NSC, HPC & Tetralith

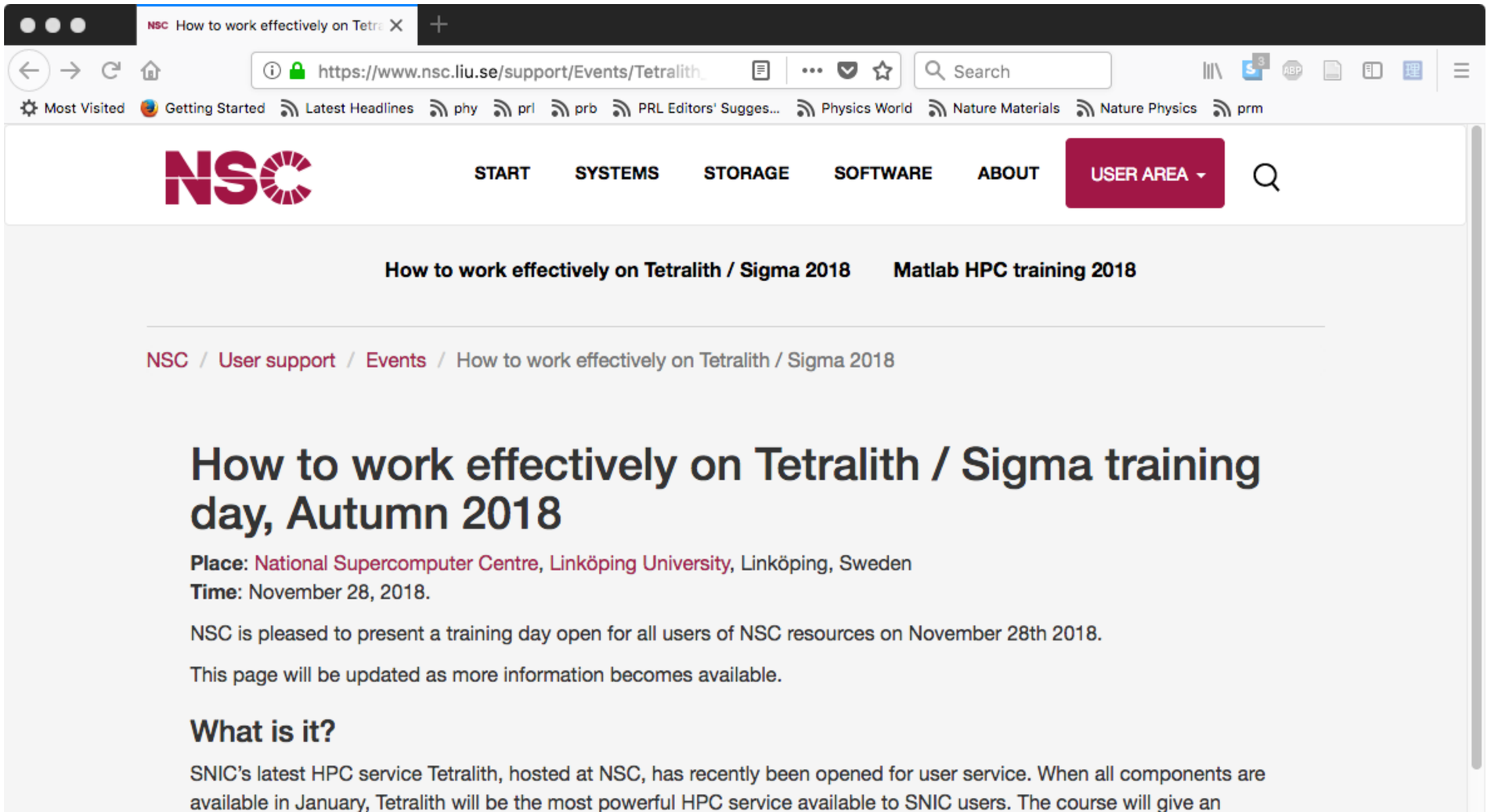
Weine Olovsson - Fridays @Fysikhuset F306
National Supercomputer Centre (NSC)

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

LINKÖPINGS UNIVERSITET

Tetralith training - Nov 28th @NSC

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



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”

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

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**.

https://www.top500.org/

When to use HPC?

