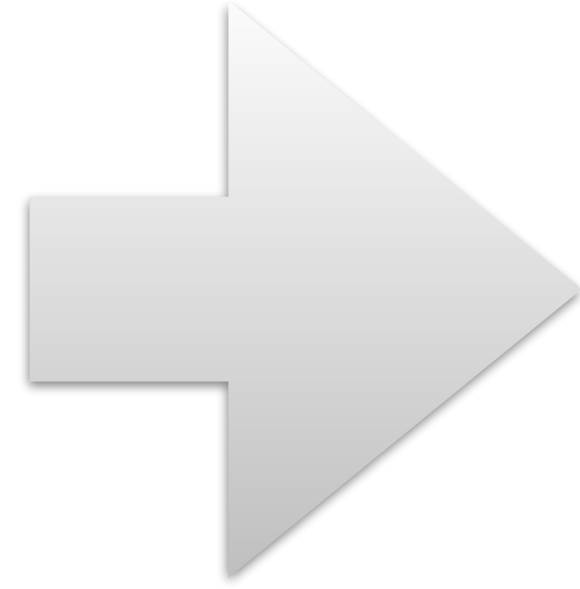


Introduction to NSC & Open Forum

National Supercomputer Centre (NSC), Linköping University

SNIC training, online @NSC 3rd Dec 2020, 10:00 - ca. 12:00

Information / Schedule



https://www.nsc.liu.se/support/Events/NSC_intro_Dec2020/

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


10:00 Introduction to NSC (Weine Olovsson)

~**10:45** Using GPUs on Tetralith and Sigma (Torben Rasmussen)

