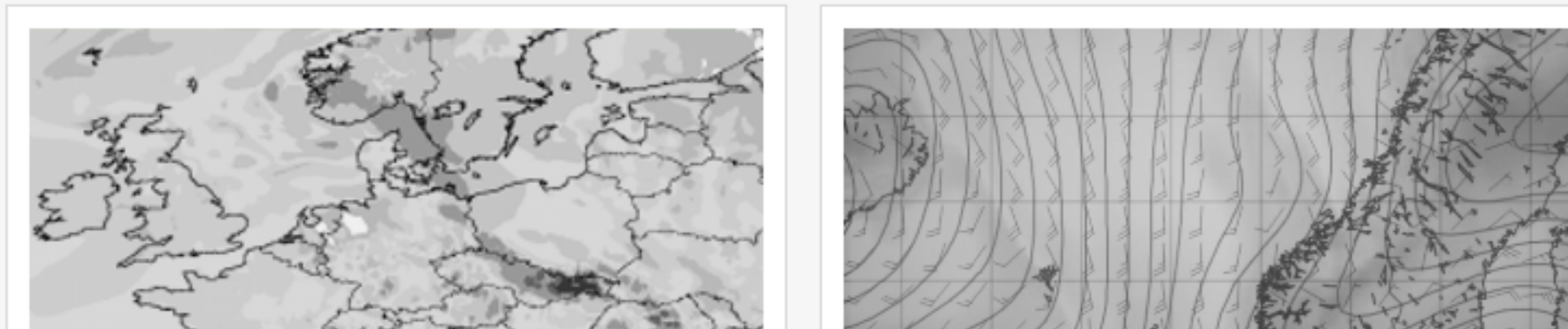
Top500 no. 102 (83)

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 screenshot shows a web browser window with the URL <https://www.nsc.liu.se/support/>. The browser's address bar and tabs are visible at the top. The website's header features the NSC logo on the left and a navigation menu with links for START, SYSTEMS, STORAGE, SOFTWARE, ABOUT, and a highlighted USER AREA dropdown menu. A search icon is also present in the header.

Below the header, the breadcrumb path reads "NSC / User support". The main content area is a light gray box with the following text:

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

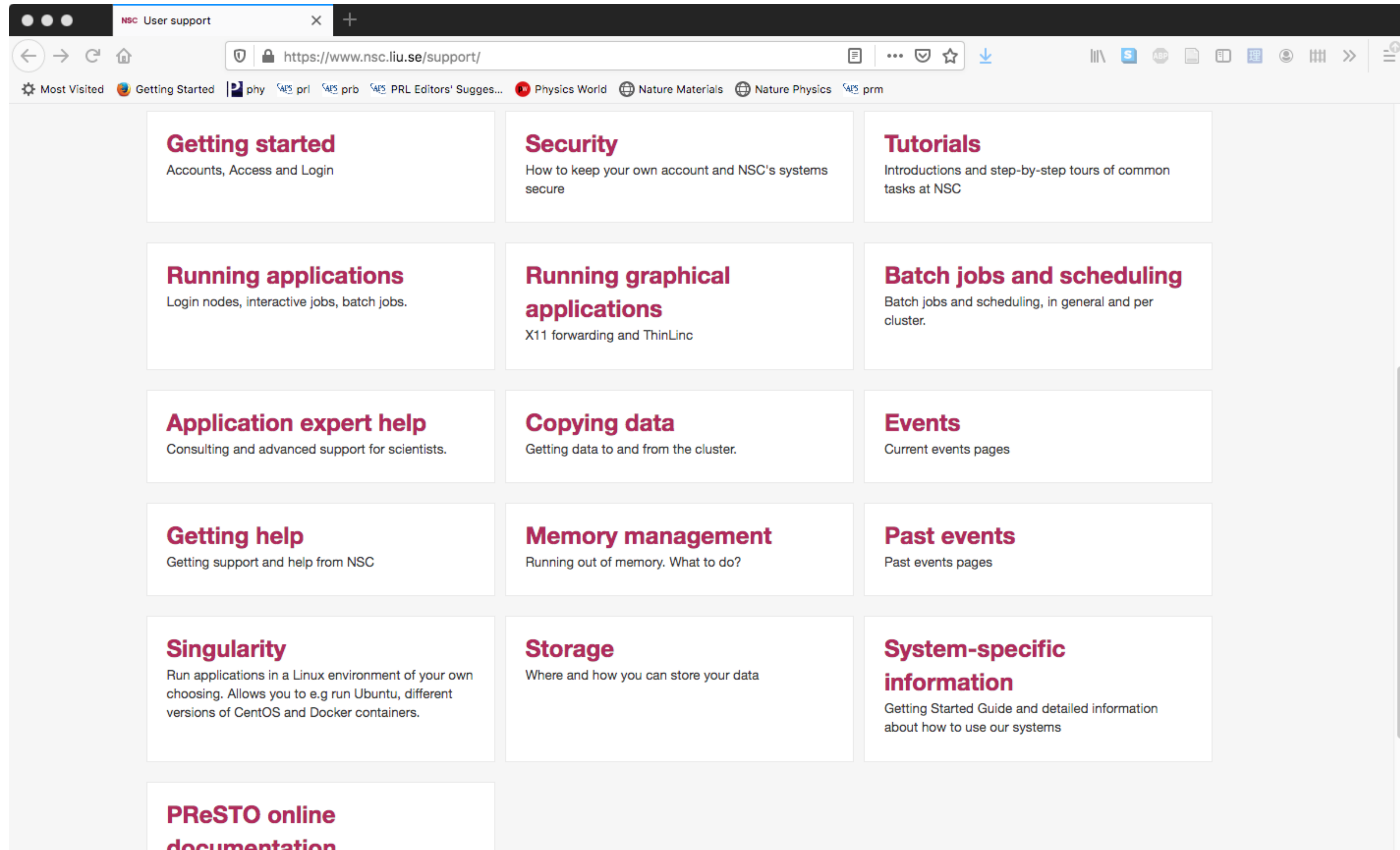
For SMHI, MetCoOp and MET users: smhi-support@nsc.liu.se

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

At the bottom of the page, there are six white boxes with red headings and black text:

- 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 14 categories, 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**: 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**: (partially visible)

Getting Access to HPC - SUPR

SNIC SUPR

Start
Rounds
Support
Login

Your are not logged in.

SUPR - SNIC User and Project Repository

SUPR is the SNIC 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 SNIC Projects

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

Current SNIC User Agreement

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

Handling of personal data within SNIC

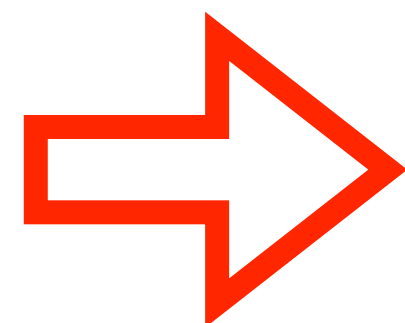
You can read about the [handling of personal data within SNIC](#) at the SNIC site without logging in.

