

# NSC introduction to Tetralith/Sigma

National Supercomputer Centre (NSC), Linköping University  
SNIC training, online @NSC 26<sup>th</sup> Apr 2022, 10:00 - ca. 12:00

# Information / Schedule



[https://www.nsc.liu.se/support/Events/NSC\\_intro\\_Apr2022/](https://www.nsc.liu.se/support/Events/NSC_intro_Apr2022/)

- 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

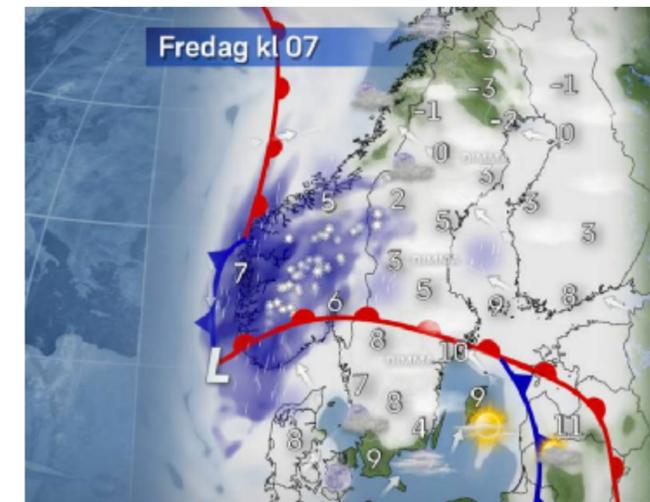


**1989** - NSC first supercomputer centre in Sweden / SAAB partner

**1996** - SMHI partner



**2016** - MET Norway partner



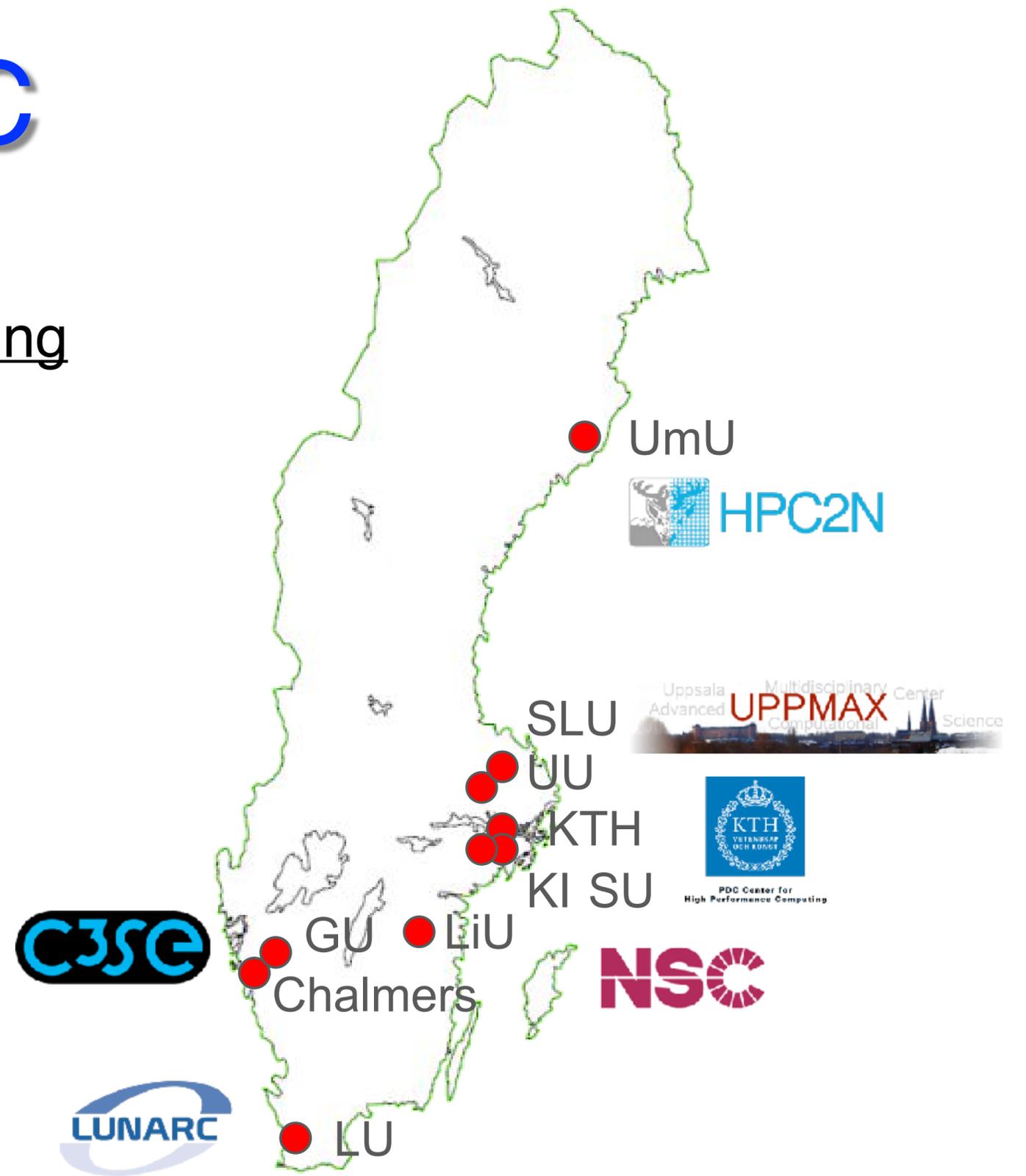


# SNIC

## 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](#)

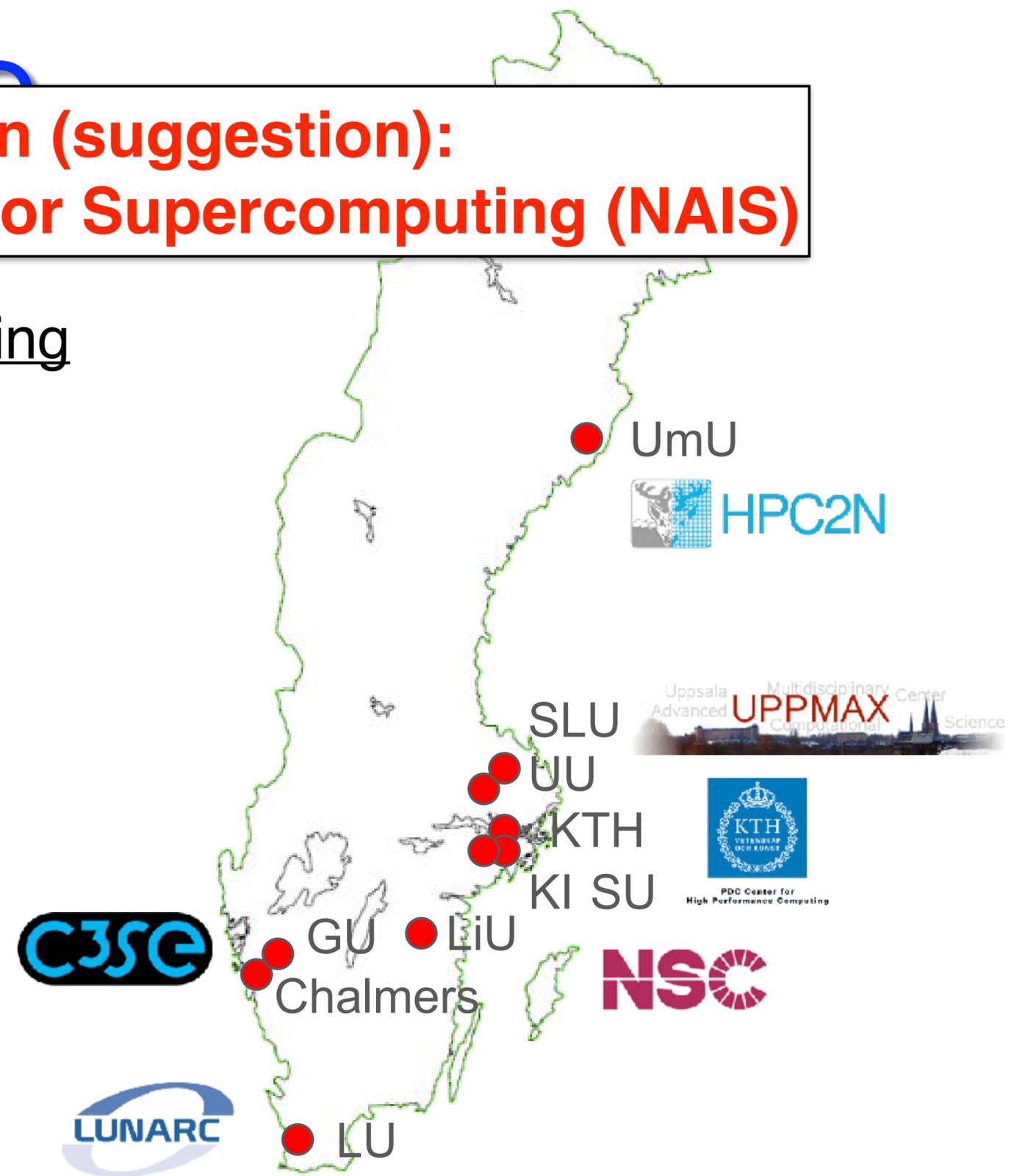


# 2023 - New organization (suggestion): National Academic Infrastructure for Supercomputing (NAIS)

## Swedish National Infrastructure for Computing

### 10 universities & 6 HPC centers:

Chalmers	<a href="#">C3SE</a>
Göteborg	
Karolinska	
KTH	<a href="#">PDC</a>
Linköping	<a href="#">NSC</a>
Lund	<a href="#">LUNARC</a>
SLU	
Stockholm	
Umeå	<a href="#">HPC2N</a>
Uppsala	<a href="#">UPPMAX</a>