~**11:00** Open Forum

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

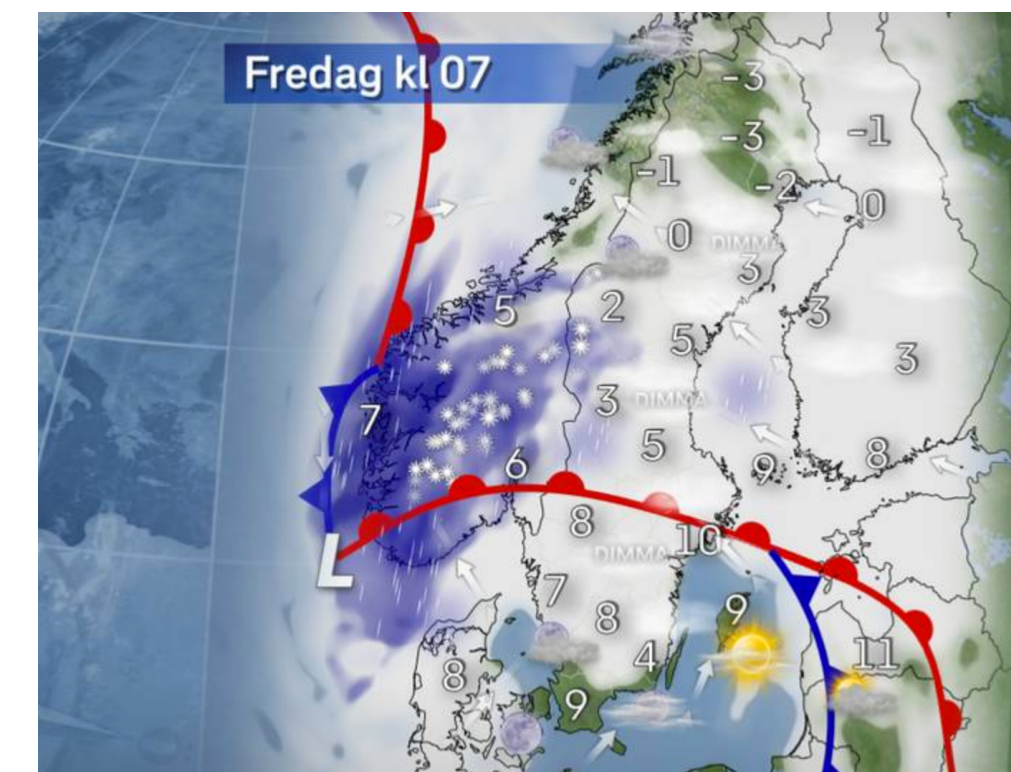


1989 - NSC first supercomputer centre in Sweden / SAAB partner

1996 - SMHI partner



2016 - MET Norway partner



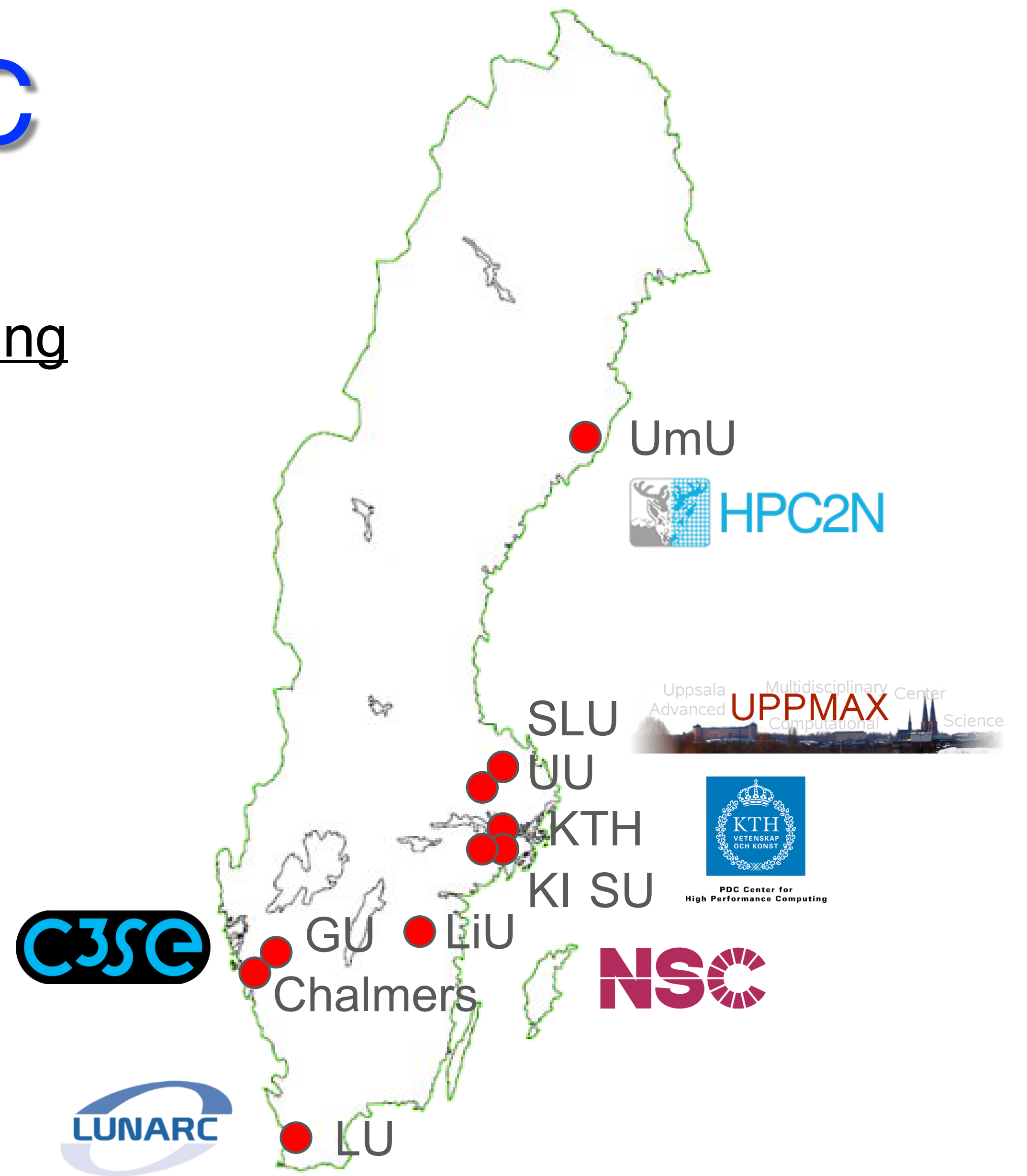


SNIC

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](#)



NSC: Quick Overview

Current Director: Matts Karlsson, Jun 2016 -

~ **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. 111 (74)

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



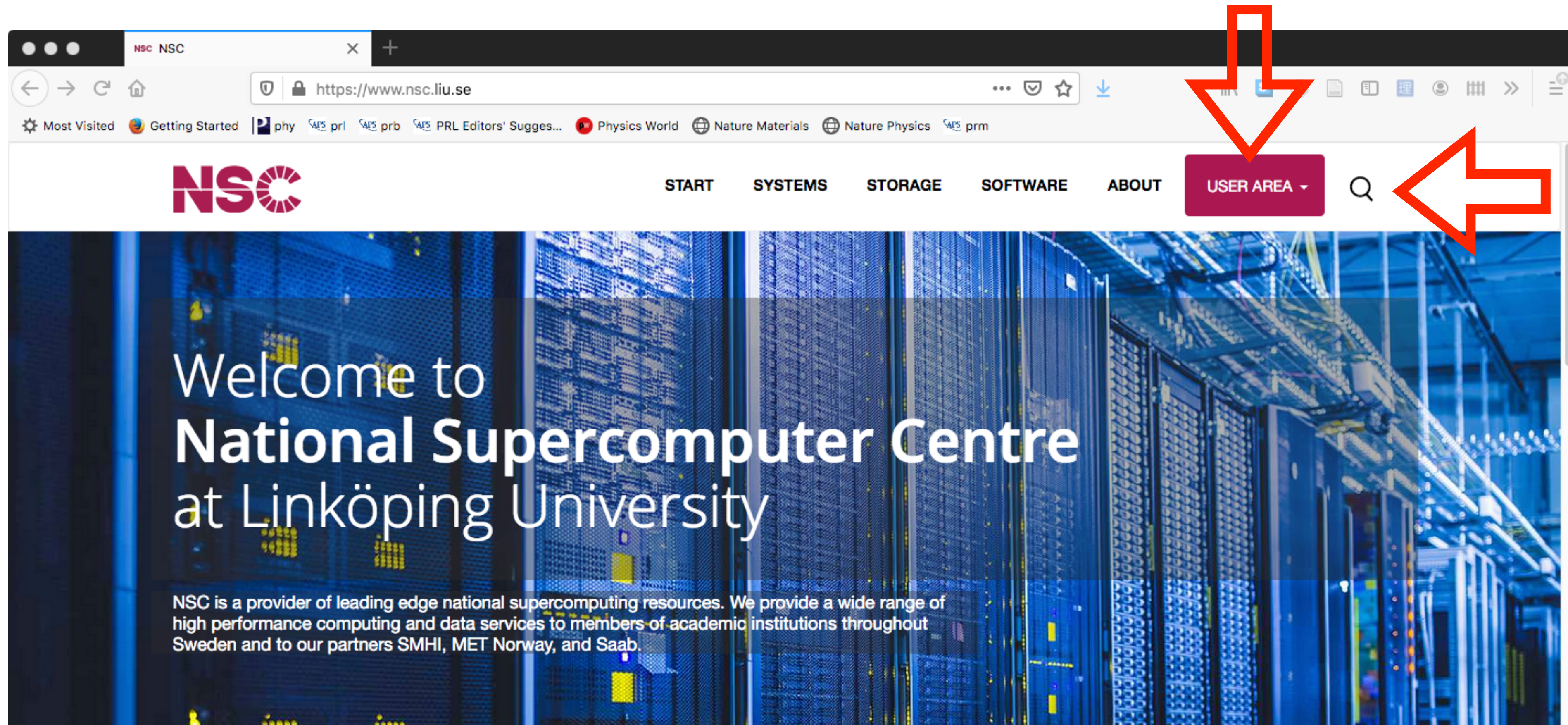
(2020 -) 2 x V100 GPU-nodes

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



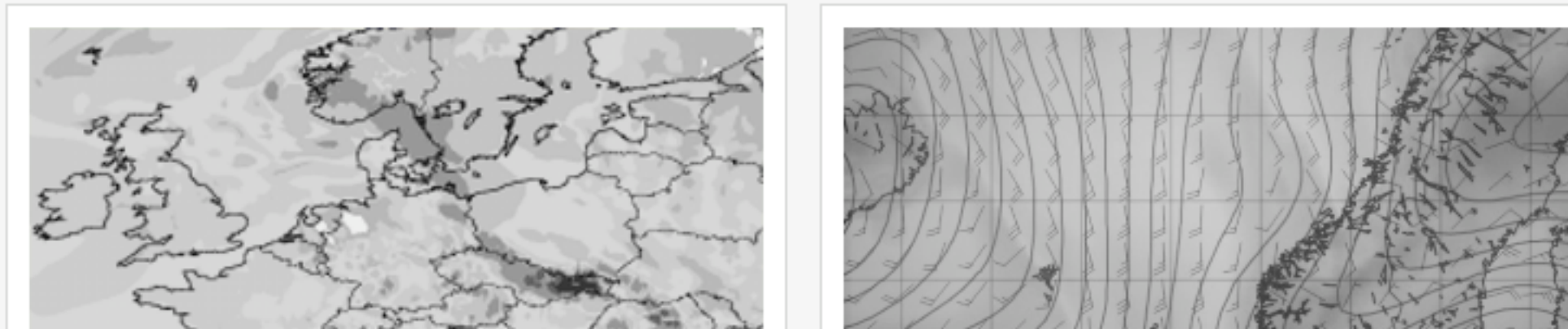
*Knut and Alice
Wallenberg
Foundation*

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). The footer contains contact information for the National Supercomputer Centre, Linköping University, and logos for Linköping University and SNIC.

NSC NSC

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

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

Latest News

New AI Supercomputer at NSC (05 Oct 2020)

USER AREA

User support
Guides, documentation and FAQ.

Getting access
Applying for projects and login accounts.