<https://supr.snic.se>

Support via SUPR

The screenshot shows a web browser window with the URL <https://supr.snic.se>. The page title is "SUPR - Weine Olovsson". The sidebar on the left contains the following navigation links: Admin, User, Start, Proposals, Rounds, Projects, Groups, Accounts, Personal Information, Support, and Logout. The main content area displays an "Activity Report Wanted" section with a table of project data.

Project	Project Title	Project Type	End Date
SNIC 2020/13-76	VASP workshop at NSC 19-20th Oct 2020	SNIC Small Compute	2020-12-01



Support via SUPR

The screenshot shows a web browser window with the URL <https://supr.snic.se/support/>. The page features the SNIC SUPR logo and a navigation menu with 'Admin' and 'User' tabs. The 'User' tab is active. The main content area is titled 'Support' and contains instructions for using the support form. It includes a 'Problem Type' section with a dropdown menu, a 'Centre and Resource' section with a dropdown menu, and a 'Project' section with a dropdown menu. A 'Summary' section is also visible at the bottom. The left sidebar contains links for 'Start', 'Proposals', 'Rounds', 'Projects', 'Groups', 'Accounts', 'Personal Information', 'Support', and 'Logout'. The user is logged in as 'Weine Olovsson' with the email 'weolo@ifm.liu.se'.

Support

Start / Support

Support

Use this form to request support for SNIC 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 weolo@ifm.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

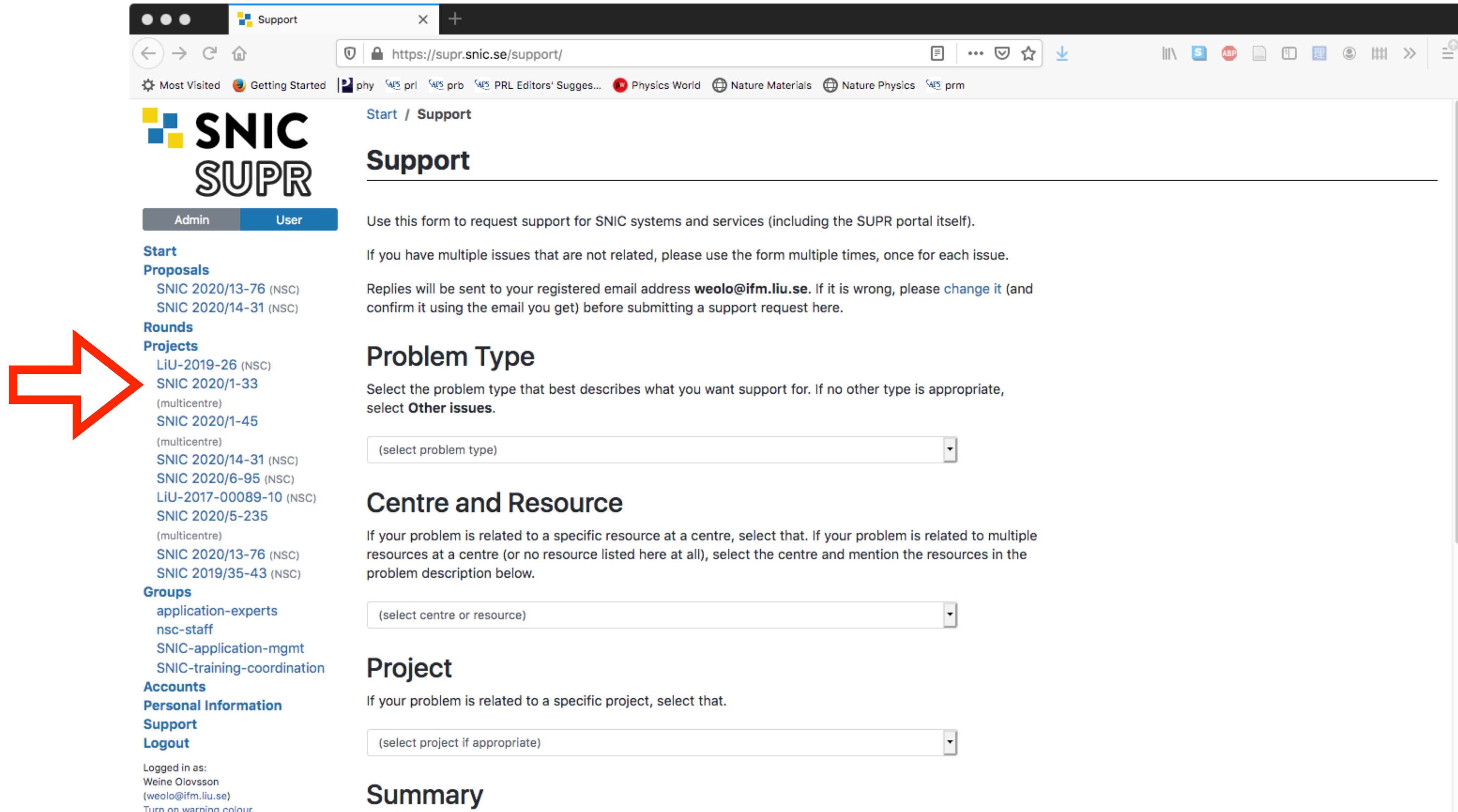
If your problem is related to a specific project, select that.

(select project if appropriate)

Summary

Logged in as:
Weine Olovsson
(weolo@ifm.liu.se)
[Turn on warning colour](#)

Projects in SUPR



The screenshot shows a web browser window with the URL <https://supr.snic.se/support/>. The page features the SNIC SUPR logo and a navigation menu with 'Admin' and 'User' tabs. The 'User' tab is active, and the 'Projects' link in the sidebar is highlighted with a red arrow. The main content area contains instructions for using the support form, a 'Problem Type' dropdown menu, a 'Centre and Resource' dropdown menu, and a 'Project' dropdown menu. The 'Summary' section is partially visible at the bottom.

Start / Support

Support

Use this form to request support for SNIC 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 weolo@ifm.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

Start

Proposals

- [SNIC 2020/13-76 \(NSC\)](#)
- [SNIC 2020/14-31 \(NSC\)](#)

Rounds

Projects

- [LiU-2019-26 \(NSC\)](#)
- [SNIC 2020/1-33 \(multicentre\)](#)
- [SNIC 2020/1-45 \(multicentre\)](#)
- [SNIC 2020/14-31 \(NSC\)](#)
- [SNIC 2020/6-95 \(NSC\)](#)
- [LiU-2017-00089-10 \(NSC\)](#)
- [SNIC 2020/5-235 \(multicentre\)](#)
- [SNIC 2020/13-76 \(NSC\)](#)
- [SNIC 2019/35-43 \(NSC\)](#)

Groups

- [application-experts](#)
- [nsc-staff](#)
- [SNIC-application-mgmt](#)
- [SNIC-training-coordination](#)

Accounts

Personal Information

Support

Logout

Logged in as:
Weine Olovsson
(weolo@ifm.liu.se)
[Turn on warning colour](#)

Projects in SUPR

Electronic theory of materials p. X

https://supr.snic.se/project/15055/

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 2020/6-95	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.