# 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. 168 (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

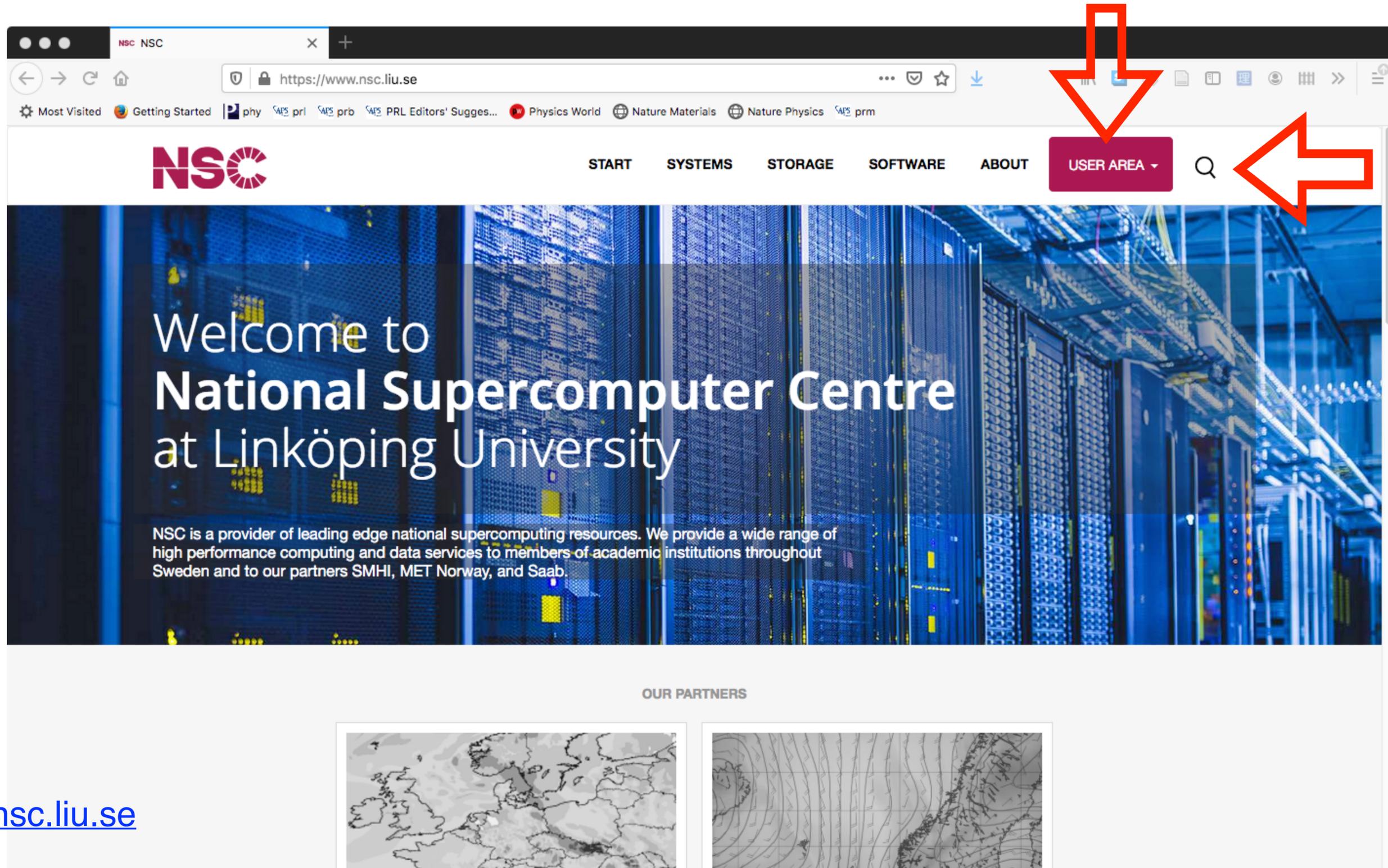


*Knut and Alice  
Wallenberg  
Foundation*



**Top500 no. 94 (83)**

# Where to find Information?



The image shows a browser window displaying the website <https://www.nsc.liu.se>. The browser's address bar and tabs are visible at the top. The website's navigation menu includes links for START, SYSTEMS, STORAGE, SOFTWARE, ABOUT, and a prominent purple button labeled 'USER AREA'. A search icon is located to the right of the 'USER AREA' button. Two red arrows are overlaid on the image: one points down to the 'USER AREA' button, and another points left to the search icon. Below the navigation menu is a large banner image of server racks with the text 'Welcome to National Supercomputer Centre at Linköping University'. A smaller text block below the banner describes NSC as a provider of leading edge national supercomputing resources. At the bottom of the page, there is a section titled 'OUR PARTNERS' with two small images: a map of Europe and a topographic map.

<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 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  
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

Org.nr: 202100-3096  
Top of Page

# Where to find Information?

The screenshot shows a web browser window with the URL <https://www.nsc.liu.se/support/>. The page features the NSC logo and a navigation menu with links for START, SYSTEMS, STORAGE, SOFTWARE, ABOUT, and a highlighted USER AREA. Below the navigation, the breadcrumb "NSC / User support" is visible. The main content area contains a section titled "Get in touch with NSC's