

# NSC, HPC & Tetralith

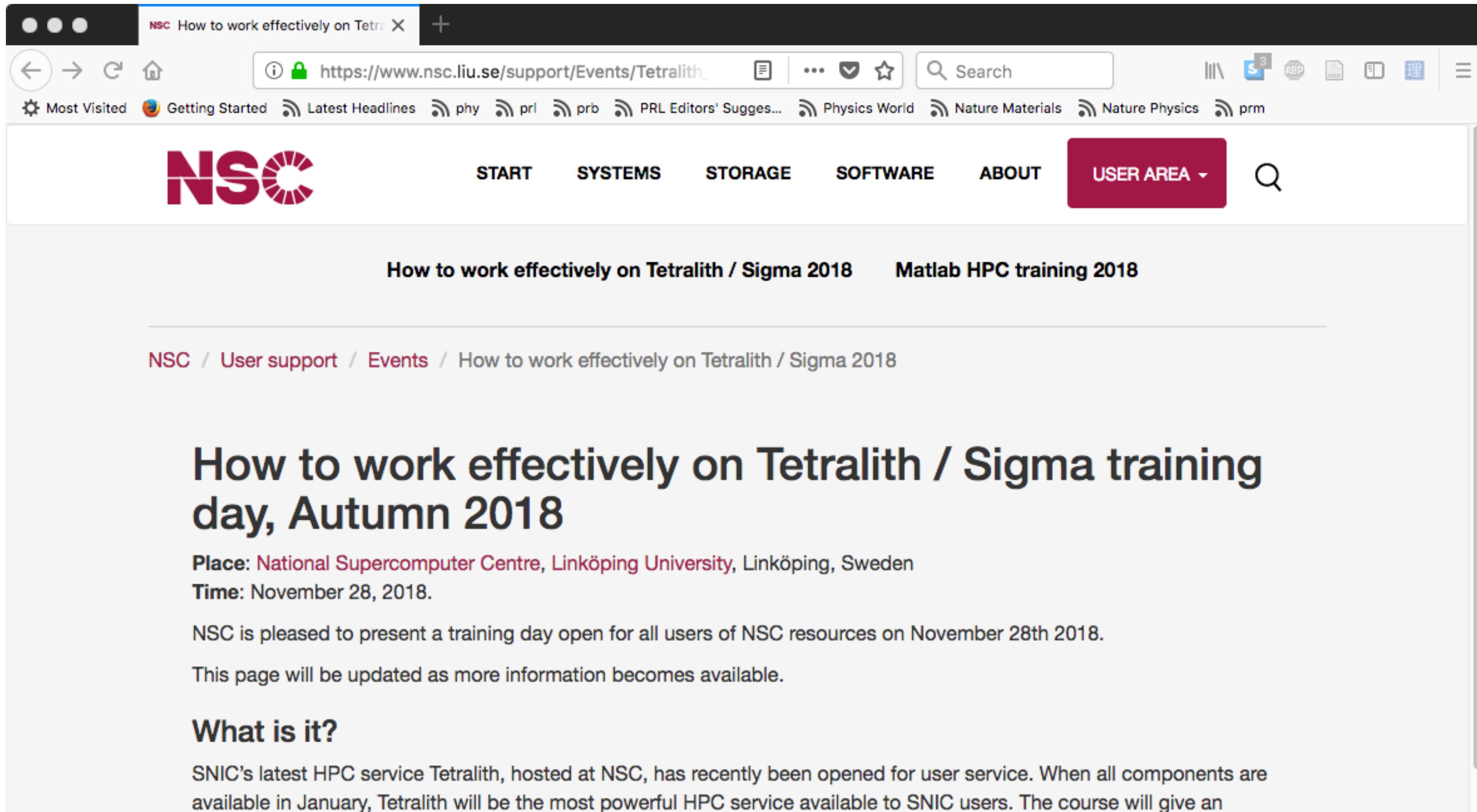
Weine Olovsson - Fridays @Fysikhuset F306

National Supercomputer Centre (NSC)

@Matlab HPC training, 24th Oct 2018, in jupiter

# Tetralith training - Nov 28th @NSC

NSC training/courses events: <https://www.nsc.liu.se/support/Events/>



The screenshot shows a web browser window with the URL <https://www.nsc.liu.se/support/Events/Tetralith>. 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 USER AREA dropdown. The main content area features a breadcrumb trail: NSC / User support / Events / How to work effectively on Tetralith / Sigma 2018. The primary heading is "How to work effectively on Tetralith / Sigma training day, Autumn 2018". Below this, the location is listed as "National Supercomputer Centre, Linköping University, Linköping, Sweden" and the time as "November 28, 2018". A paragraph states: "NSC is pleased to present a training day open for all users of NSC resources on November 28th 2018. This page will be updated as more information becomes available." A section titled "What is it?" begins with the text: "SNIC's latest HPC service Tetralith, hosted at NSC, has recently been opened for user service. When all components are available in January, Tetralith will be the most powerful HPC service available to SNIC users. The course will give an

# About NSC

- NSC is a **National HPC center** hosted at Linköping University (LiU)
- NSC is an **independent organization** at LiU under direct control of the Vice-Chancellor (Rector)

“NSC is a provider of leading edge **national supercomputing** resources. We provide a wide range of **high performance computing** and data services to members of academic institutions throughout Sweden and to our partners SMHI, MET Norway, and Saab”

# What is HPC?

**High Performance Computing** is the application of "**supercomputers**" (or high performance computers) to **computational problems** that are either **too large** for desktop/workstation computers or would take **too long time** on such computers.

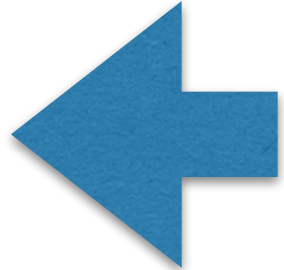
A Supercomputer or a High Performance Computer refers to a system that somehow **aggregates computing power** in a way that delivers much higher performance than one could get out of a typical desktop/workstation computer.

Today most High Performance Computers are really **clusters of powerful workstations**.

# When to use HPC?

- **High number** of simulation or data analysis jobs
- Simulations or data analysis jobs which are **too large** for desktop PC