System status
Everything OK!
No reported problems

Self-service

SUPR NSC Express

NSC

National Supercomputer Centre
Linköping University
581 83 LINKÖPING
SWEDEN

Org.nr: 202100-3096

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

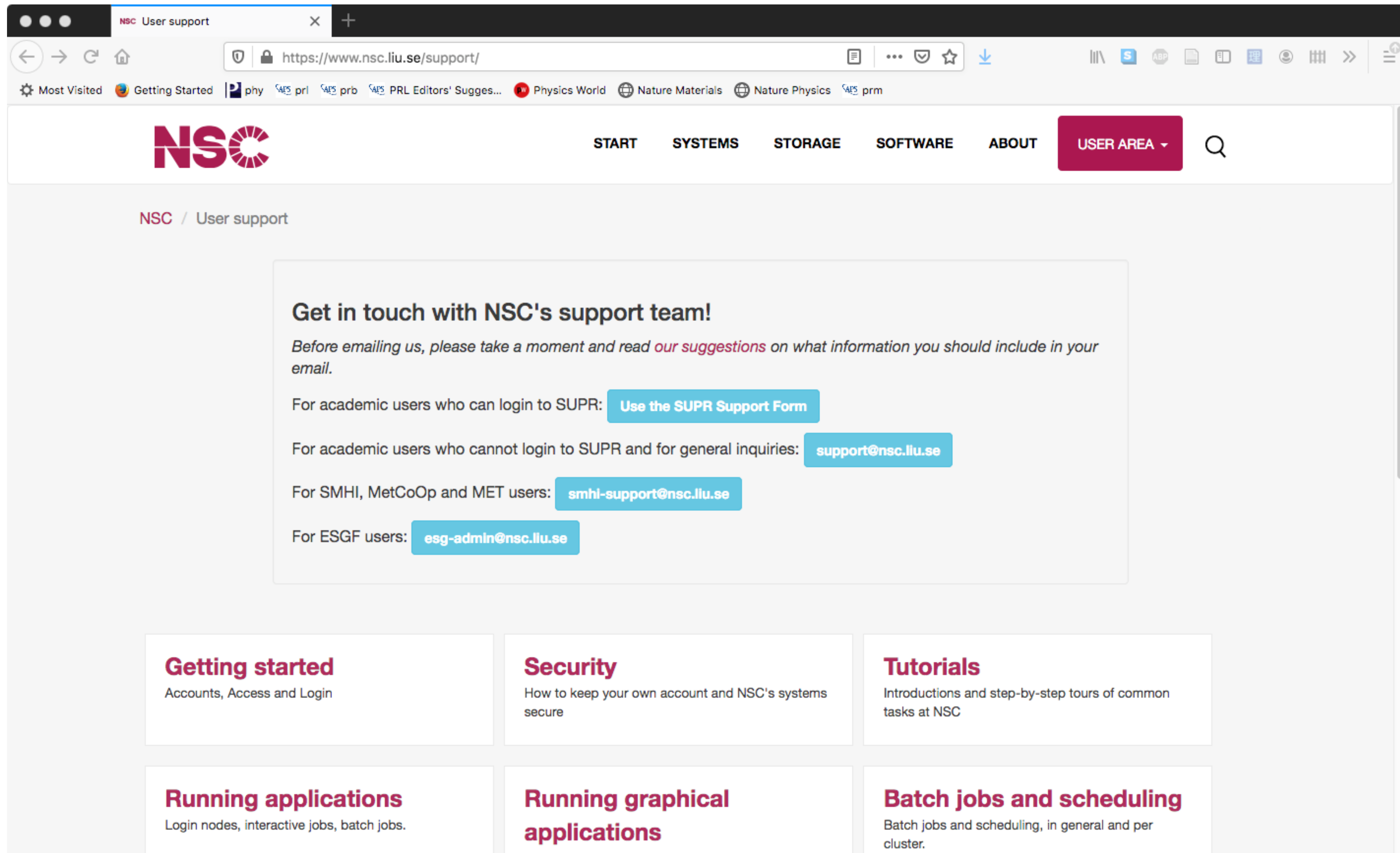
NSC is part of Linköping University and the Swedish National Infrastructure for Computing (SNIC).

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 brief descriptions: "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

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

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

Getting started

Accounts, Access and Login

Security

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

Tutorials

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

Running applications

Login nodes, interactive jobs, batch jobs.

Running graphical applications

Batch jobs and scheduling

Batch jobs and scheduling, in general and per cluster.

Where to find Information?

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 tabs, including "Most Visited" and "Getting Started". The main content area of the page is a grid of 15 white boxes, each containing a title and a brief description of a help topic. The topics are arranged in a 5x3 grid, with the last cell in the bottom row being empty.

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

Getting Access to HPC - SUPR

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

SNIC SUPR

Admin User

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](#)

Start

SUPR - Weine Olovsson

Activity Report Wanted

The Swedish Research Council requires SNIC to provide reporting of results from all SNIC projects. As a consequence, starting in 2020, SNIC requires you to provide activity reports within three months after the end of your SNIC 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
SNIC 2020/13-76	VASP workshop at NSC 19-20th Oct 2020	SNIC Small Compute	2020-12-01

Proposals

You have no proposals in preparation or pending committee decision.

Rounds

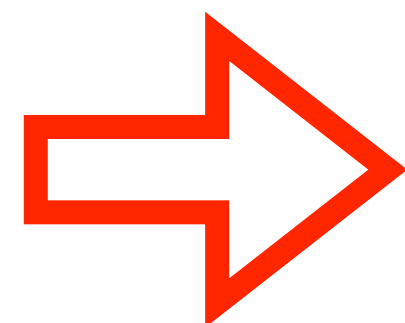
[View Rounds](#)

Projects and Project Membership Requests

[View and Manage](#)

Groups

[View and Manage](#)