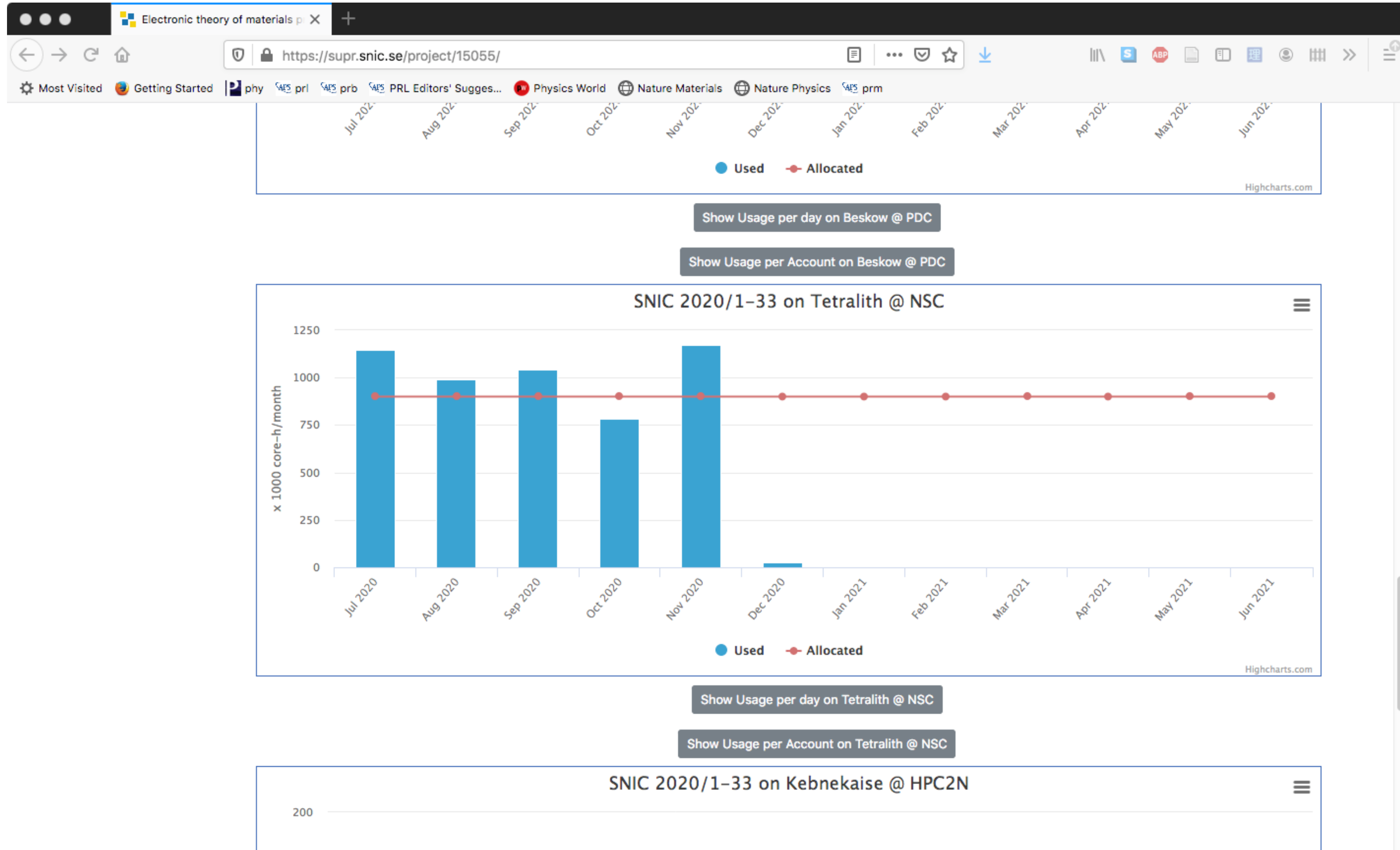
Resource	Allocation Unit	Total Usage	Allocation until Today	Percentage	Total Allocation	Percentage
Beskow @ PDC	1 400 x 1000 core-h/month	6 797.0	7 000.0	97.1 %	16 800.0	40.5 %
Tetralith @ NSC	900 x 1000 core-h/month	5 163.2	4 500.0	114.7 %	10 800.0	47.8 %
Kebnekaise @ HPC2N	150 x 1000 core-h/month	554.7	750.0	74.0 %	1 800.0	30.8 %
Tegner @ PDC	23 x 1000 core-h/month	0.0	115.0		276.0	

Storage

Percentage field to the right, compares **Usage** with the allocation. **Last Updated** shows the time at which the usage was last updated.

Resource	Allocation	Usage	Unit	Percentage	Allocation	Usage	Unit	Percentage	Last Updated
Centre Storage @ NSC	0		GiB		0		files		

Projects in SUPR



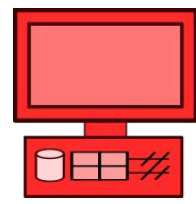
When & Why to use HPC?