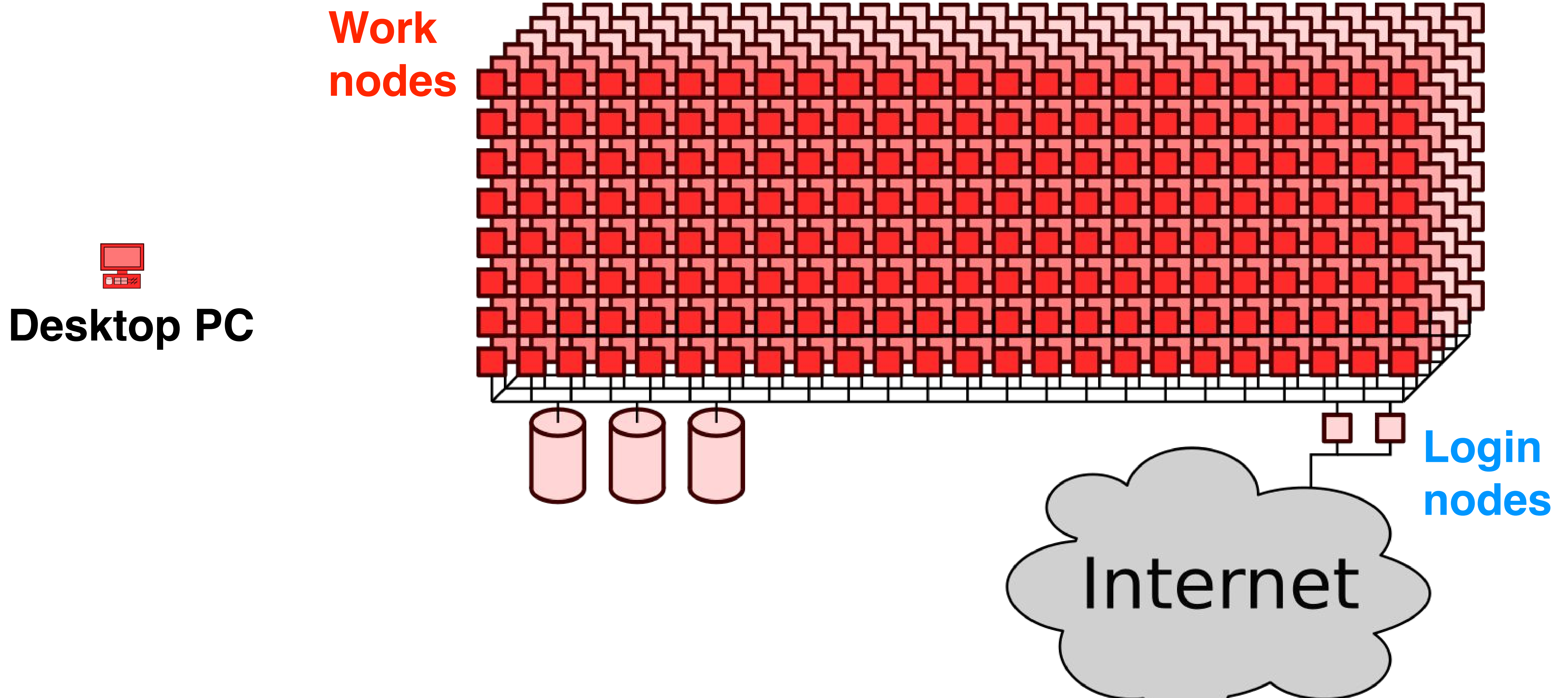
# What is HPC used for?

- Materials science  Largest part of NSC academic usage
- Many disciplines within chemistry, physics and biology
- Numerical weather prediction simulations - weather forecasts
- Climate simulations
- Flow simulations - car, truck, train, aeroplane etc. construction
- ...



# Desktop PC vs HPC: Scale

**Tetralith cluster at NSC**



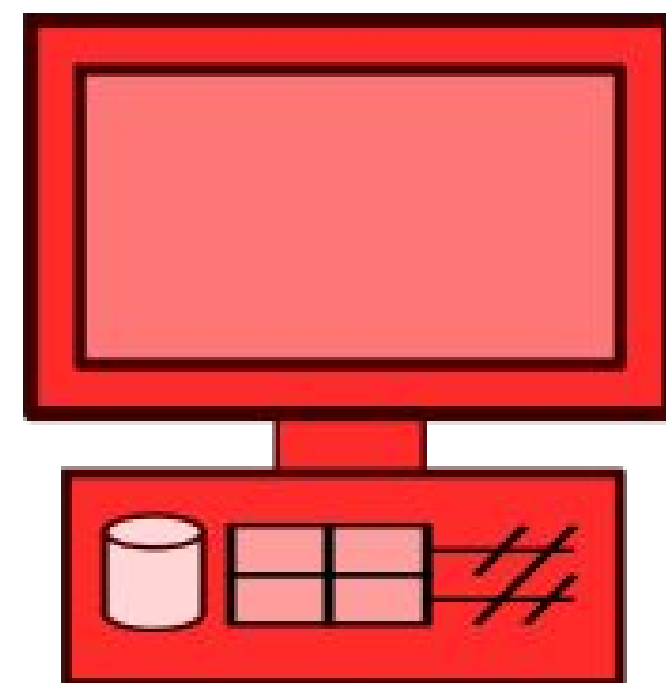
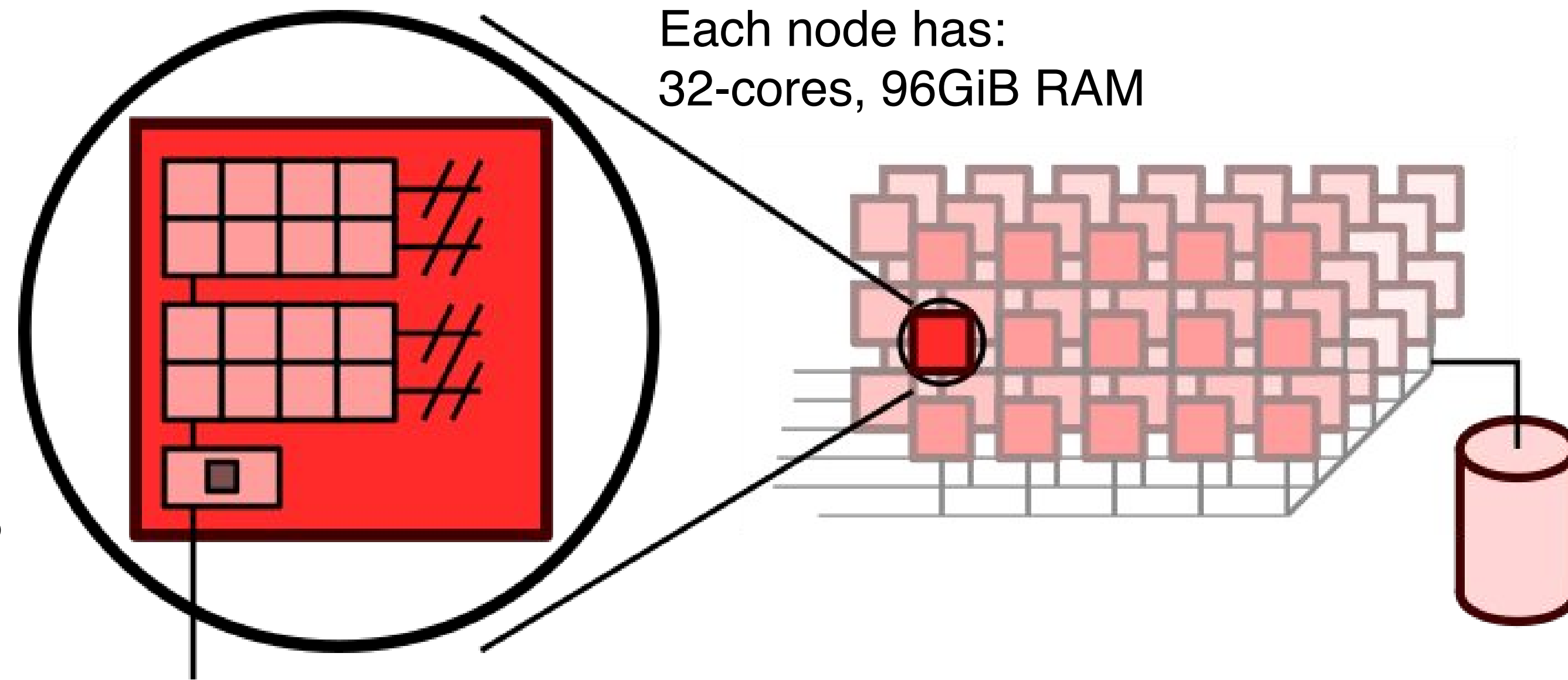
# Desktop PC vs HPC: Scale