support team!" with a sub-header "Before emailing us, please take a moment and read our suggestions on what information you should include in your email." This section lists contact methods for different user groups: academic users who can login to SUPR (Use the SUPR Support Form), academic users who cannot login to SUPR and for general inquiries (support@nsc.liu.se), SMHI, MetCoOp and MET users (smhi-support@nsc.liu.se), and ESGF users (esg-admin@nsc.liu.se). At the bottom, there are six categorized links: 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

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 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 are several bookmarked sites: Most Visited, Getting Started, phy, SPS pri, SPS prb, PRL Editors' Sugges..., Physics World, Nature Materials, Nature Physics, and prm. The main content area is a grid of 15 white boxes, each containing a topic title and a brief description. The topics are arranged in a 5x3 grid, with the last cell in the bottom row being empty.

<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

**SNIC SUPR**

Start  
Rounds  
Support  
Login

Your are not logged in.

Start

## 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

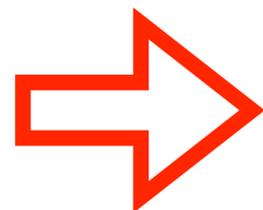
You can read about the [handling of personal data within SNIC](#) at the SNIC site without logging in.

<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 details.

Project	Project Title	Project Type	End Date
<a href="#">SNIC 2020/13-76</a>	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](mailto: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

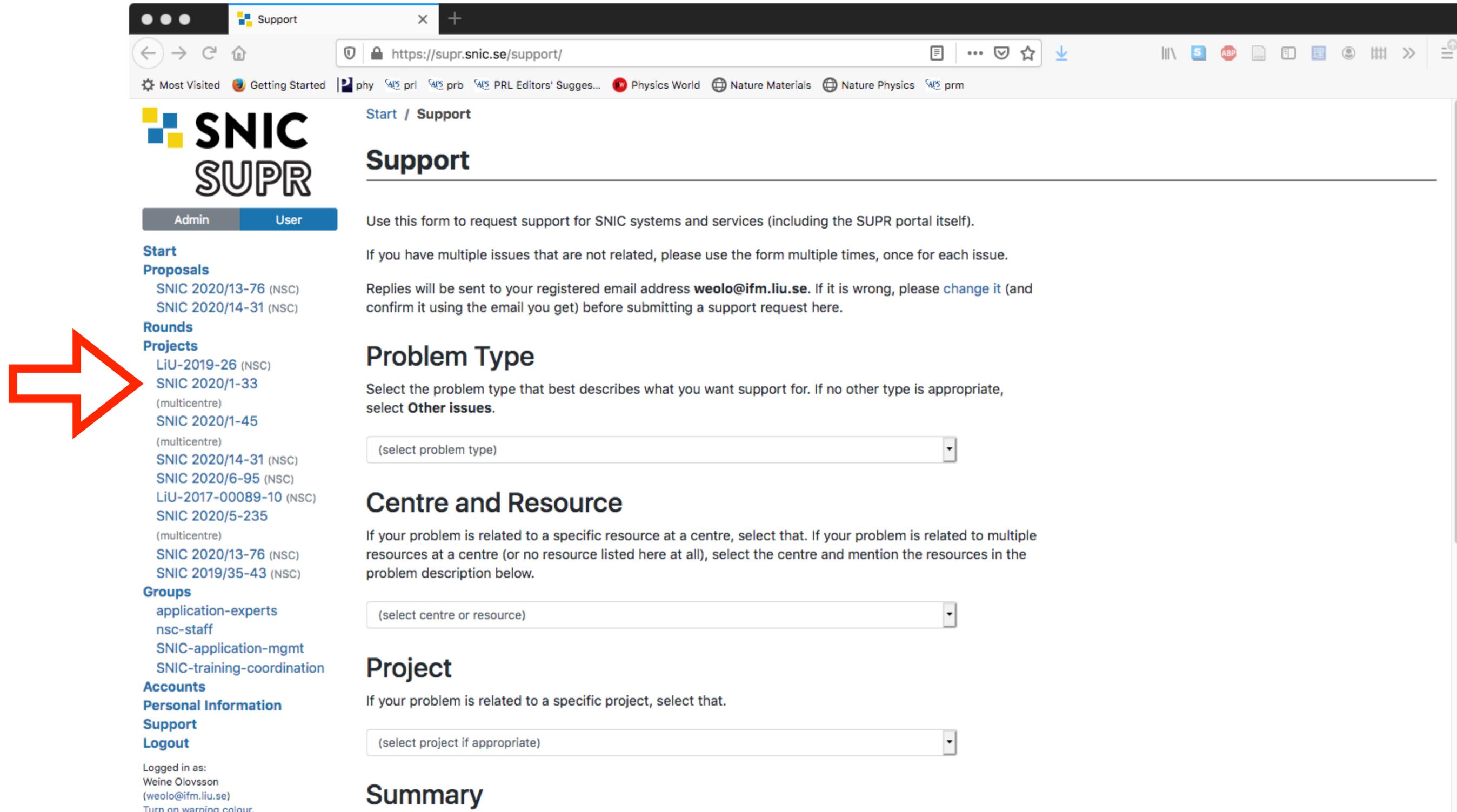
If your problem is related to a specific project, select that.