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

Tetralith: 1908 nodes, Sigma: 110 nodes



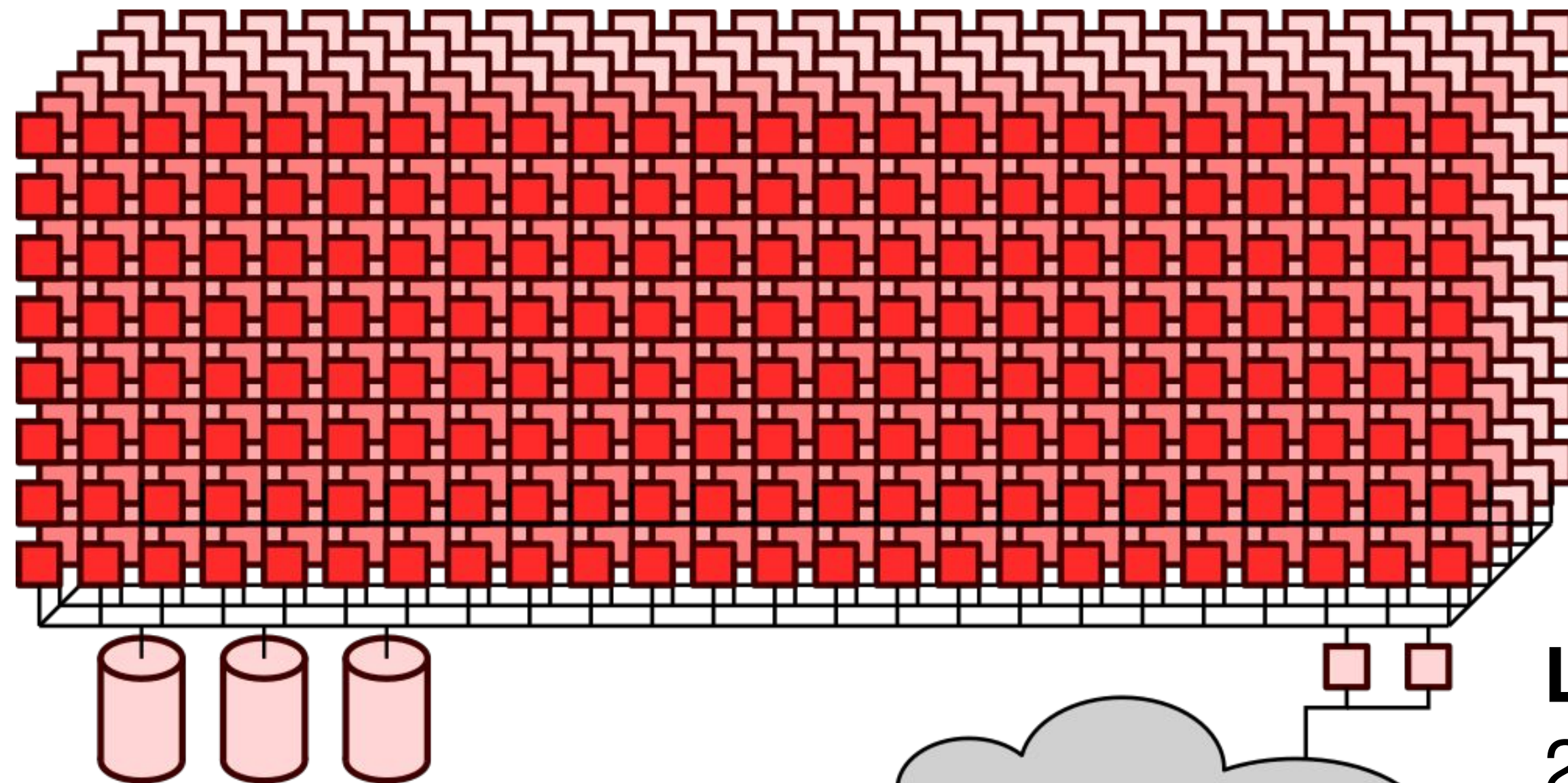
Desktop/laptop:

8 cores

16 GB RAM

Windows, MacOS (Unix), Linux

1 user



Work node:

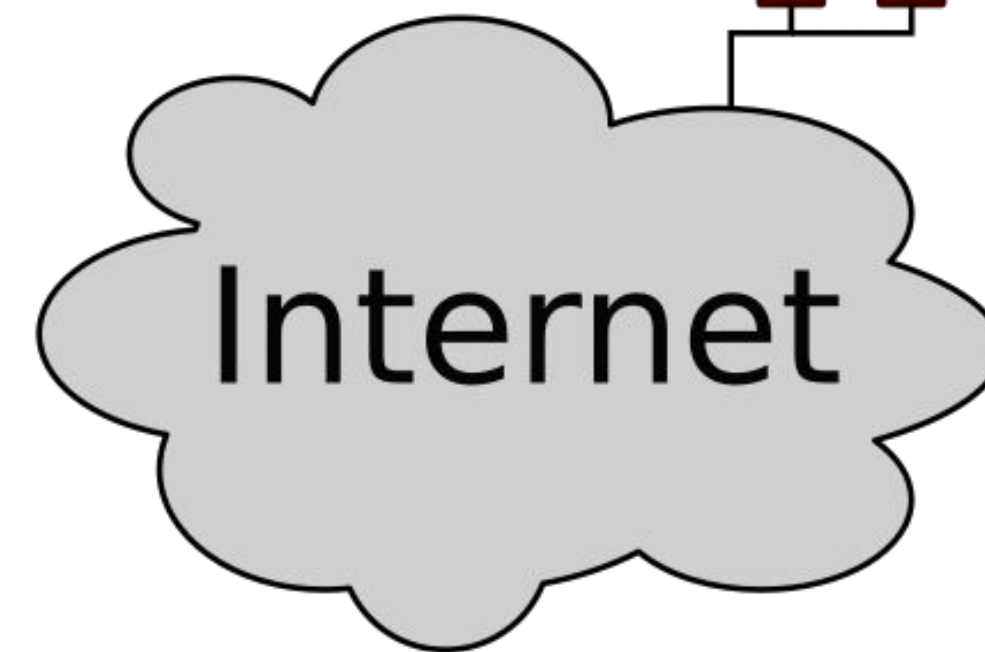
32 cores

96 (384) GB RAM

Linux

Omni-Path network

1 - few users at a time



Login nodes:

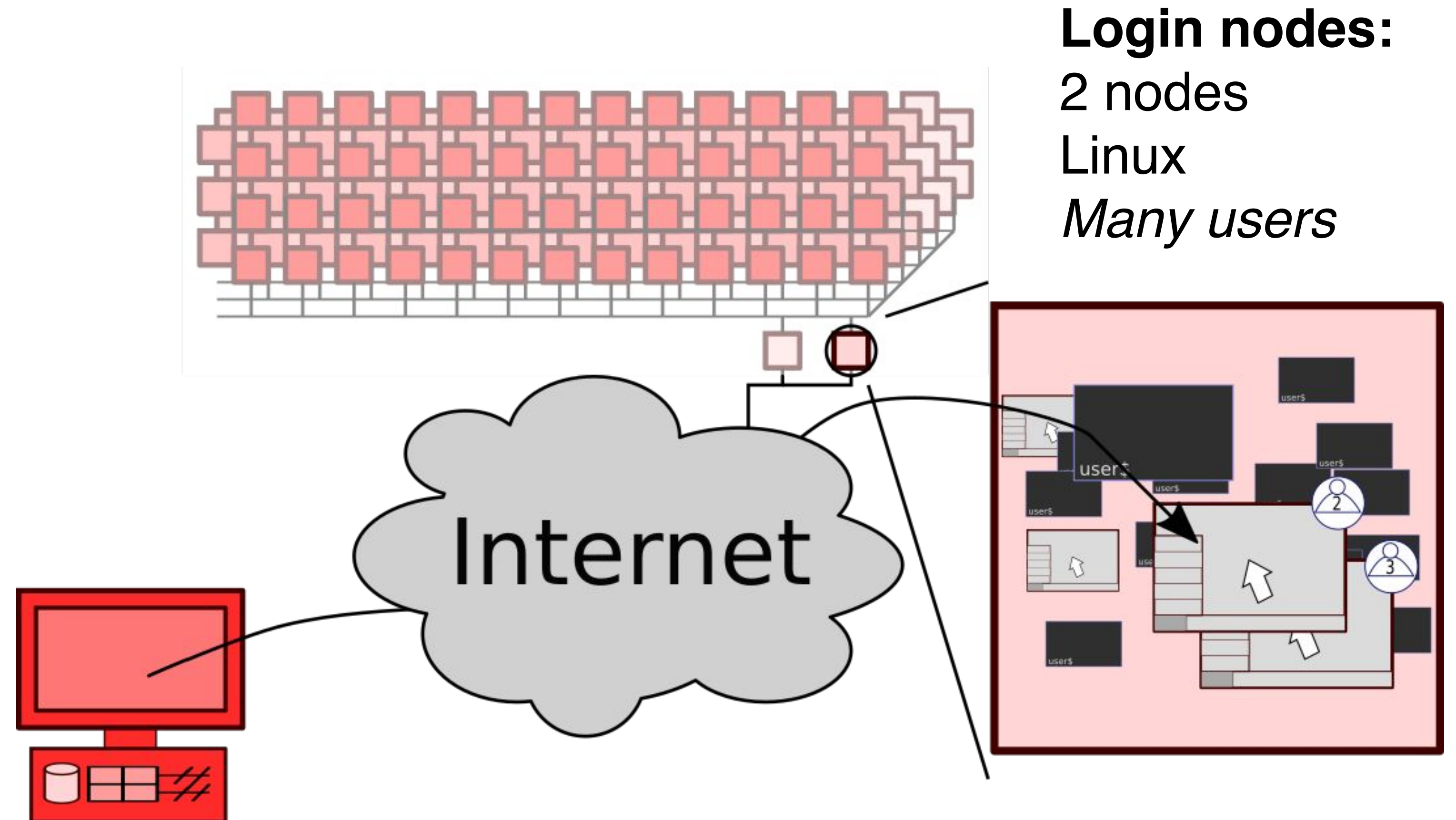
2 nodes

Linux

Many users

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

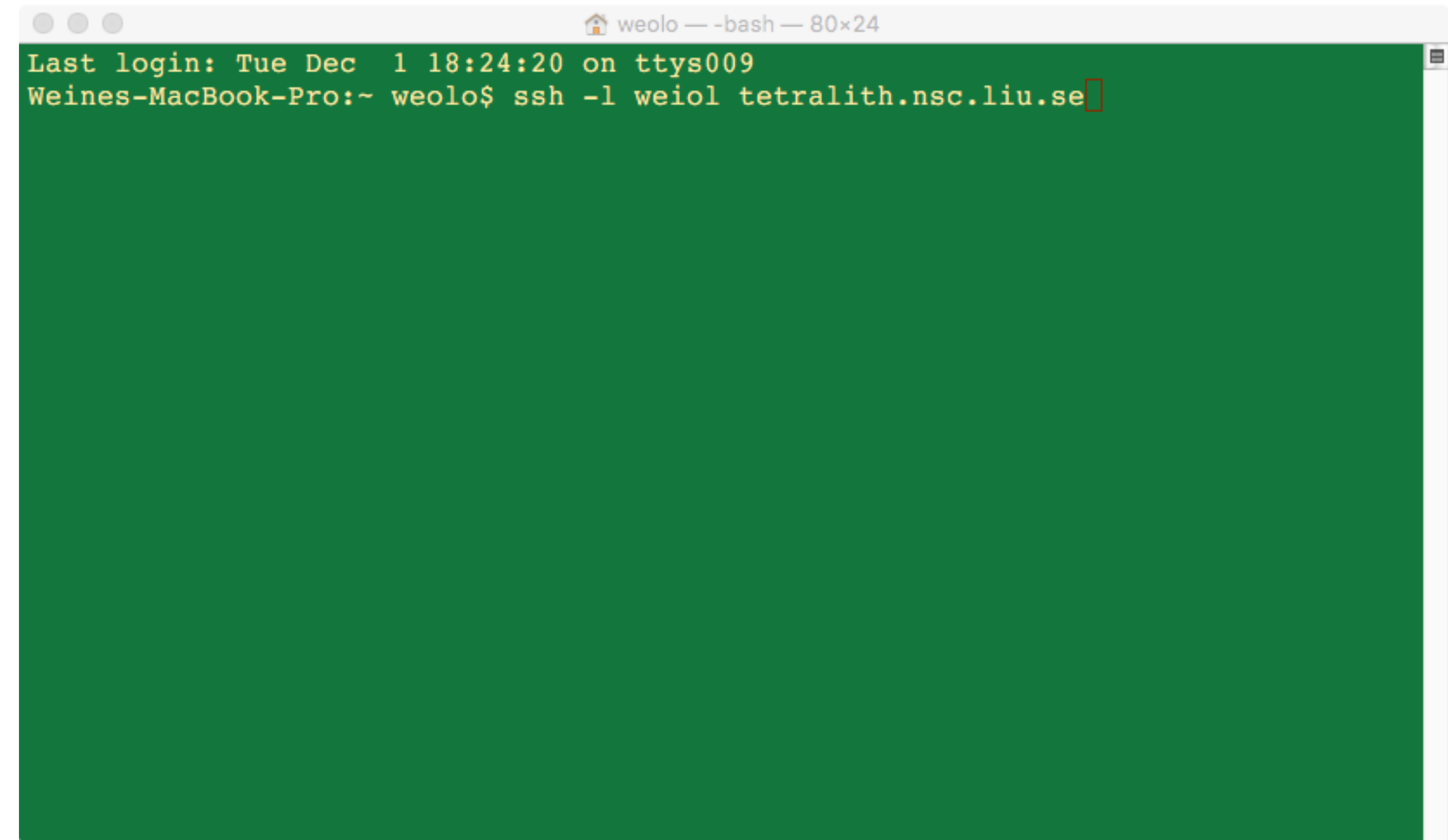
Typical login via terminal from Linux / Mac:

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

- Windows: can use PuTTY

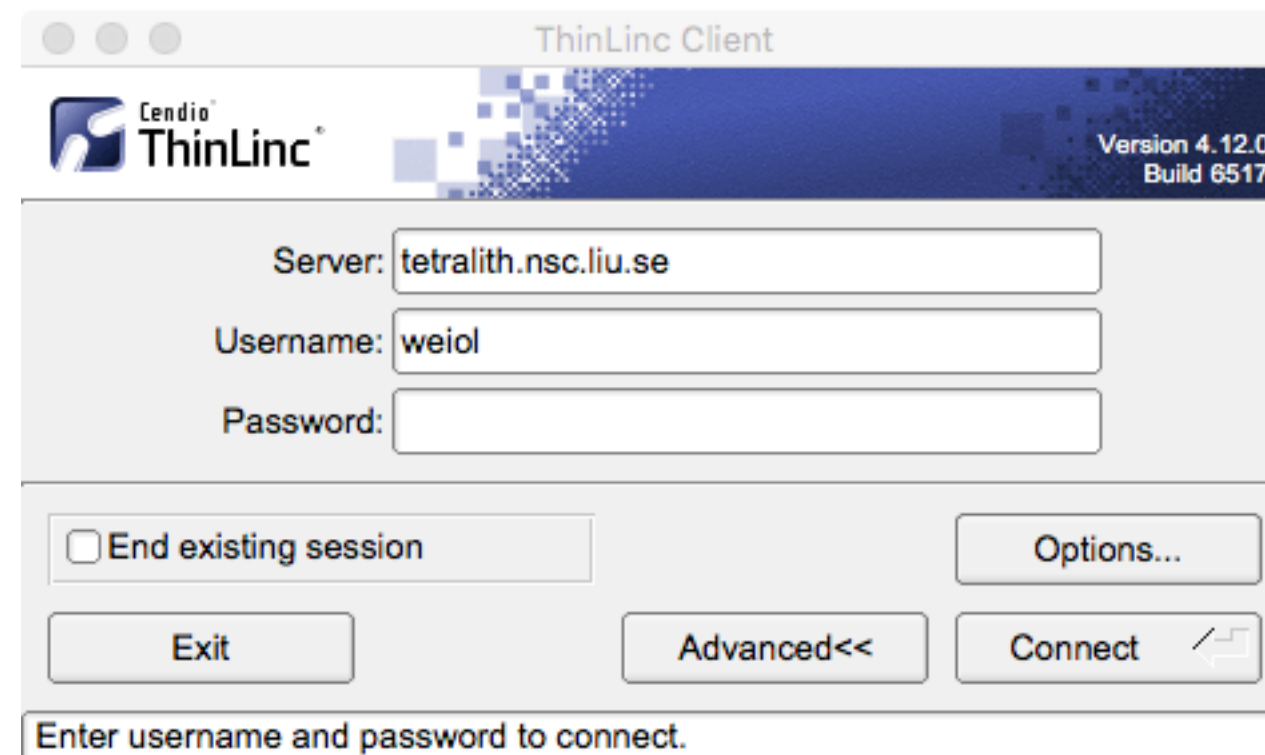
Note: to end up on a specific login node use:

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

A terminal window with a dark 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.

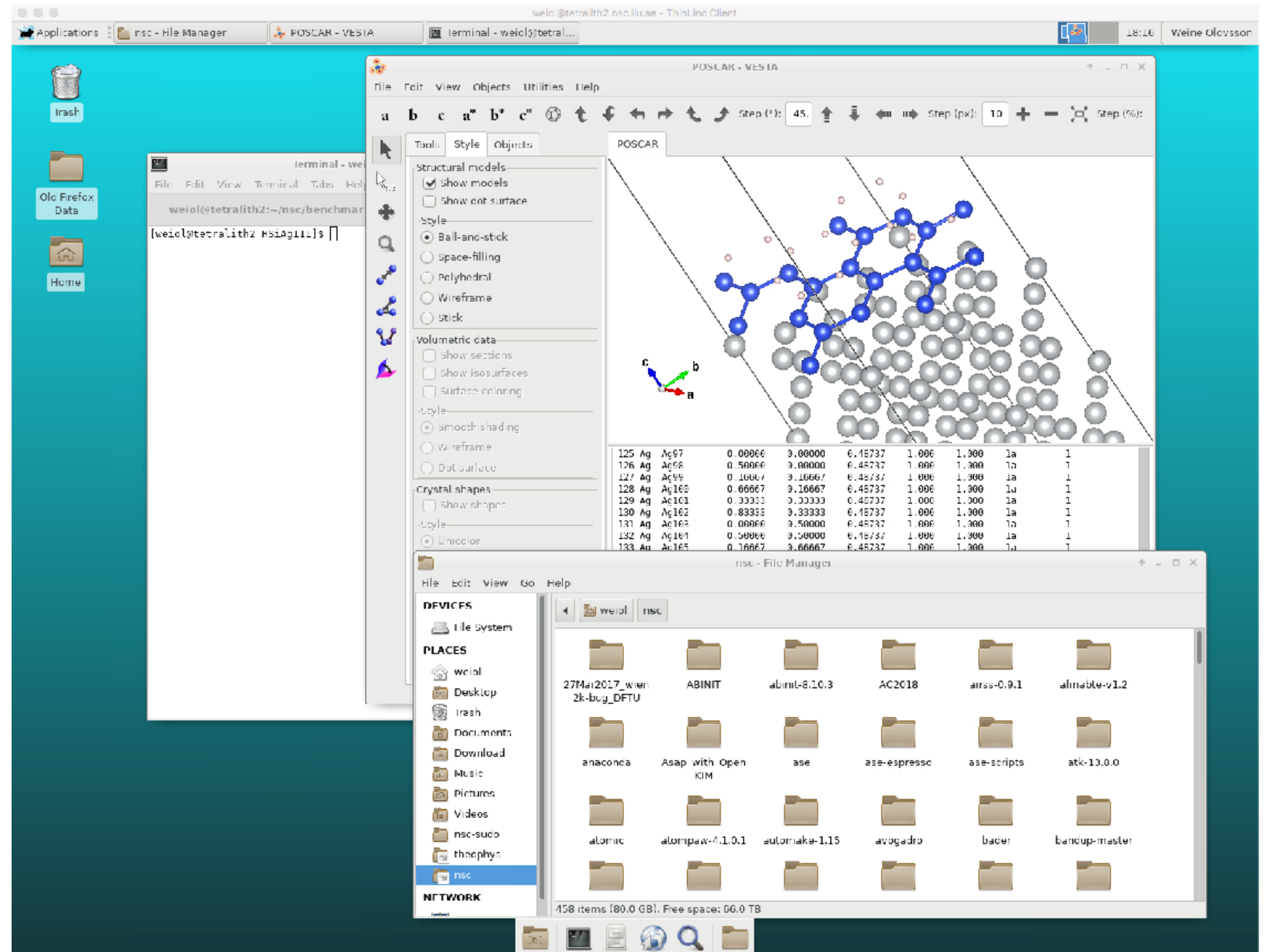
```
weolo - bash - 80x24  
Last login: Tue Dec 1 18:24:20 on ttys009  
Weines-MacBook-Pro:~ weolo$ ssh -l weiol tetralith.nsc.liu.se
```

Access to Tetralith: ThinLinc

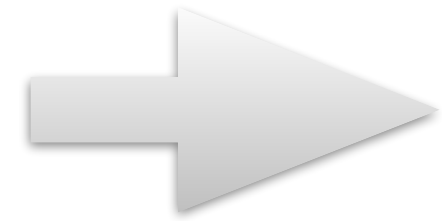


- ThinLinc - *virtual desktop*
- Persistent sessions (compare screen, tmux)
- Recommended for graphics
- Hardware acc. graphics (vglrun) in some cases