## **Sigma (LiU)**

108 nodes

## **Tetralith (SNIC)**

652 -> 1892 nodes



Typical PC has  
4-cores, 8GiB RAM



# Desktop PC vs HPC

## Shared resource

- Your desktop is your own, it's not shared
- Typical national level HPC systems are shared by **hundreds of researchers**

## Workflow

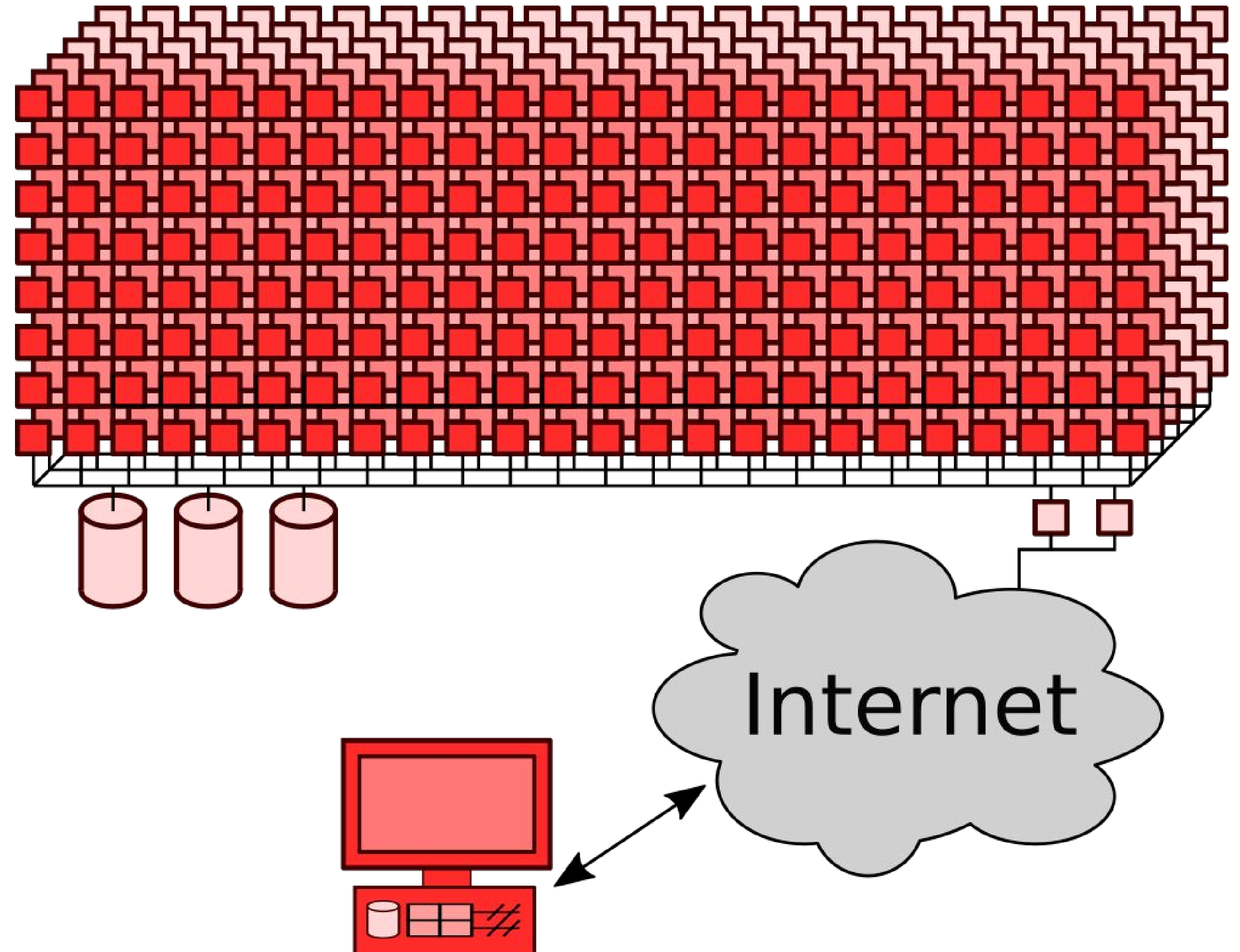
- On a desktop the interfaces are direct and immediate
- On an HPC resource work typically happens in “batch mode”. Most work is prepared and **queued to run** when resources become available

# Access to HPC: login

Tetralith has 2 login nodes

Login nodes sit on the edge between the real compute resource and the network

Storage visible across the entire system



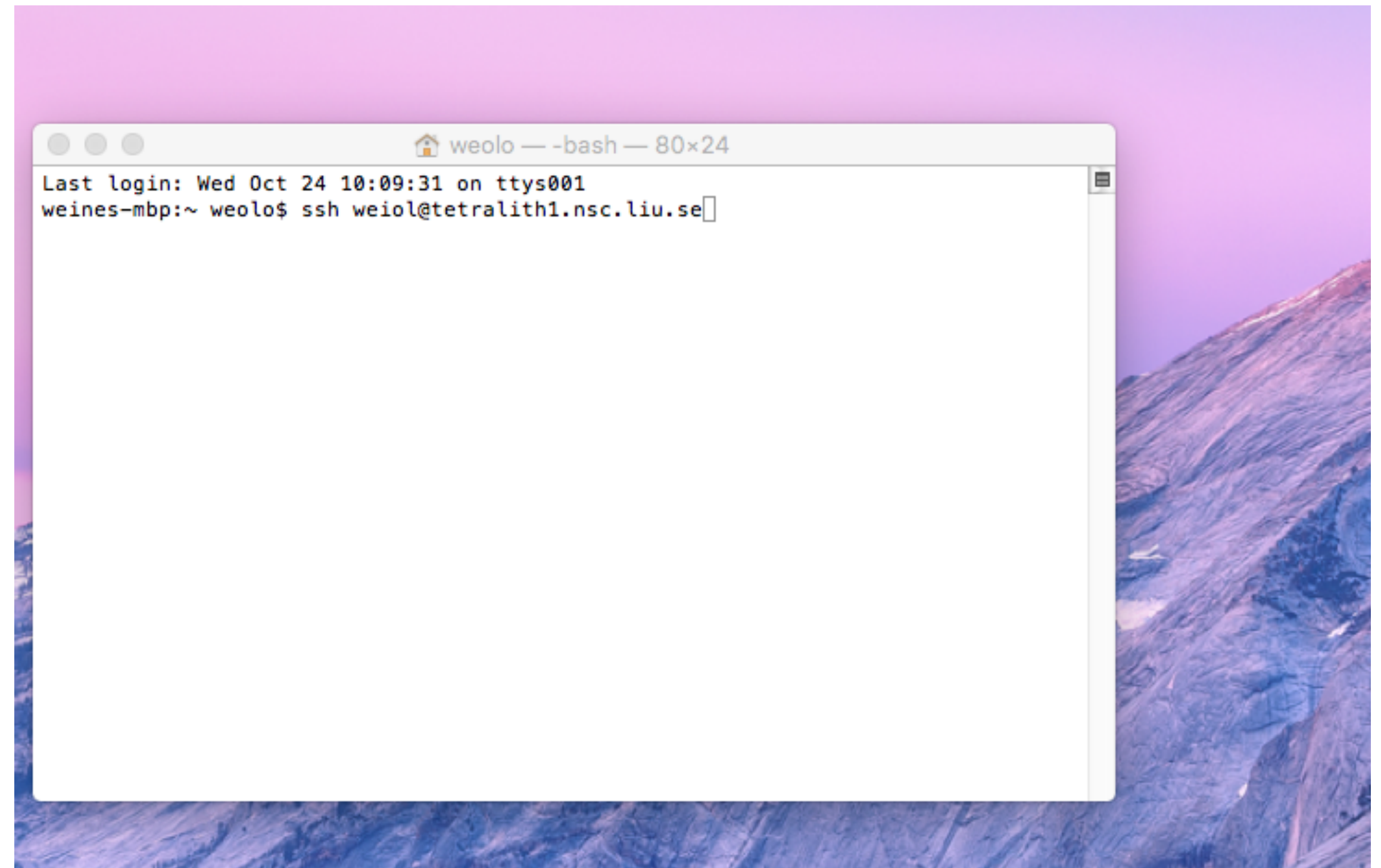
# Access to HPC: login, classical way

Typical login via terminal from Linux / Mac:

```
ssh username@tetralith1.nsc.liu.se
```