(select project if appropriate)

### Summary

Logged in as:  
Weine Olovsson  
([weolo@ifm.liu.se](mailto: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

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If you have multiple issues that are not related, please use the form multiple times, once for each issue.

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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](mailto: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
<a href="#">SNIC 2020/6-95</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.

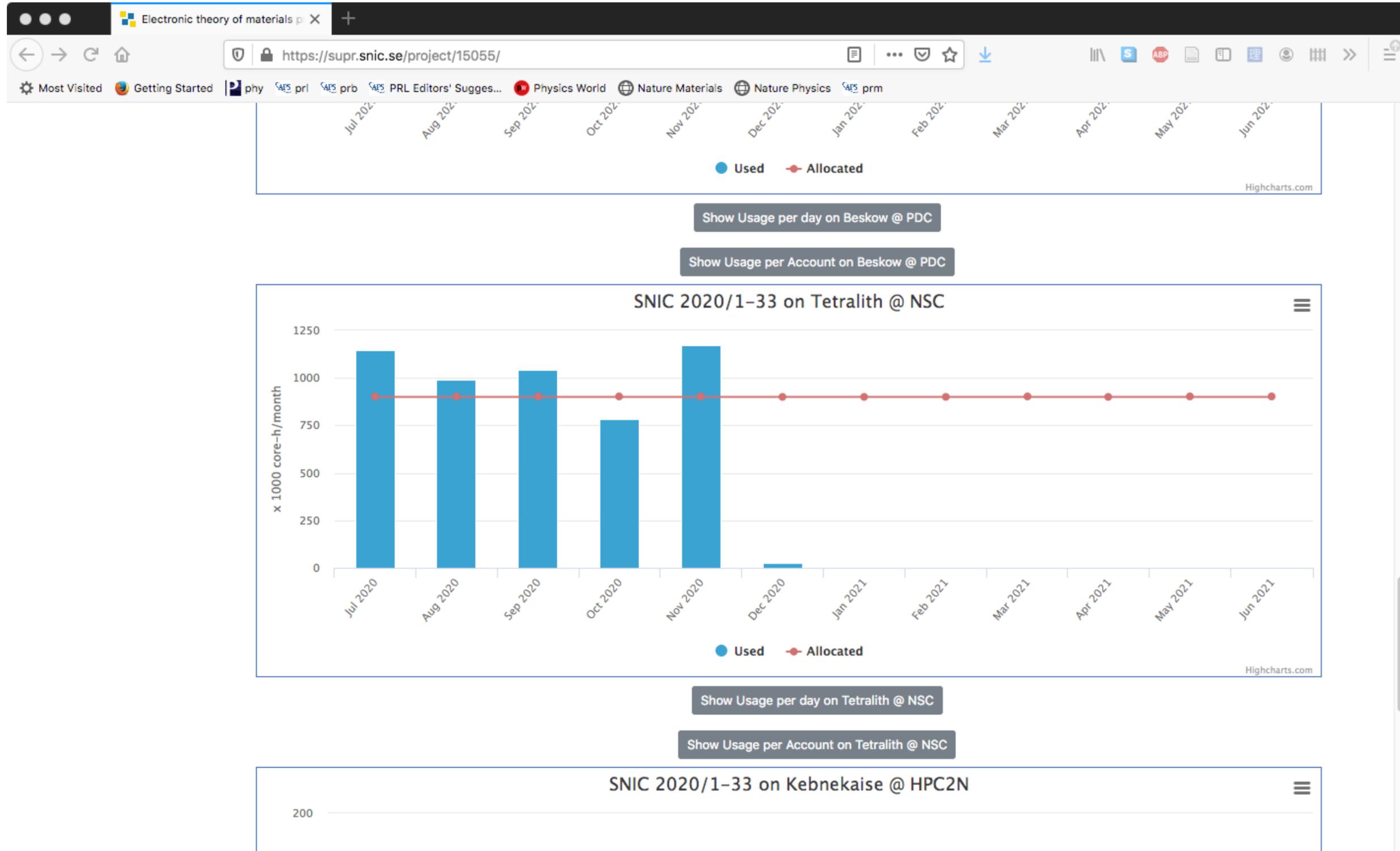
Resource	Allocation Unit	Total Usage	Allocation until Today	Percentage	Total Allocation	Percentage
Beskow @ PDC	1 400 x 1000 core-h/month	6 797.0	7 000.0	97.1 %	16 800.0	40.5 %
Tetralith @ NSC	900 x 1000 core-h/month	5 163.2	4 500.0	114.7 %	10 800.0	47.8 %
Kebnekaise @ HPC2N	150 x 1000 core-h/month	554.7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



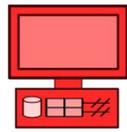
# When & Why to use HPC?