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

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

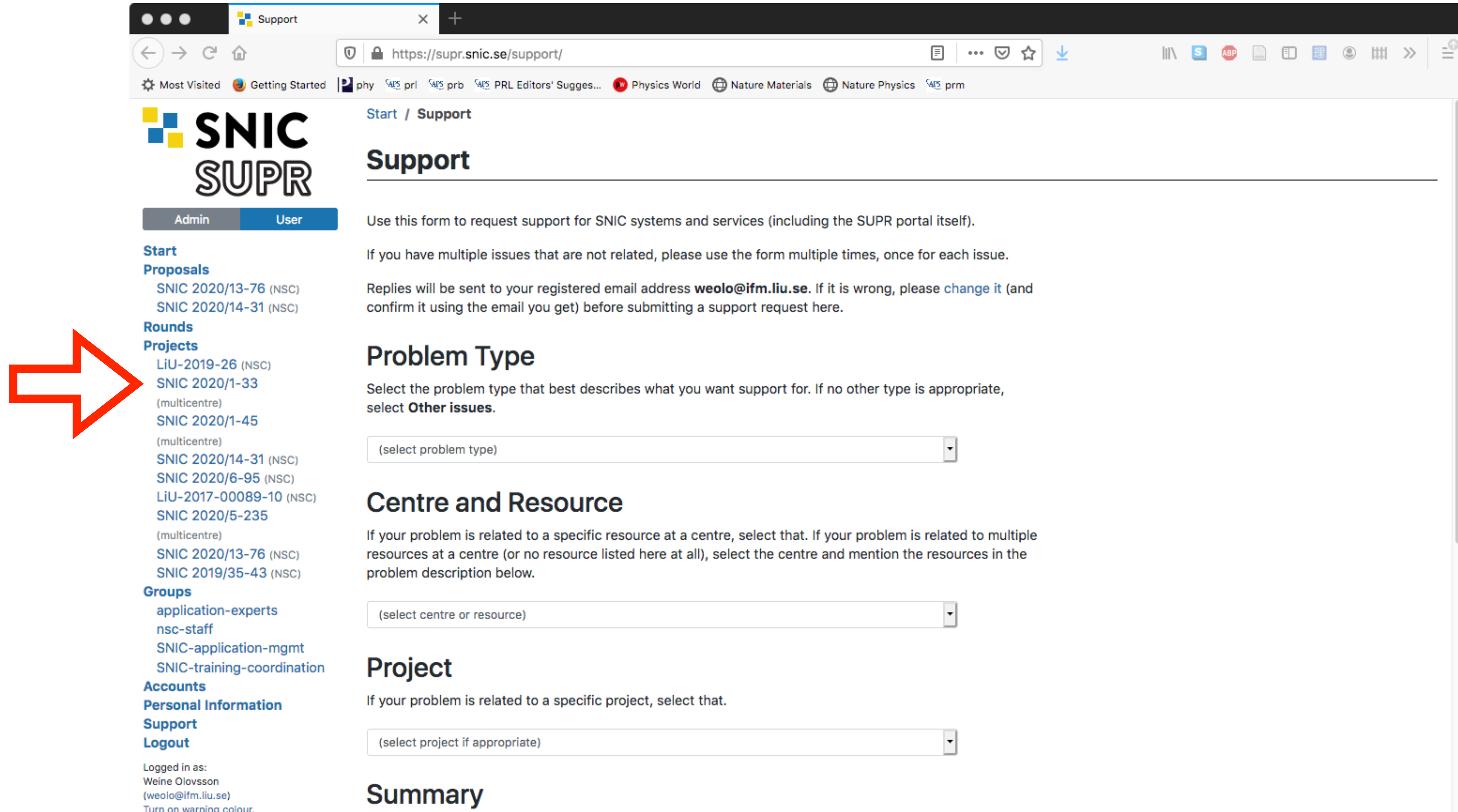
Personal Information

Support

Logout

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

Projects in SUPR



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:
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(weolo@ifm.liu.se)
[Turn on warning colour](#)

Projects in SUPR

The screenshot shows a web browser window with the address bar displaying `https://supr.snic.se/project/15055/`. The page title is "Electronic theory of materials". The browser's address bar includes navigation icons (back, forward, refresh, home) and a search bar. Below the address bar, there are several tabs, including "Most Visited", "Getting Started", and "phy". The main content of the page is as follows:

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.

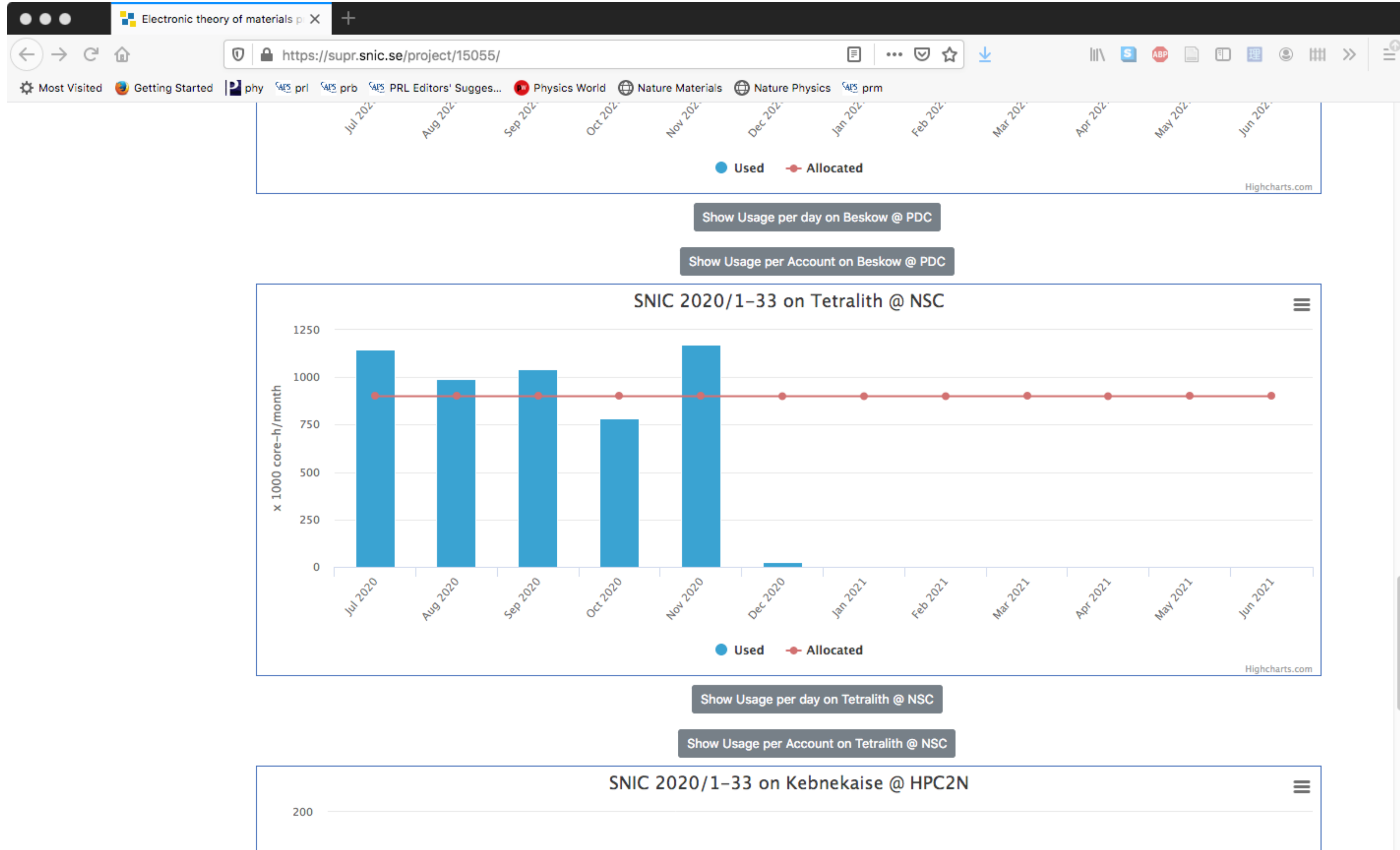
Resource	Allocation Unit	Total Usage	Allocation until Today	Percentage	Total Allocation	Percentage
Beskow @ PDC	1 400 x 1000 core-h/month	6 797.0	7 000.0	97.1 %	16 800.0	40.5 %
Tetralith @ NSC	900 x 1000 core-h/month	5 163.2	4 500.0	114.7 %	10 800.0	47.8 %
Kebnekaise @ HPC2N	150 x 1000 core-h/month	554.7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



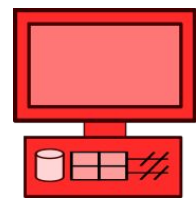
When & Why to use HPC?