also: tetralith2

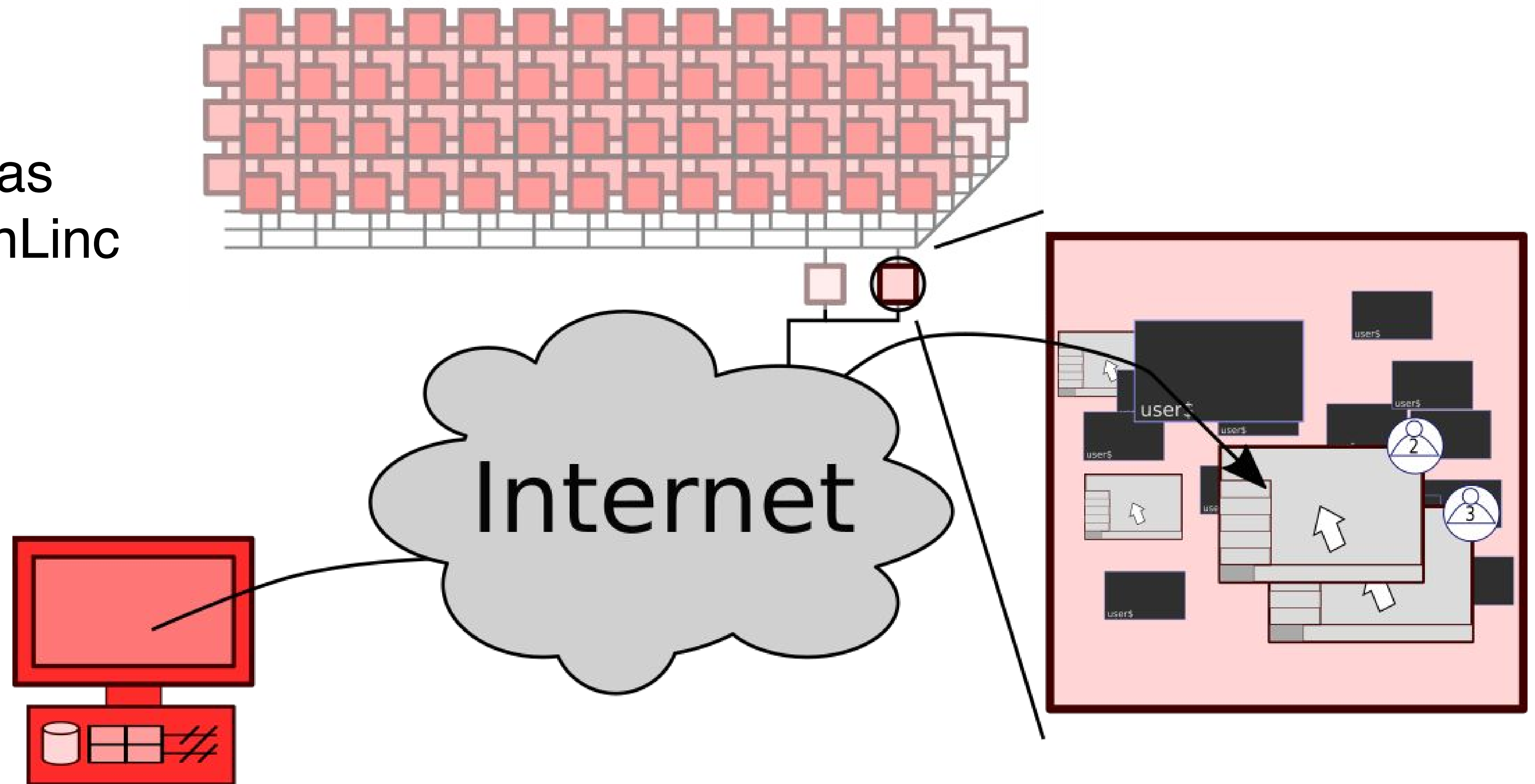
Windows: can use PuTTY



More information: <https://www.nsc.liu.se/support/getting-started/>

# Access to HPC: login, virtual desktop

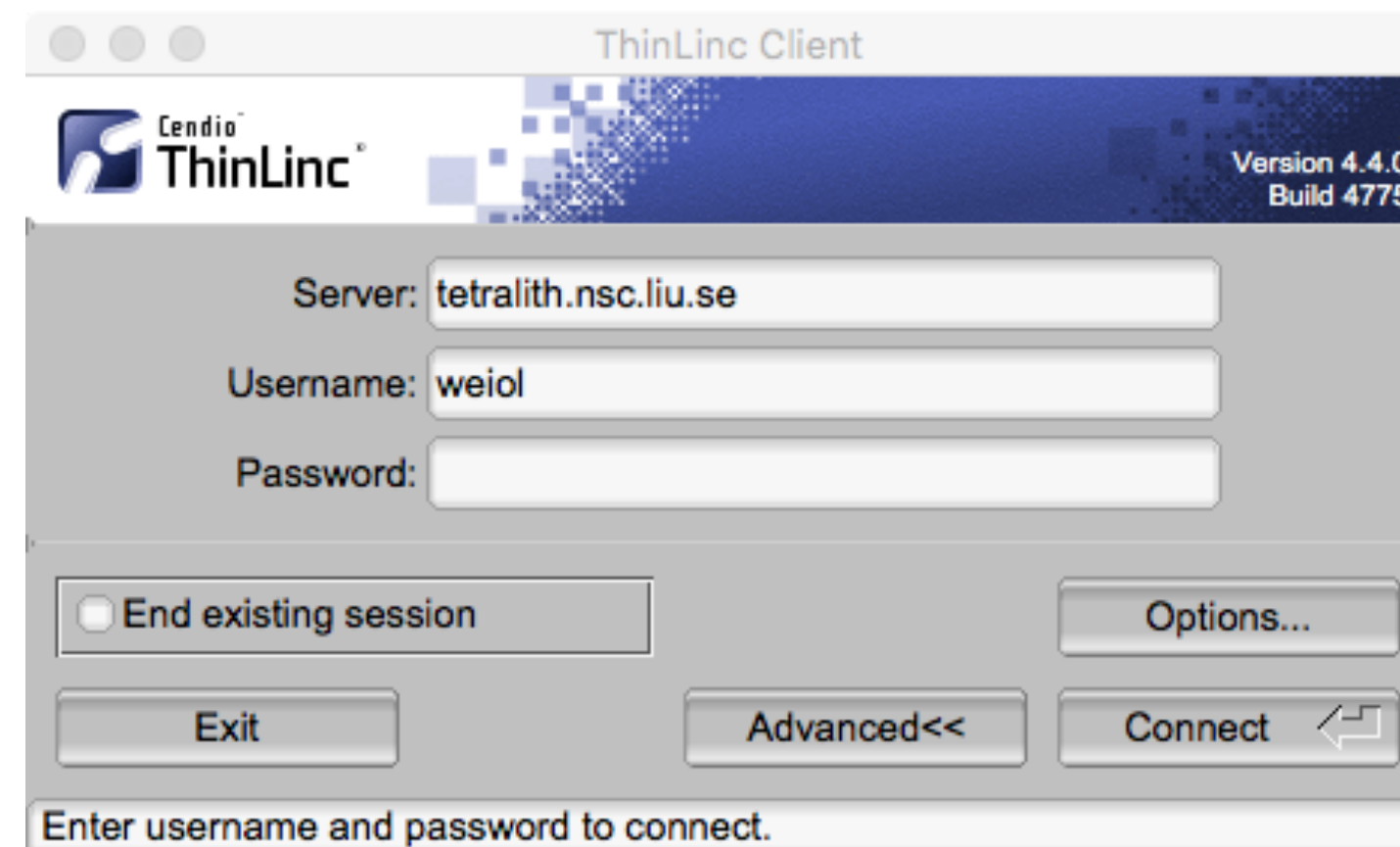
Each login node has many ssh and ThinLinc users at once