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**



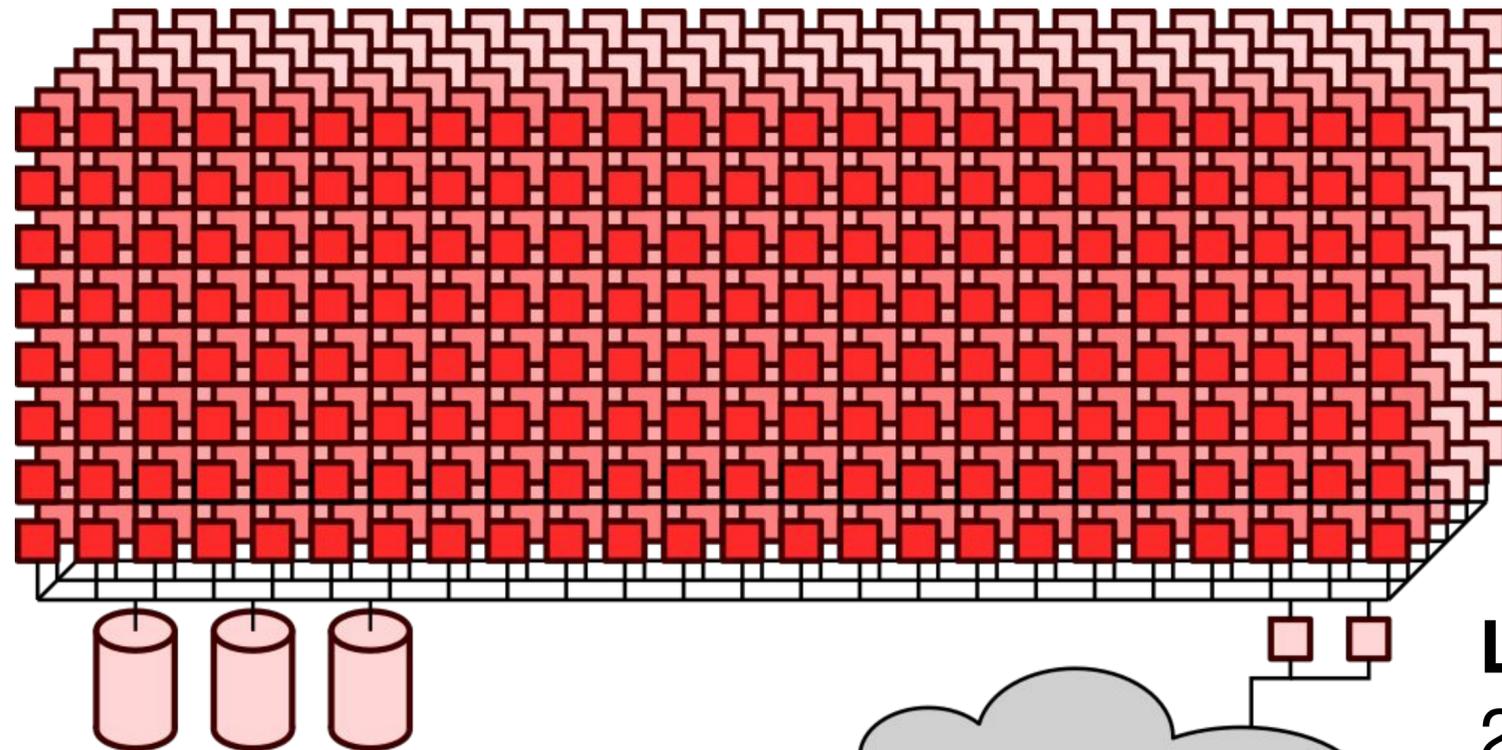
## Desktop/laptop:

8 cores

16 GB RAM

Windows, MacOS (Unix), Linux

*1 user*



## Work node:

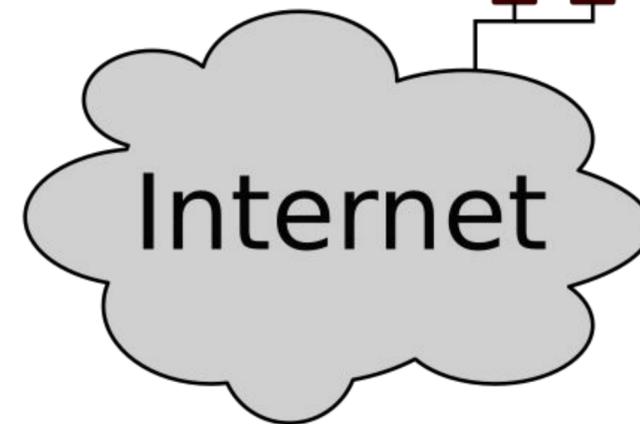
32 cores

96 (384) GB RAM

Linux

Omni-Path network

*1 - few users at a time*



## Login nodes:

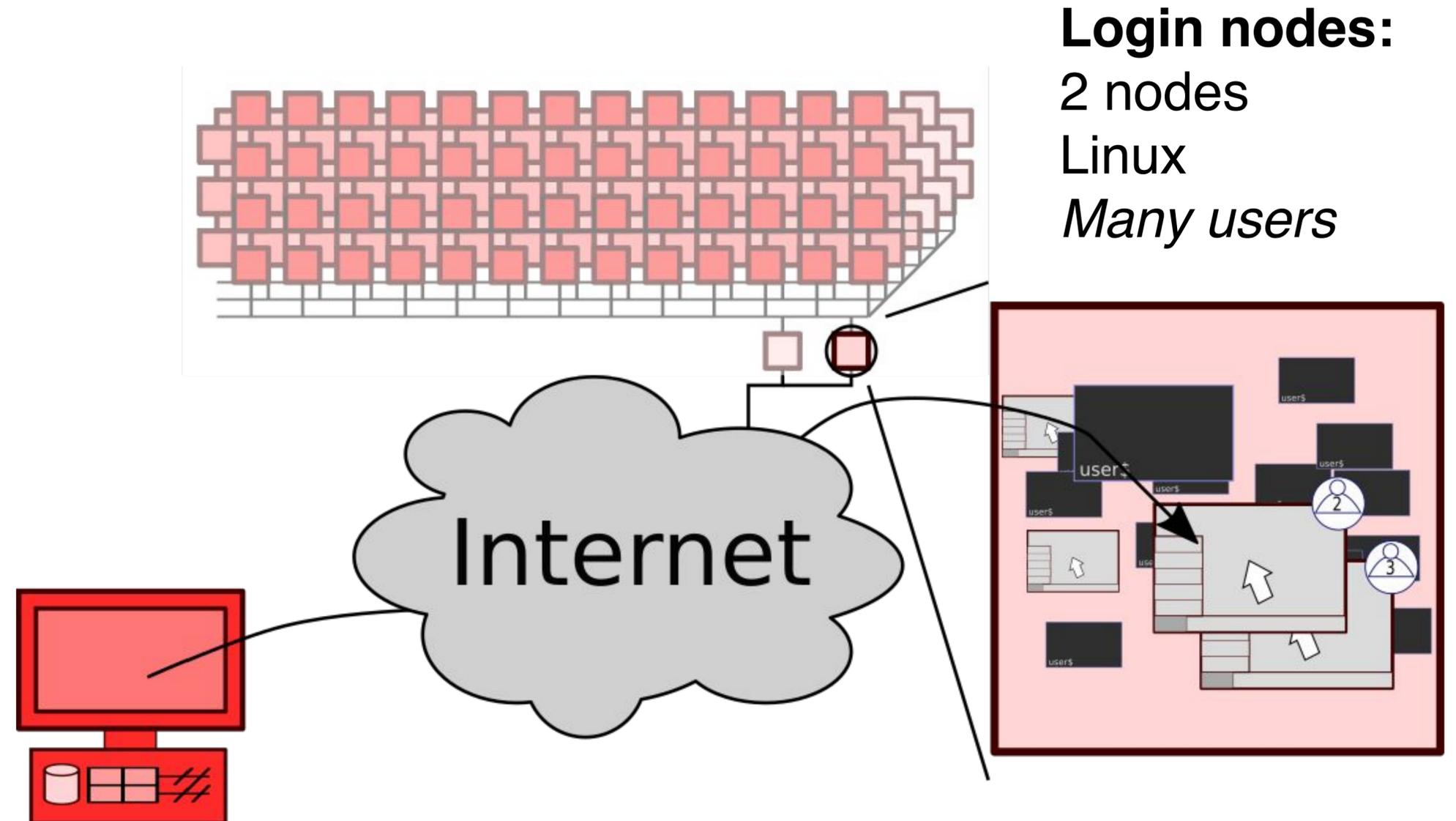
2 nodes

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

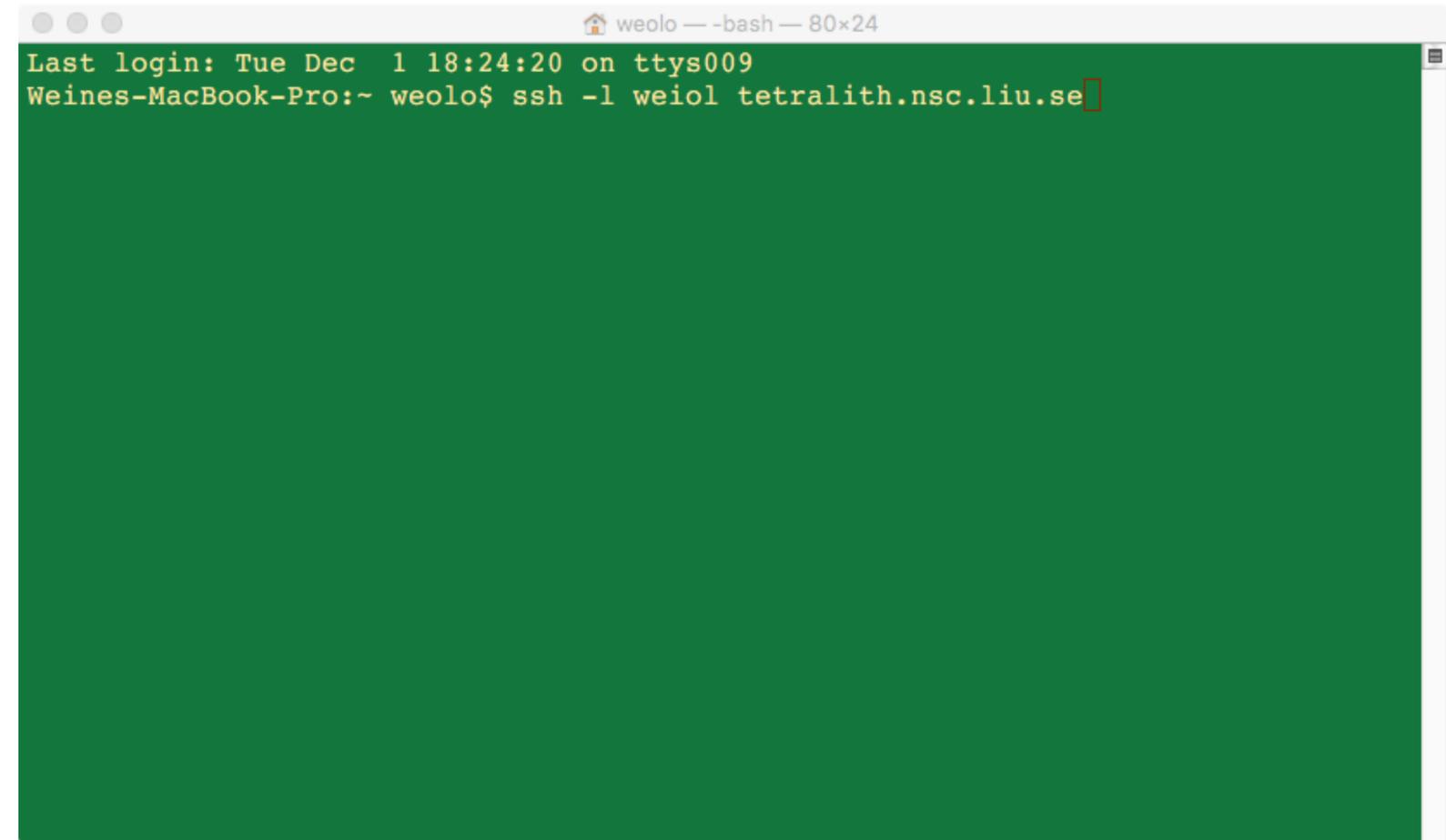
Typical login via terminal from Linux / Mac:

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

- Windows: can use PuTTY

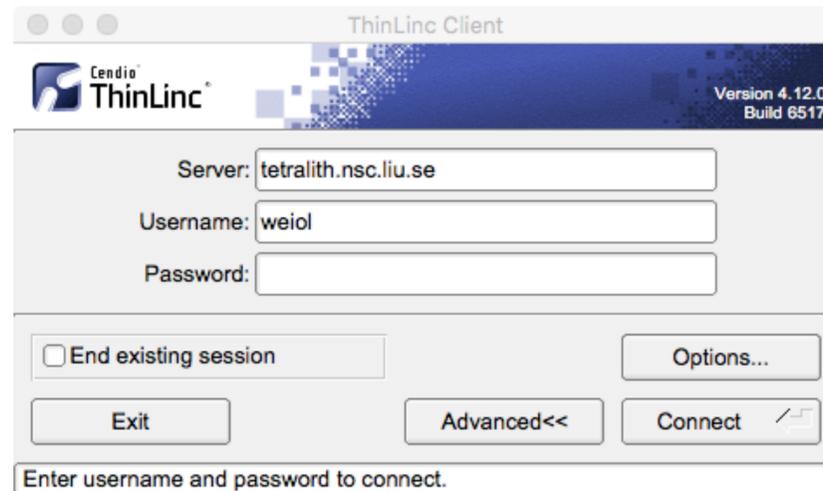
Note: to end up on a specific login node use:

```
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.

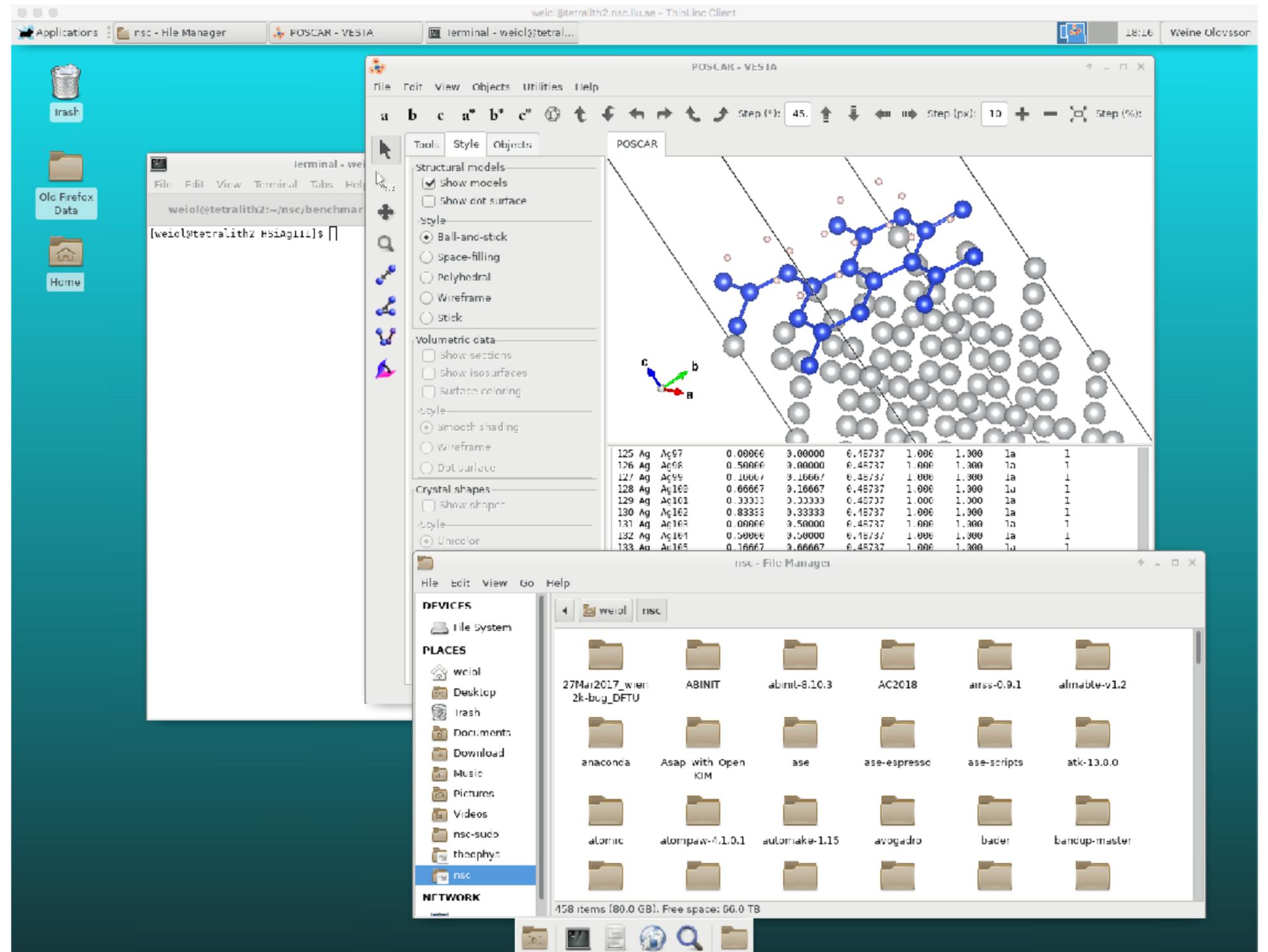
```
weolo — -bash — 80x24  
Last login: Tue Dec 1 18:24:20 on ttys009  
Weines-MacBook-Pro:~ weolo$ ssh -l weiol tetralith.nsc.liu.se
```

# 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/tetralith/>

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

# Software: Installation Webpage

The screenshot shows a web browser window with the URL <https://www.nsc.liu.se/software/installed/tetralith/>. The page features the NSC logo and a navigation menu with links for START, SYSTEMS, STORAGE, SOFTWARE, ABOUT, and a USER AREA dropdown. The main content area is titled "Tetralith & Sigma Software" and includes a breadcrumb trail: NSC / Software / Installed software / Tetralith & Sigma Software. A prominent section header reads "Tetralith & Sigma Software List". Below this, a light blue box contains a disclaimer: "DISCLAIMER: Please note that the software catalogue is a work in progress! If your application is missing, please request it by sending e-mail to NSC Support". The text explains that the list of centrally installed scientific applications under `/software/sse/` may not be 100% up to date and suggests using the `module avail` command for the most reliable source, possibly augmented by `ls /software/sse/manual/` to show manually performed installations. It also notes that some software is licensed and may not be available for everyone, requiring a license from NSC. The list was last updated on 2020-03-16. Under the heading "Electronic structure", a list of software packages is provided: Abinit, ASE, CASTEP, Elk, EPW, exciting, and GPAW.

NSC Tetralith & Sigma Software

START SYSTEMS STORAGE SOFTWARE ABOUT USER AREA

## Tetralith & Sigma Software

NSC / Software / Installed software / Tetralith & Sigma Software