<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: `snicquota`

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:

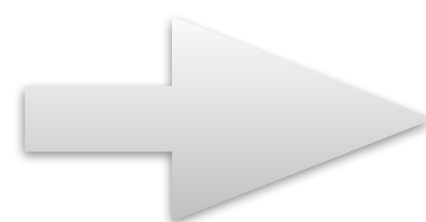
- Use `snicquota` to check available disk space
- Project storage is linked to specific project allocation and life time
- Good idea to have your own backup
- **Data is never 100% safe, there's always some risk**

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

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

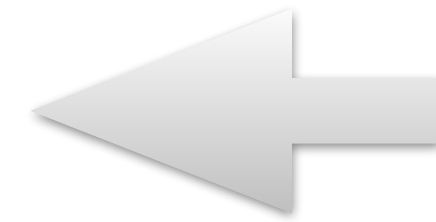
Basic Security

- 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

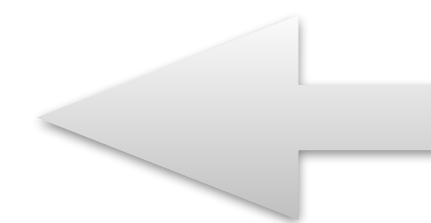
2. Check module system (module avail)

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

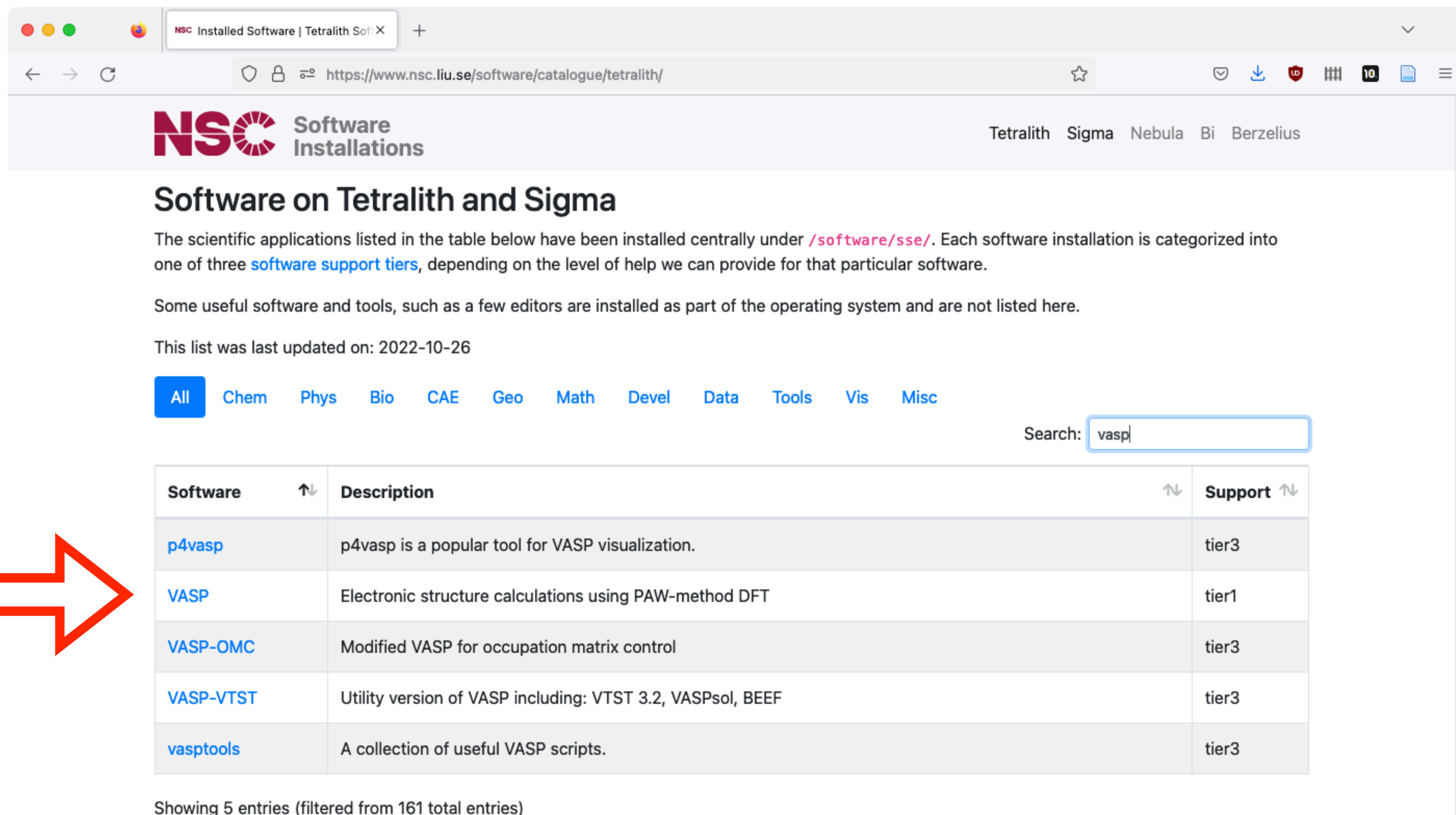
[All](#) [Chem](#) [Phys](#) [Bio](#) [CAE](#) [Geo](#) [Math](#) [Devel](#) [Data](#) [Tools](#) [Vis](#) [Misc](#)

Search:

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

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

Software: Installation Webpage



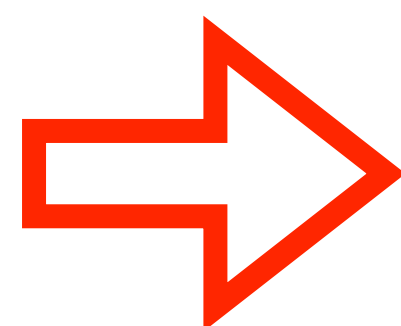
The screenshot shows a web browser window with the URL <https://www.nsc.liu.se/software/catalogue/tetralith/>. The page title is "NSC Software Installations". The navigation menu includes "Tetralith", "Sigma", "Nebula", "Bi", and "Berzelius". The main heading is "Software on Tetralith and Sigma".

The text explains that scientific applications are listed in a table, categorized into three software support tiers based on the level of help provided. It notes 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 (selected), Chem, Phys, Bio, CAE, Geo, Math, Devel, Data, Tools, Vis, Misc. A search bar contains the text "vasp".