# ThinLinc: The ThinLinc client

First step: you need a ThinLinc client installed on your computer

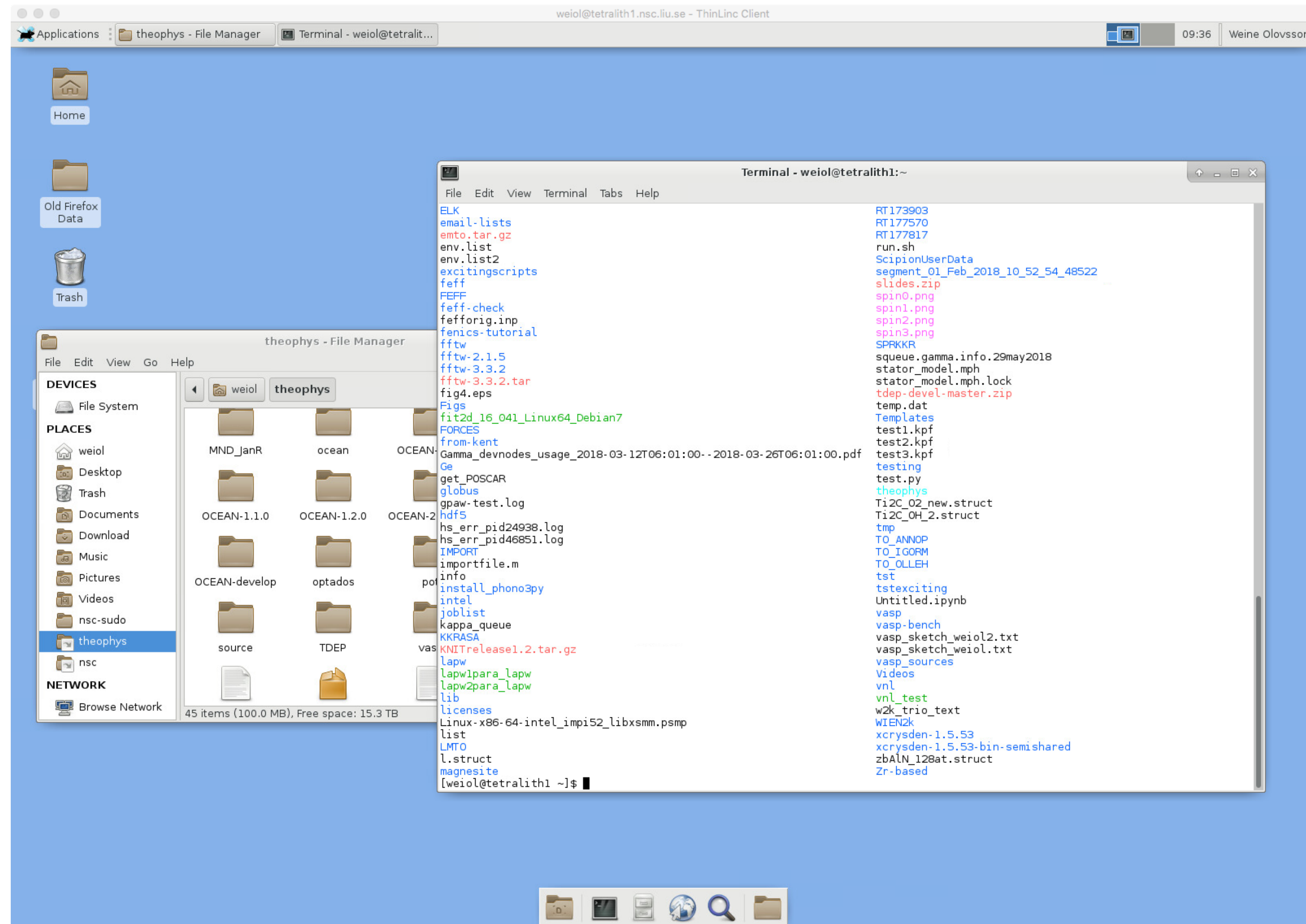


ThinLinc download: <https://www.cendio.com/thinlinc/download>

Cendio webpage: <https://www.cendio.com/thinlinc/what-is-thinlinc>

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

# ThinLinc: The ThinLinc desktop



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



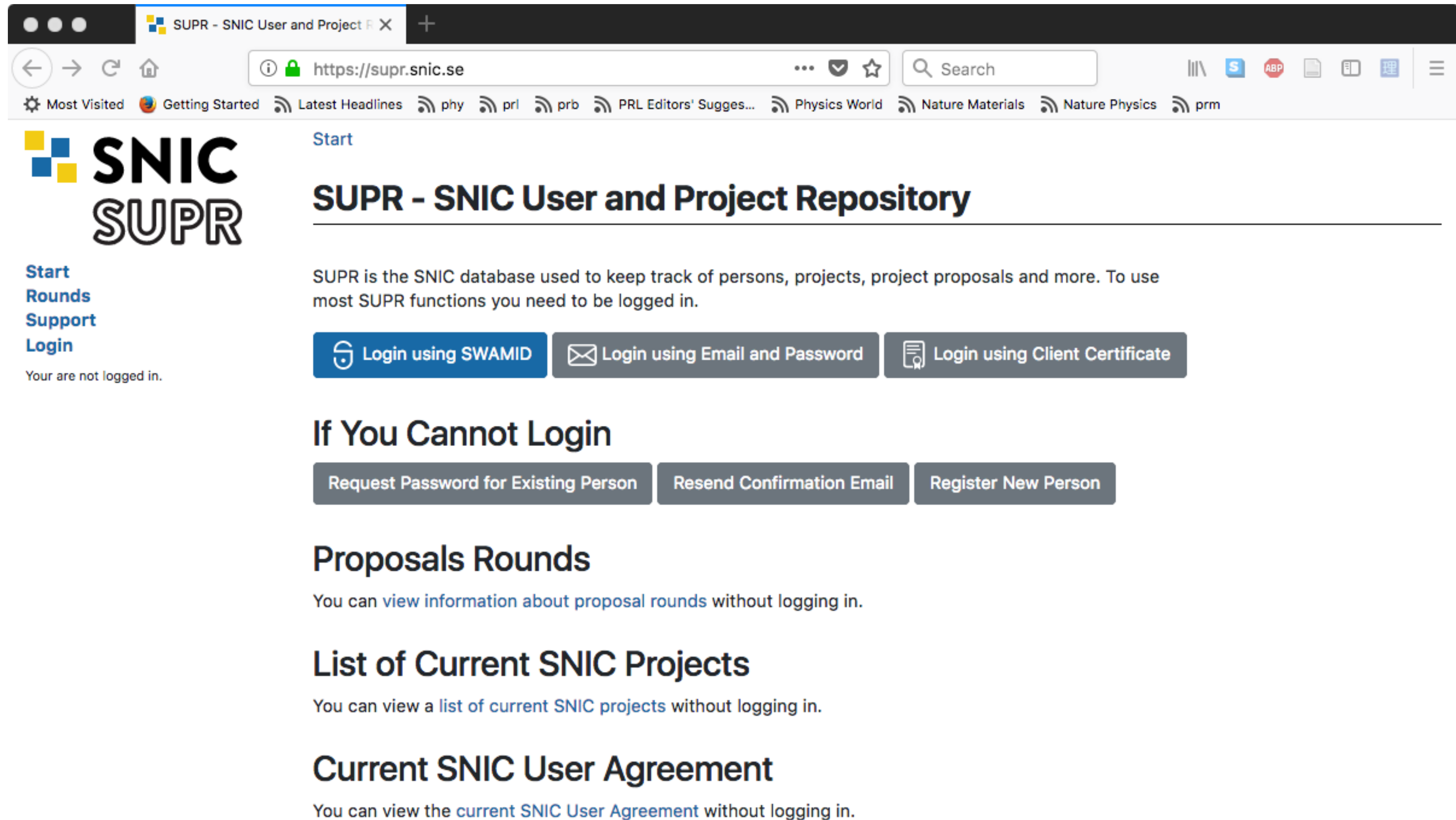