### Tetralith & Sigma Software List

**DISCLAIMER:** Please note that the software catalogue is a work in progress! If your application is missing, please request it by sending e-mail to [NSC Support](#)

The following scientific applications have been installed centrally under `/software/sse/`. This list may not always be 100% up to date. The most reliable source is running the command `module avail` while logged into Tetralith or Sigma, possibly augmented by `ls /software/sse/manual/` to show additional manually performed installations without modules. Please note that some of this software is licensed, and may not be available for everyone. You need ask NSC for access, which is typically granted upon some proof of having a license.

The list was last updated: 2020-03-16

#### Electronic structure

- Abinit
- ASE
- CASTEP
- Elk
- EPW
- exciting
- GPAW

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

# 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@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: 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-intel/recommendation (D)  
buildenv-gcc/7.3.0-bare buildenv-intel/2015.1.133-impi-2018.1.163-eb  
buildenv-gcc/2016b-eb buildenv-intel/2016b-eb  
buildenv-gcc/2018a-eb buildenv-intel/2017.u7-bare  
buildenv-gcccuda/recommendation (D) buildenv-intel/2018a-eb  
buildenv-gcccuda/10.2-7.3.0-bare buildenv-intel/2018b-eb  
buildenv-impi-gcc/recommendation (D) buildenv-intel/2018.u1-bare  
buildenv-impi-gcc/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@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:

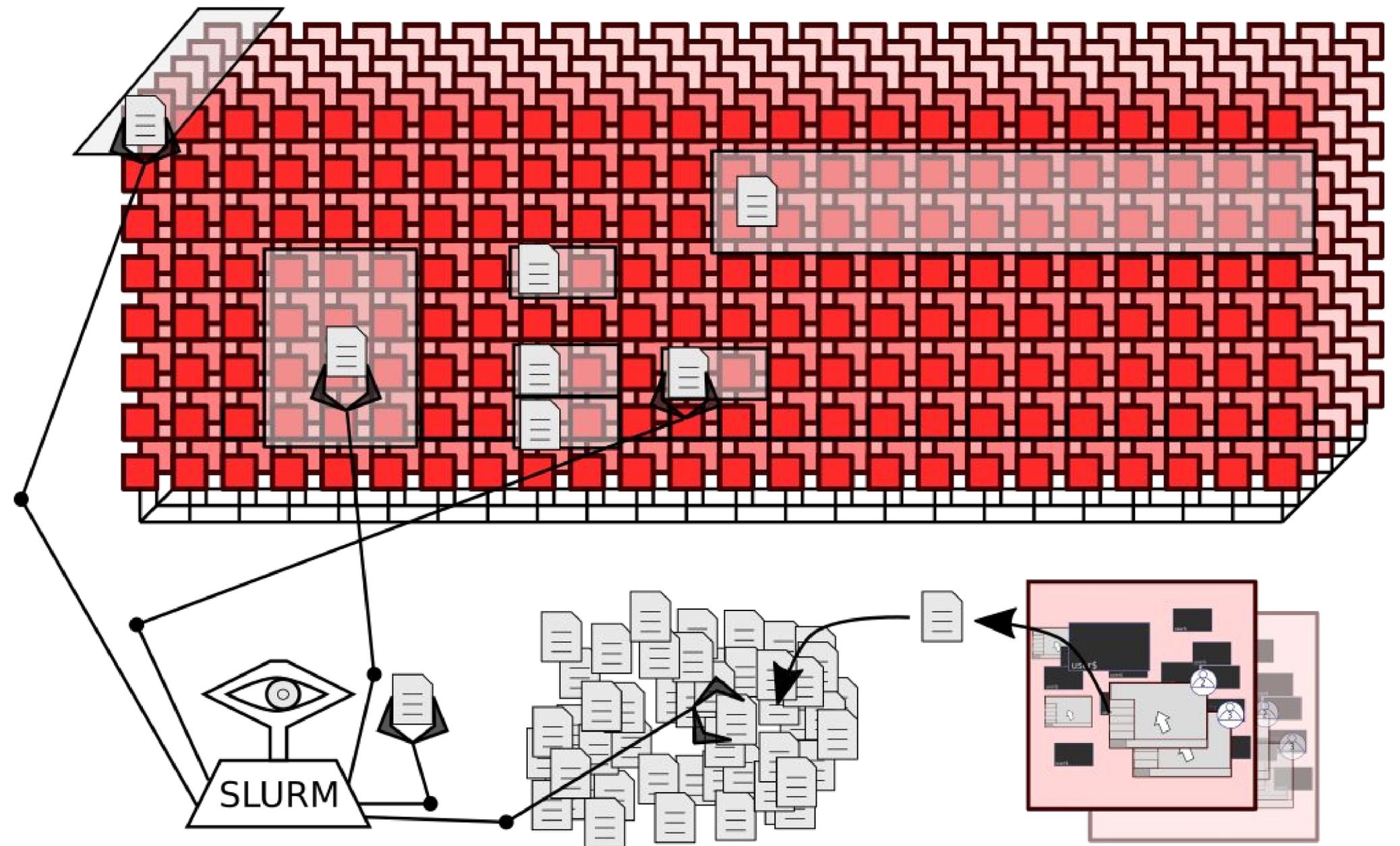
**S:** Module is Sticky, requires `--force` to unload or purge

**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



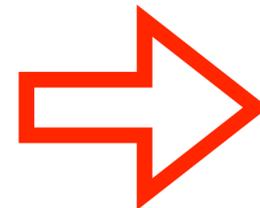
# Slurm: Running Batch Job

- 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/6.2.1.29042021-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](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.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](#)