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



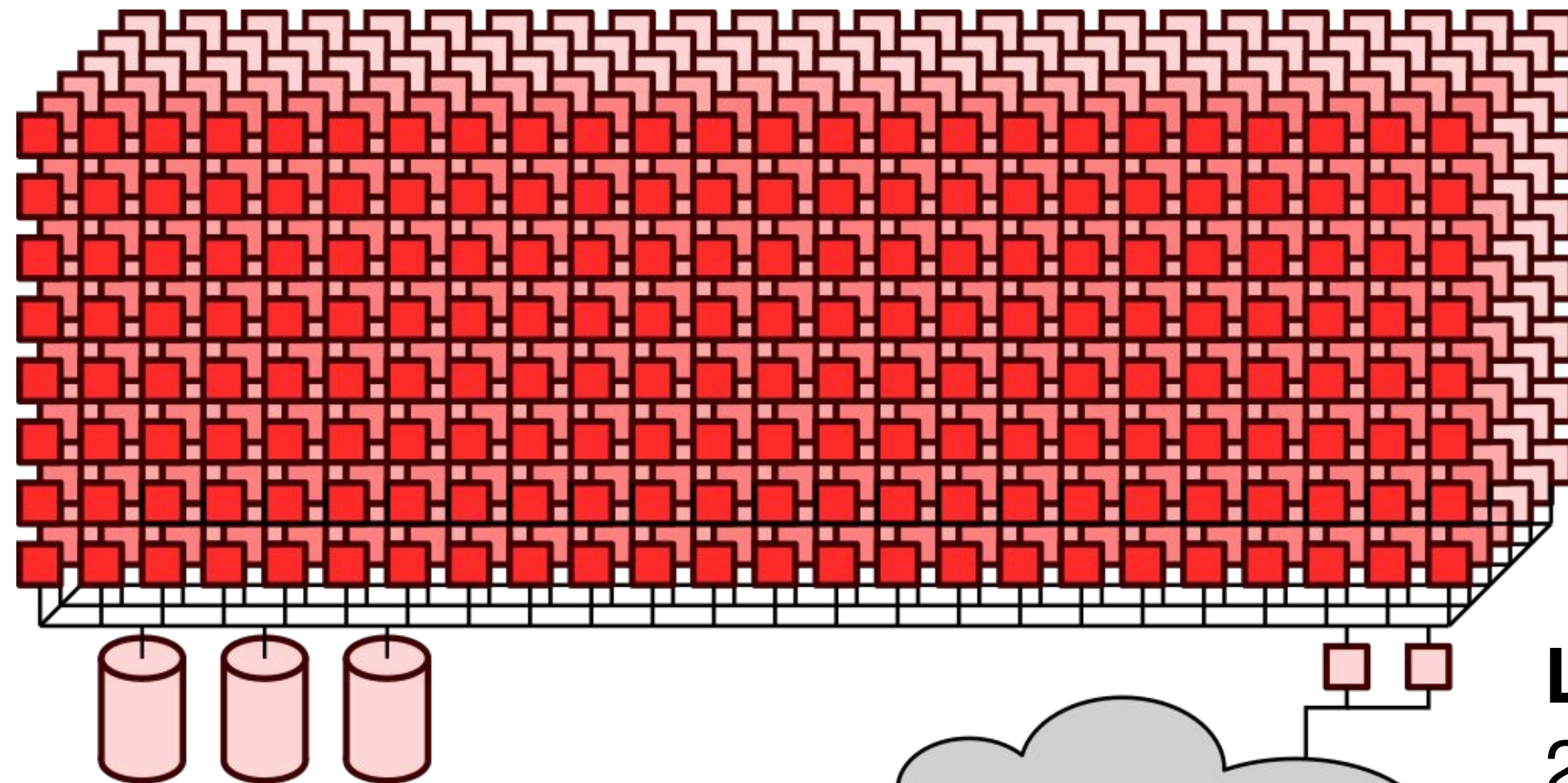
Desktop/laptop:

8 cores

16 GB RAM

Windows, MacOS (Unix), Linux

1 user



Work node:

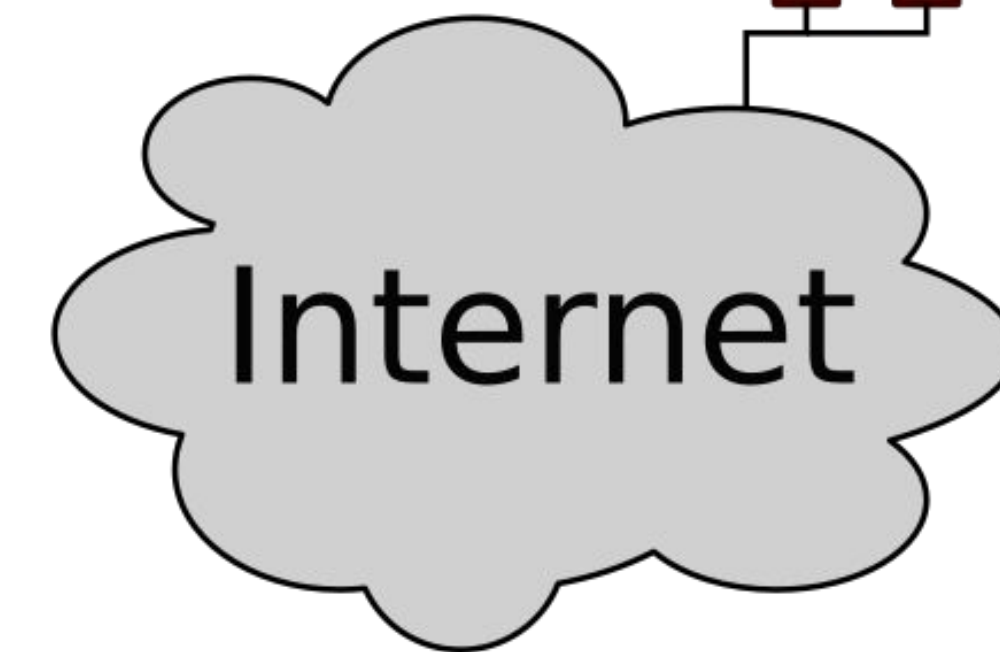
32 cores

96 (384) GB RAM

Linux

Omni-Path network

1 - few users at a time



Login nodes:

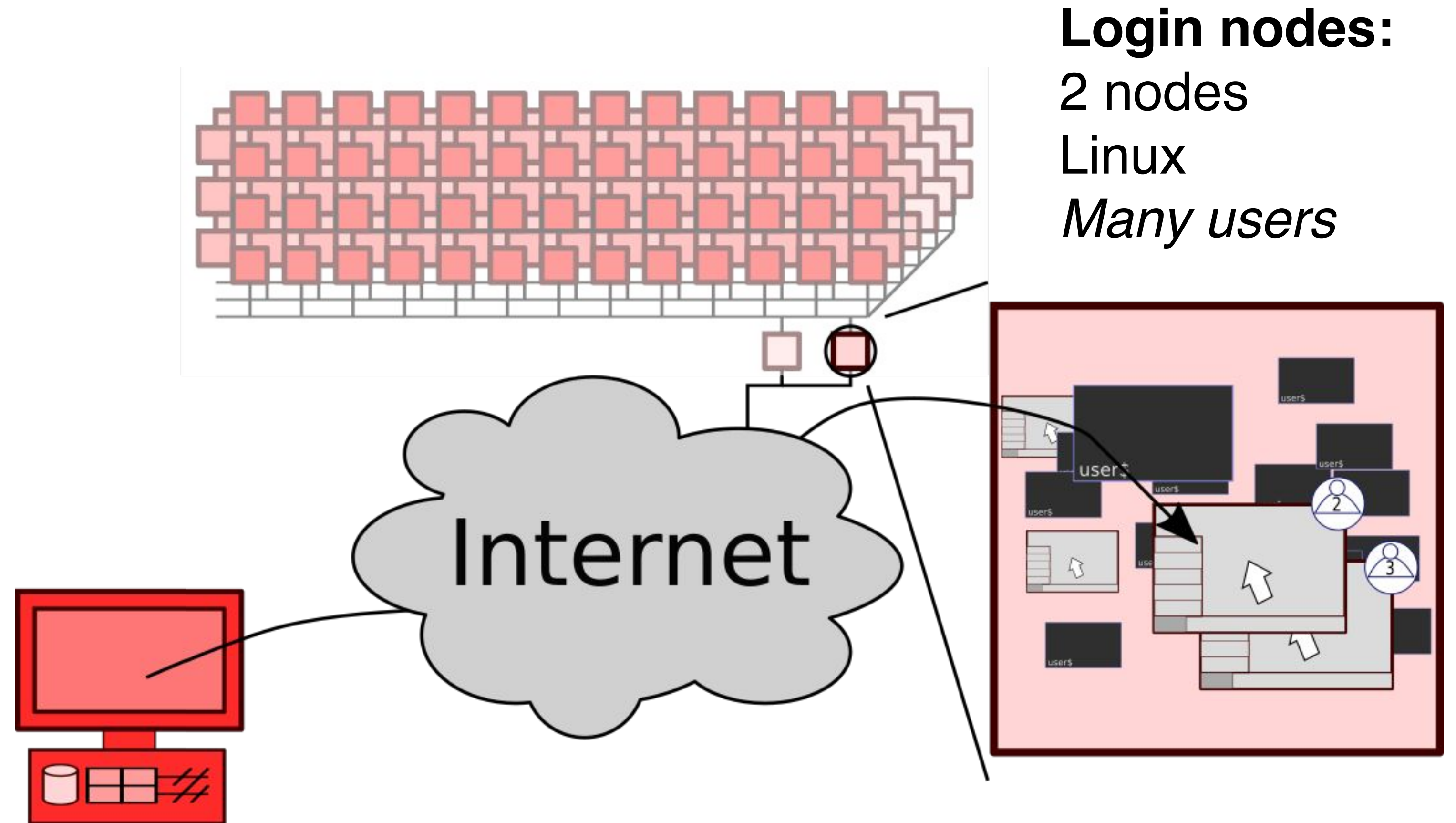
2 nodes

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

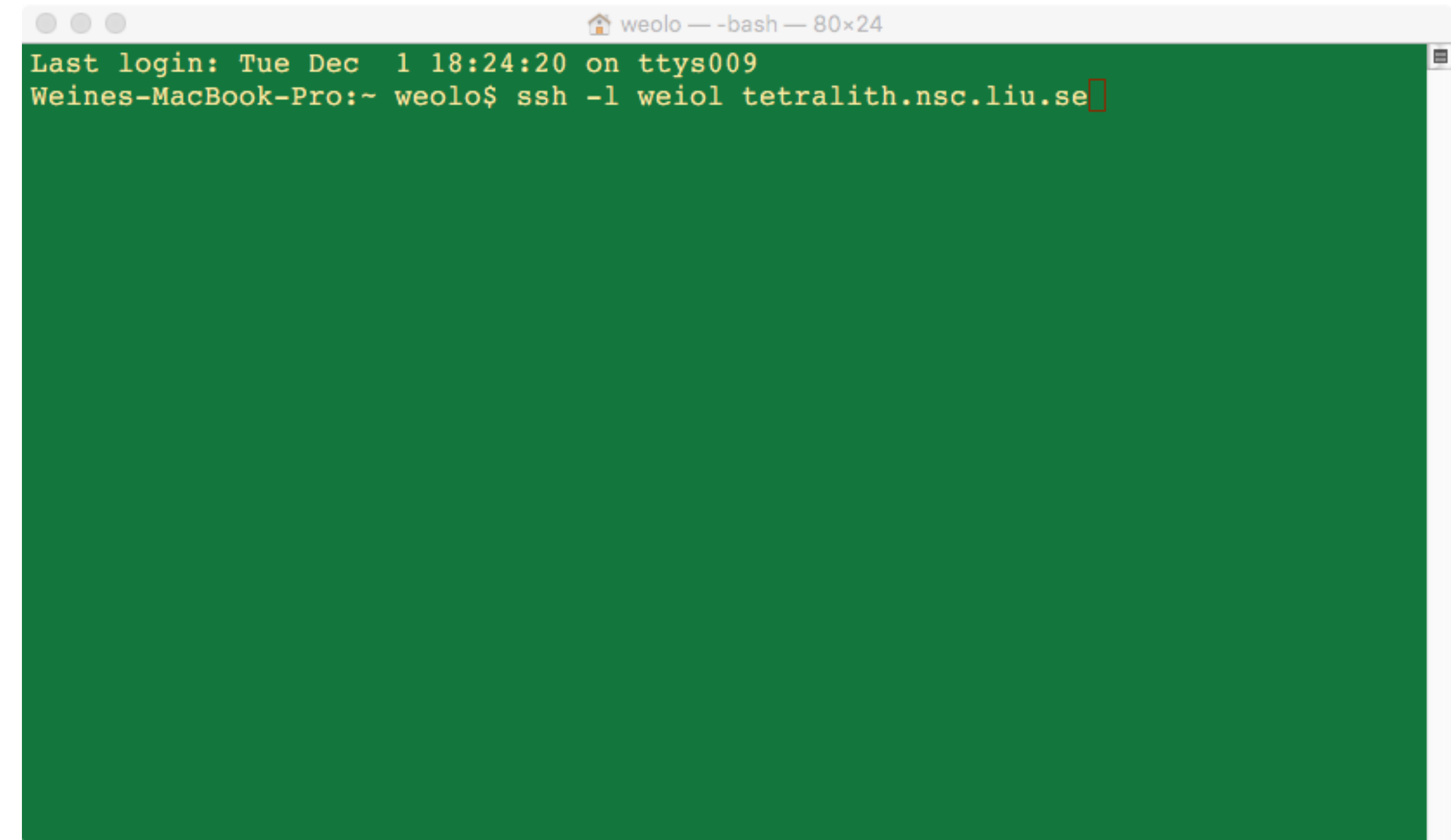
Typical login via terminal from Linux / Mac:

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

- Windows: can use PuTTY

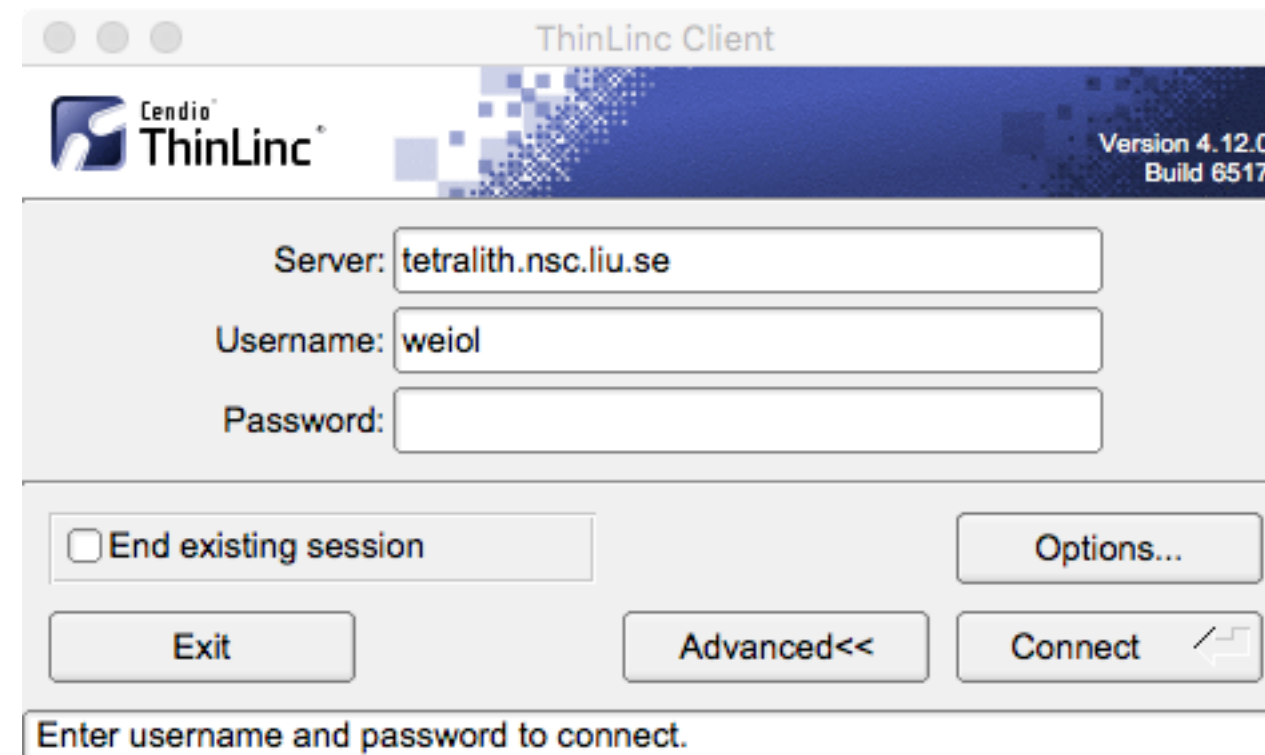
Note: to end up on a specific login node use:

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

A terminal window with a 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" and the command "ssh -l weiol tetralith.nsc.liu.se" being entered at the prompt "Weines-MacBook-Pro:~ weolo\$".

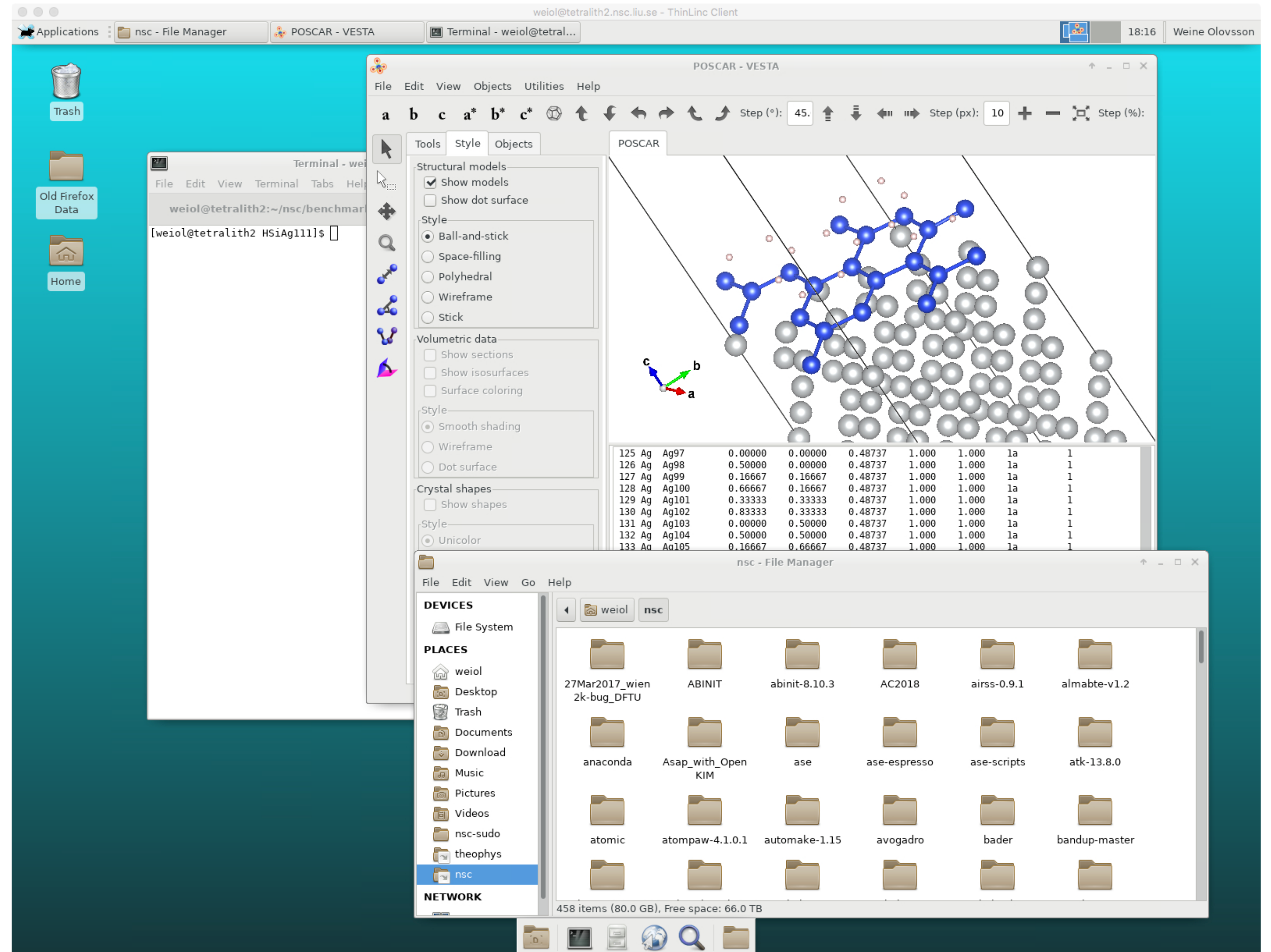
```
weolo - bash - 80x24  
Last login: Tue Dec 1 18:24:20 on ttys009  
Weines-MacBook-Pro:~ weolo$ ssh -l weiol tetralith.nsc.liu.se
```