# ThinLinc: Advantages

- Provides a desktop interface to the system
- Allows for persistent sessions

(similar functionality can be had in a text terminal using screen or tmux)

- **NSC recommends** ThinLinc for graphical applications (vs. x-forwarding)
- Hardware accelerated 3D graphics possible (vglrun)

# Get HPC Access <https://supr.snic.se/>



**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

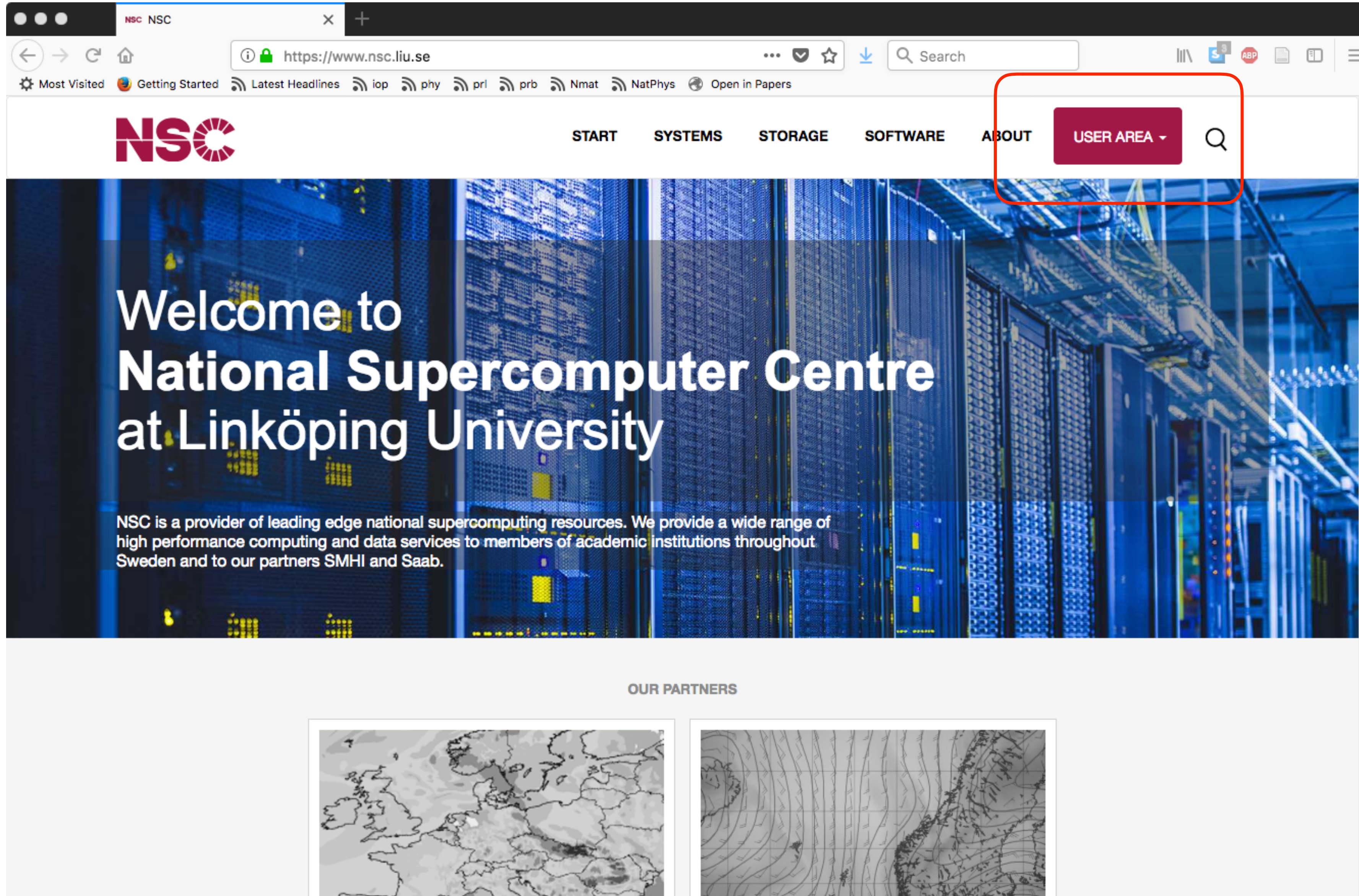
You can view a [list of current SNIC projects](#) without logging in.