Software	Description	Support
p4vasp	p4vasp is a popular tool for VASP visualization.	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
vasptools	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/tetalith/modules/vasp.html>. The page header includes the NSC Software Installations logo and navigation links for Tetralith, Sigma, Nebula, Bi, and Berzelius. 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/

Homepage: 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

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@tetralith1 ~]$ module avail vasp
```

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

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: 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".

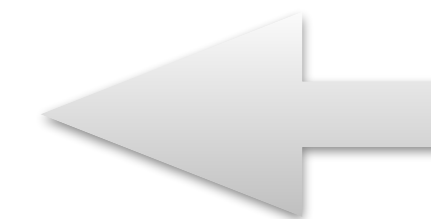
```
[weiol@tetralith2 ~]$
```

<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/2018a-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:

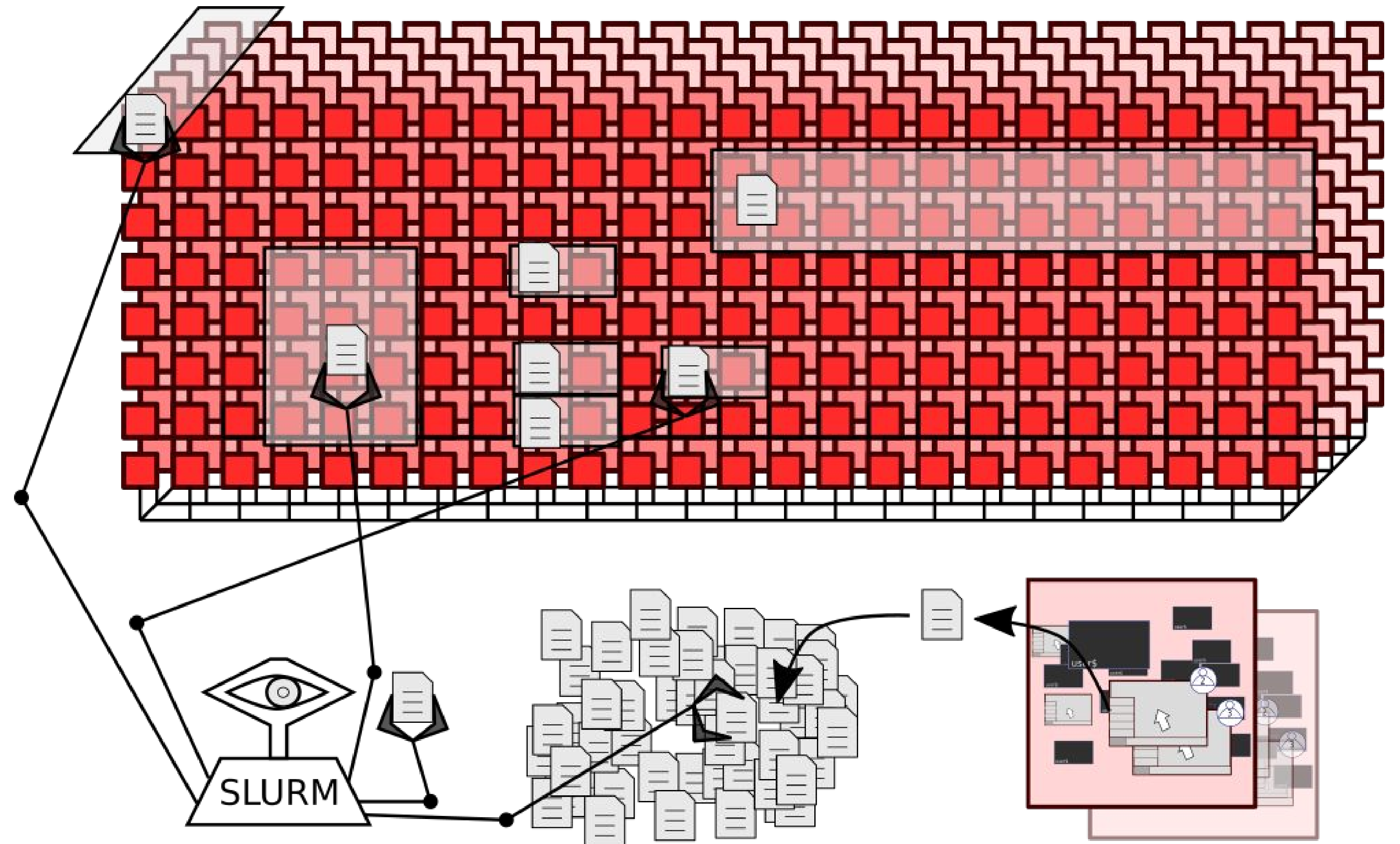
S: Module is Sticky, requires `--force` to unload or purge

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



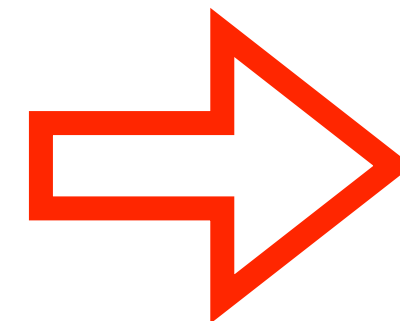
Slurm: Running Batch Job

- 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 snic2020-13-76
#SBATCH -t 1:00:00
#SBATCH -n 32
#SBATCH -J vaspstst

module load VASP/6.3.2.27062022-omp-nsc1-intel-2018a-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 ~]$interactive -A snic2020-13-76 -n 32 -t 1:00:00
salloc: Pending job allocation 11193334
salloc: job 11193334 queued and waiting for resources
salloc: job 11193334 has been allocated resources
salloc: Granted job allocation 11193334
srun: Step created for job 11193334
[weiol@n405 ~]$
```

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

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 for help/questions

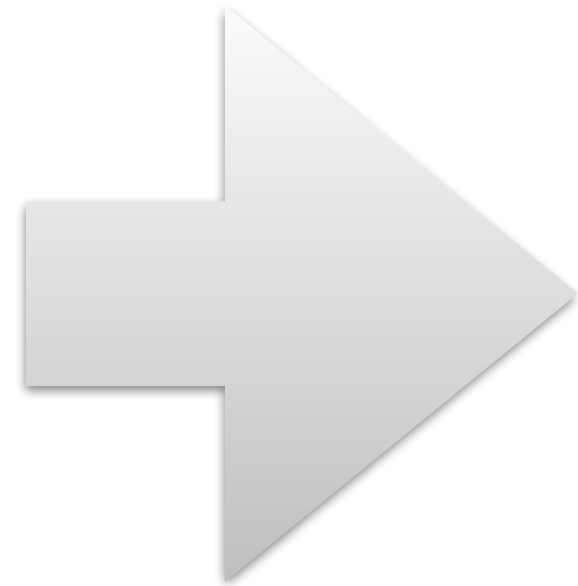
Best Practices & Suggestions

Common problems:

- My job **failed/crashed**. What now?
 - First, try to understand the cause
 - Contact support@nsc.liu.se / fill in form <https://supr.snic.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=devel`

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](#)