Access to Tetralith: ThinLinc

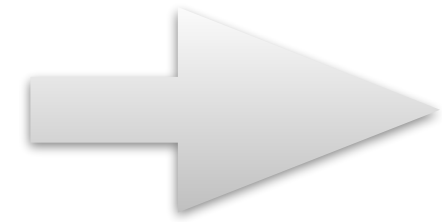


- ThinLinc - *virtual desktop*
- Persistent sessions (compare screen, tmux)
- Recommended for graphics
- Hardware acc. graphics (vglrun) in some cases

<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:

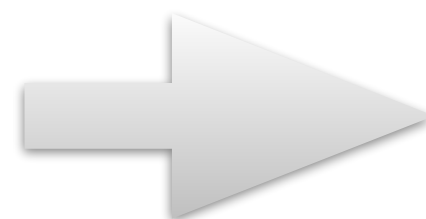
- Use `snicquota` to check available disk space
- Project storage is linked to specific project allocation and life time
- Good idea to have your own backup
- **Data is never 100% safe, there's always some risk**

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

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

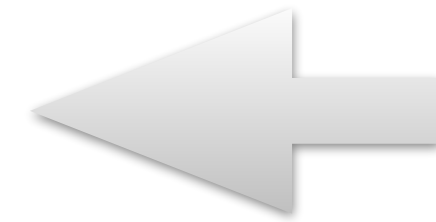
Basic Security

- 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 heading is "Tetralith & Sigma Software". A breadcrumb trail reads "NSC / Software / Installed software / Tetralith & Sigma Software". Below this is a section titled "Tetralith & Sigma Software List" containing 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 scientific applications are installed centrally under `/software/sse/` and may not be up to date. It provides instructions on how to check for updates using `module avail` and `ls /software/sse/manual/`. It also notes that some software is licensed and may require access from NSC. The list was last updated on 2020-03-16. Under the heading "Electronic structure", a list of software packages is shown: 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

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.

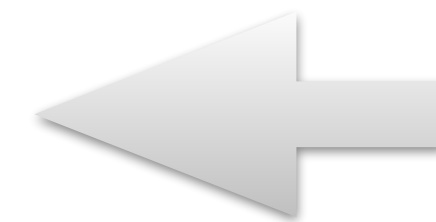
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".

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

Software: 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:

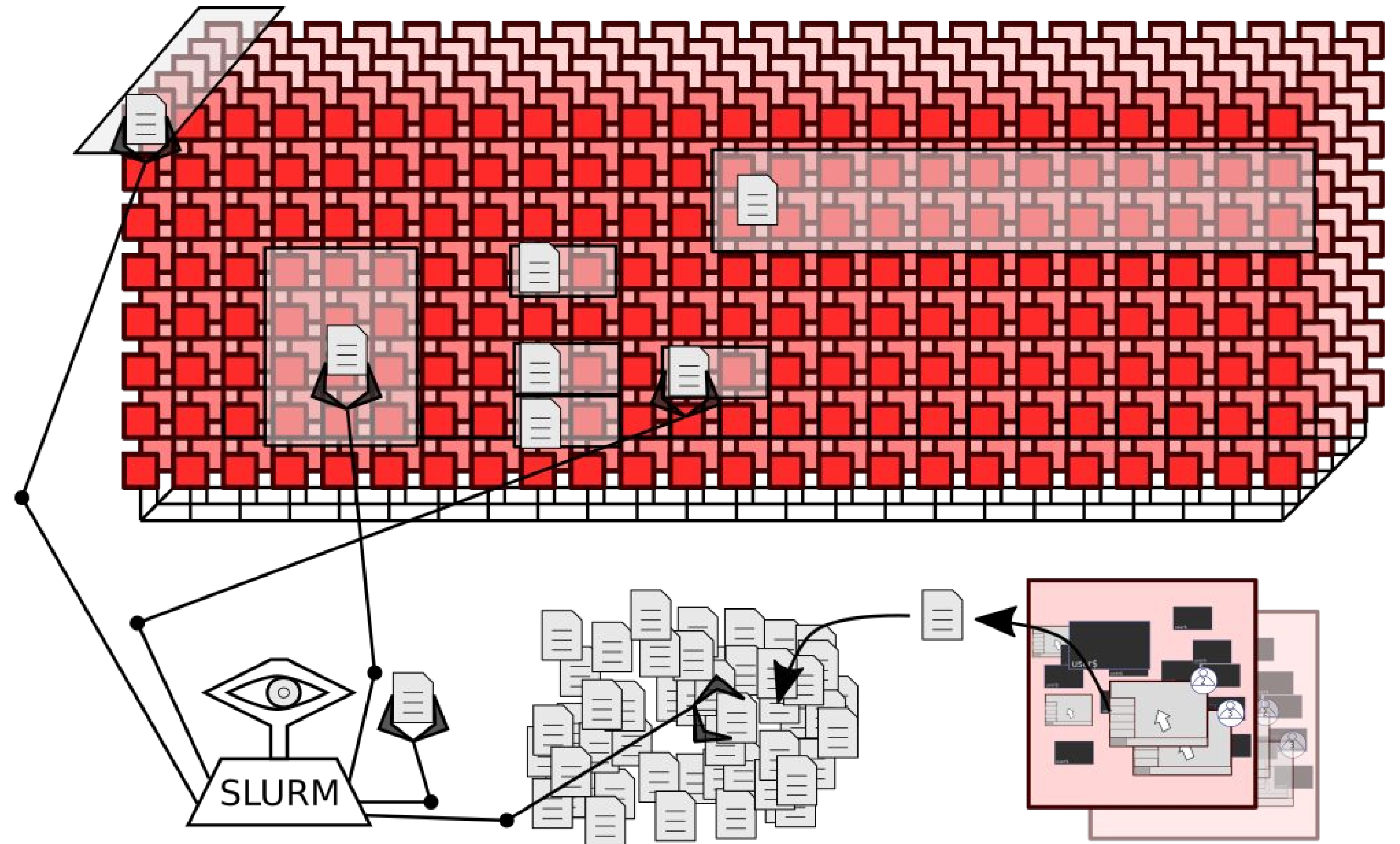
S: Module is Sticky, requires `--force` to unload or purge

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



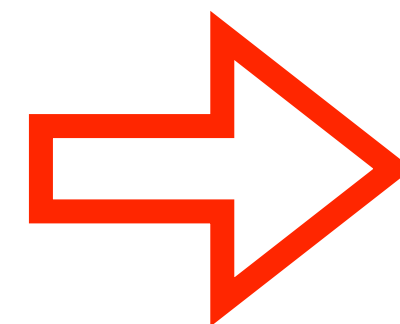
Slurm: Running Batch Job

- 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/6.1.0.28012020-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)