### Current SNIC User Agreement

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



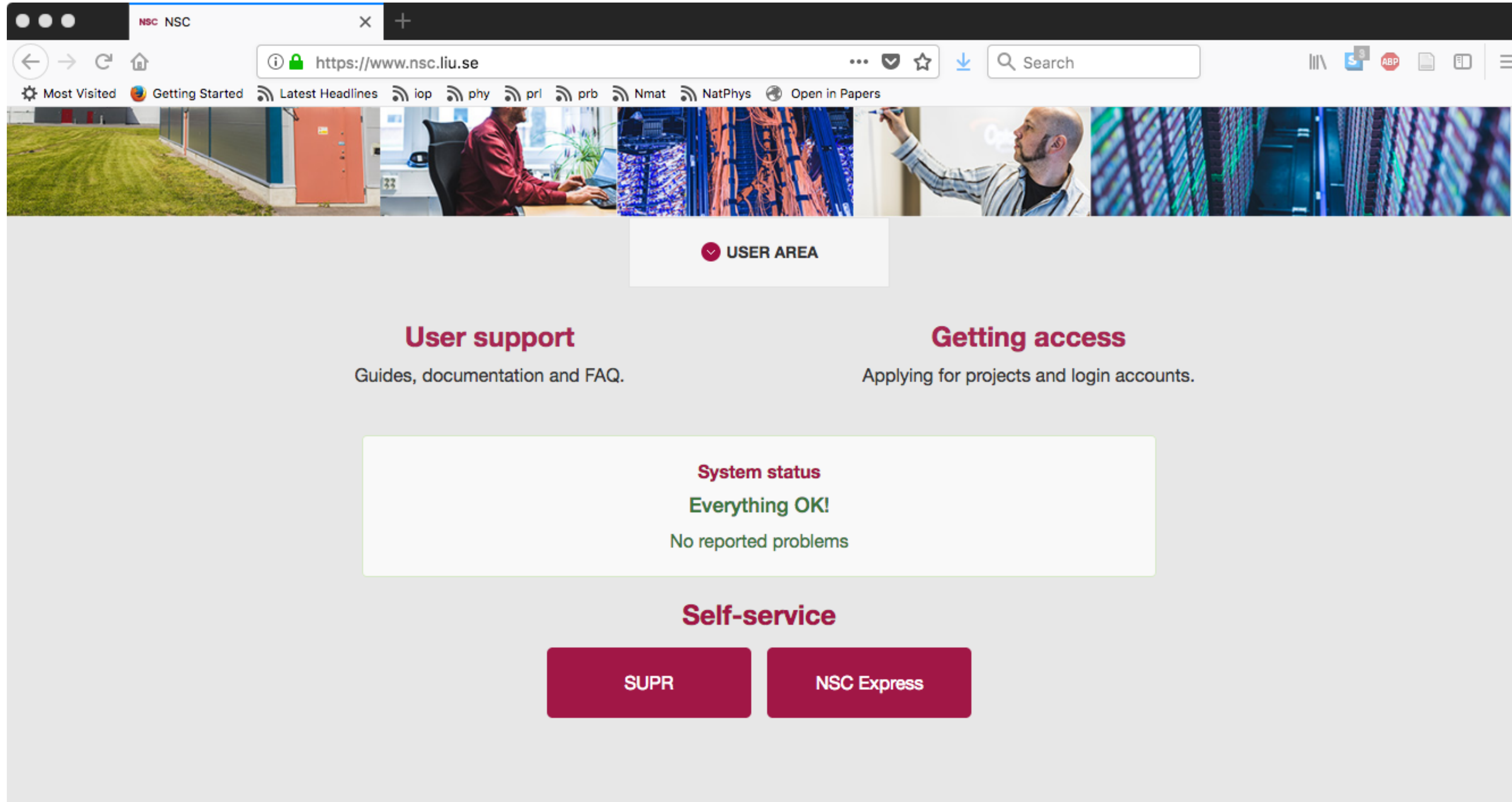
# Documentation & Support



The image shows a browser window displaying the homepage of the National Supercomputer Centre at Linköping University (NSC). The browser's address bar shows the URL <https://www.nsc.liu.se>. The website's navigation menu includes links for START, SYSTEMS, STORAGE, SOFTWARE, and ABOUT. A red rectangular box highlights the 'USER AREA' dropdown menu, which is currently closed. Below the navigation menu, the main content area features a large blue-tinted image of server racks. Overlaid on this image is the text: 'Welcome to National Supercomputer Centre at Linköping University'. Below this, a smaller text block states: 'NSC is a provider of leading edge national supercomputing resources. We provide a wide range of high performance computing and data services to members of academic institutions throughout Sweden and to our partners SMHI and Saab.' At the bottom of the page, there is a section titled 'OUR PARTNERS' which contains two grayscale images: a map of Europe and a technical diagram or map.



# Documentation & Support



The screenshot shows a web browser window with the URL <https://www.nsc.liu.se>. The browser's address bar and navigation icons are visible. Below the browser, a navigation menu includes links for 'Most Visited', 'Getting Started', 'Latest Headlines', and various research groups like 'iop', 'phy', 'prl', 'prb', 'Nmat', and 'NatPhys'. A banner image at the top features a person working at a computer, server racks, and a person pointing at a screen. Below the banner, a 'USER AREA' button is centered. The main content area is divided into four 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').



**National Supercomputer Centre**  
Linköping University  
581 83 LINKÖPING  
SWEDEN

Org.nr: 202100-3096  
VAT.nr: SE202100309601

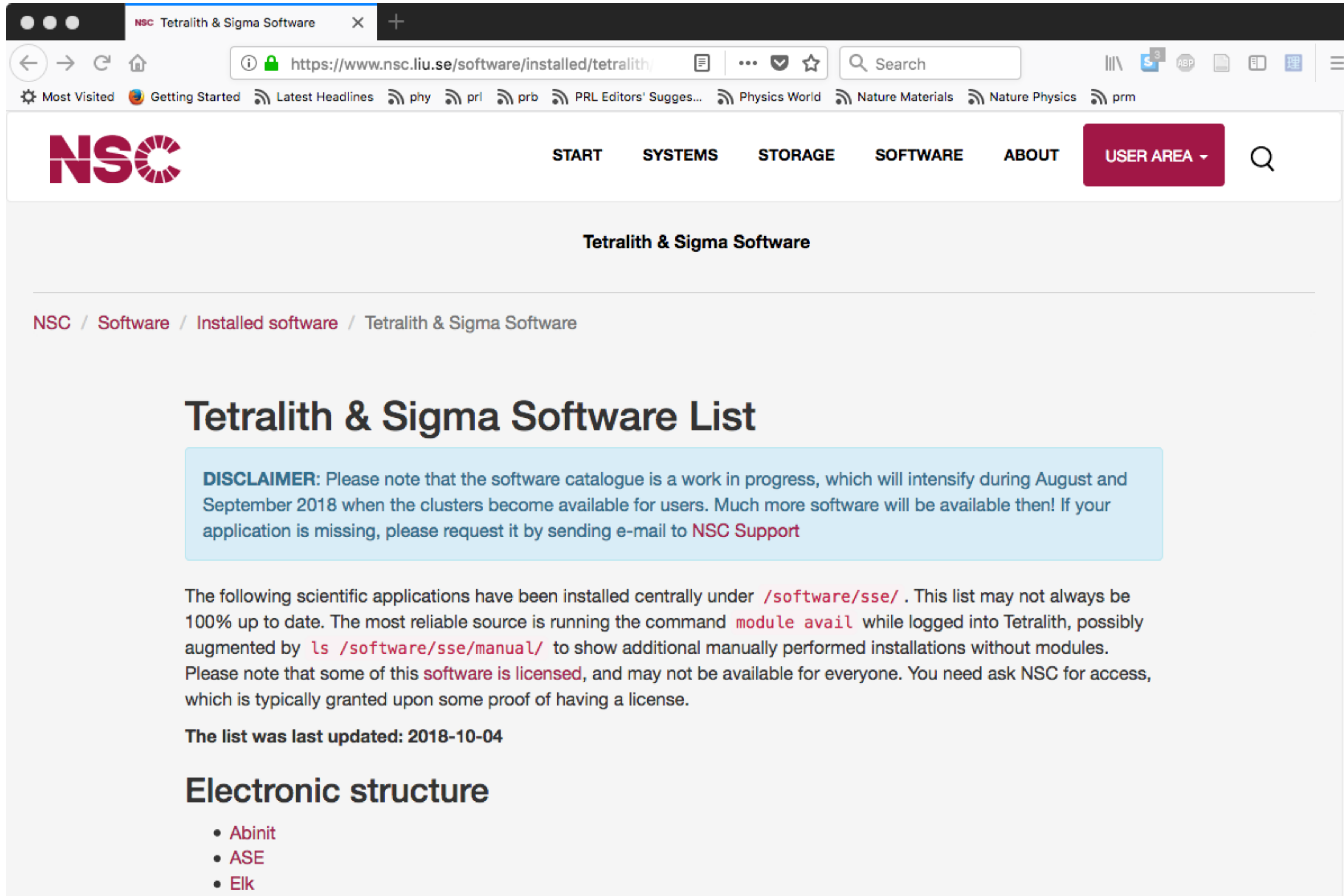
E-mail: [support@nsc.liu.se](mailto:support@nsc.liu.se)  
Tel.: 013-281000 (switchboard)  
Fax.: 013-149403  
Further address information

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



[Top of Page](#)

# Documentation & Support



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. The primary heading is "Tetralith & Sigma Software List". A light blue disclaimer box states: "DISCLAIMER: Please note that the software catalogue is a work in progress, which will intensify during August and September 2018 when the clusters become available for users. Much more software will be available then! If your application is missing, please request it by sending e-mail to NSC Support". Below this, a paragraph explains that the list of centrally installed scientific applications under `/software/sse/` may not be 100% up to date and provides instructions for using the `module avail` command and `ls /software/sse/manual/` to check for manually performed installations. It also notes that some software is licensed and requires access from NSC. The list was last updated on 2018-10-04. The section "Electronic structure" is partially visible, listing [Abinit](#), [ASE](#), and [Elk](#).

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, which will intensify during August and September 2018 when the clusters become available for users. Much more software will be available then! 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, 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: 2018-10-04

### Electronic structure

- [Abinit](#)
- [ASE](#)
- [Elk](#)

# About NSC: Staff

- Current director: Matts Karlsson (Jun 2016 - )
- Currently 37 individuals (not all full-time)
- Mostly **system experts** and **application experts**
- Some management and administration



# Application Experts @NSC

## Application Expert:

Rickard Armiento (30%)

Chandan Basu

Frank Bramkamp

Martin Moche (20%)

Weine Olovsson (90%)

Johan Raber

Torben Rasmussen

Hamish Struthers

Wei Zhang

## PhD:

Physics

Cond. mat. physics

Mechanics

Str. biology

Physics

Chemistry

Chemistry

Chemical physics

HPC

## Work at NSC:

Hadoop/EasyBuild

Comp. sci.

Comp. fluid dynamics

Str. biology

Comp. materials sci.

Comp. chemistry

Comp. chemistry

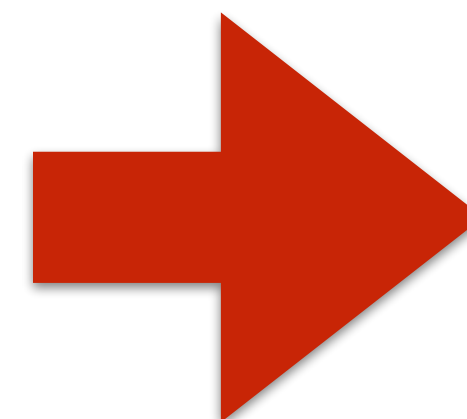
Climate research

Comp. sci.

# How NSC can help

- Provide computational resources (apply via SUPR)  
<https://supr.snic.se/>
- Software installation (global / local)
- Troubleshooting / advice
- Training (SNIC, local and other)  
<https://www.nsc.liu.se/support/Events/>

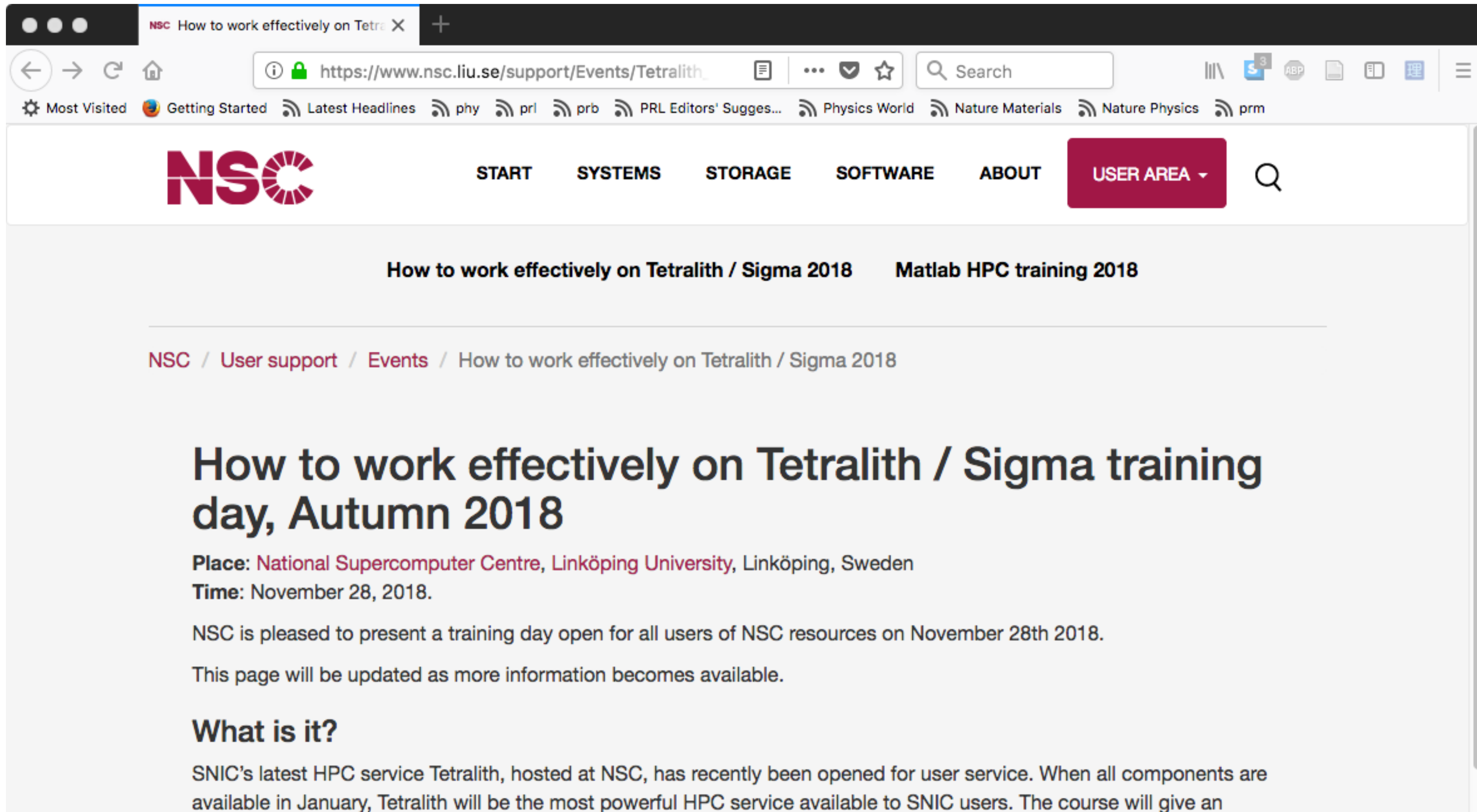
**Questions**



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

# Tetralith training - Nov 28th @NSC

NSC training/courses events: <https://www.nsc.liu.se/support/Events/>



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