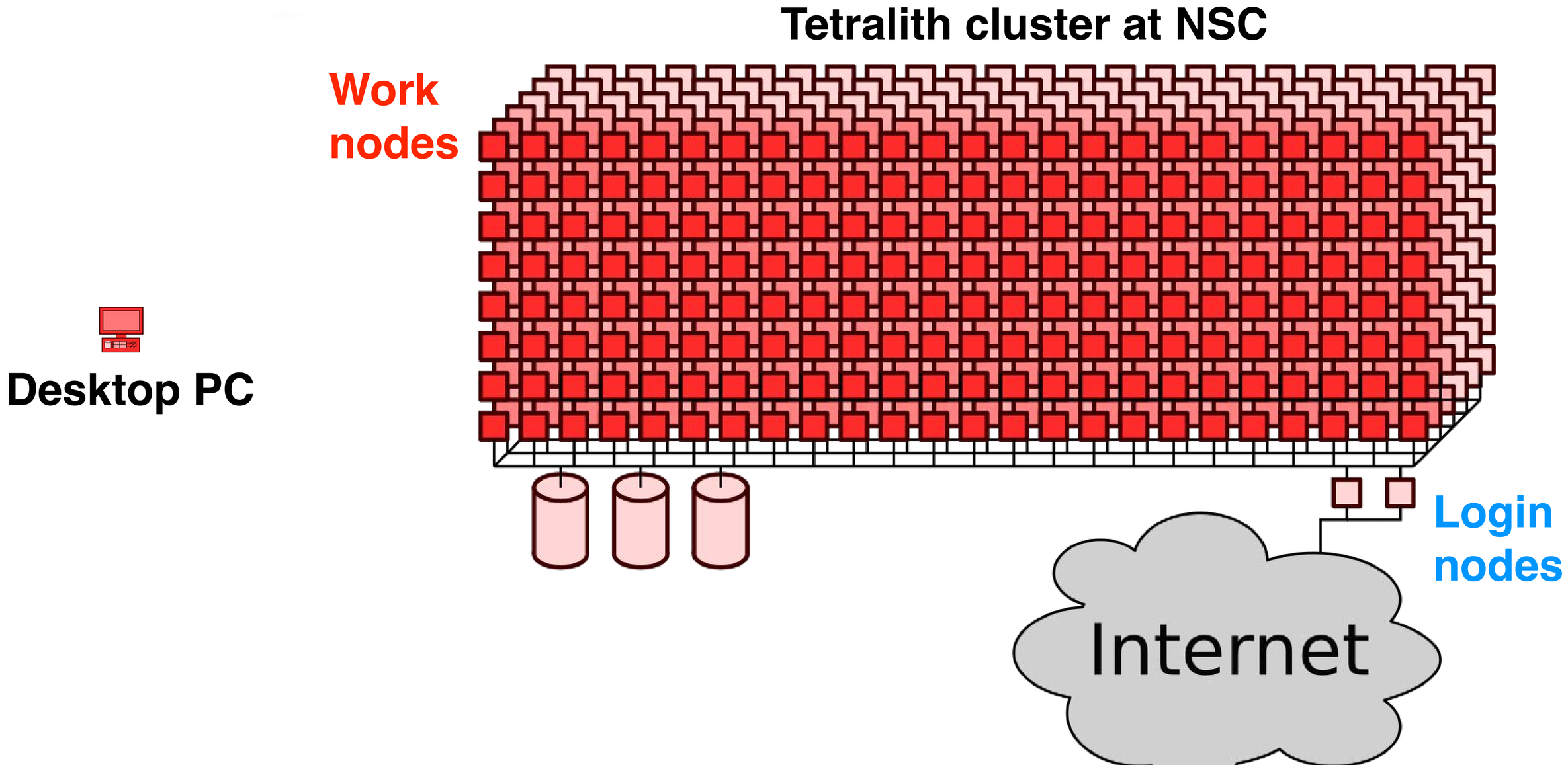
- **High number** of simulation or data analysis jobs

- 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 forcasts
- Climate simulations
- Flow simulations - car, truck, train, aeroplane etc. construction
- …

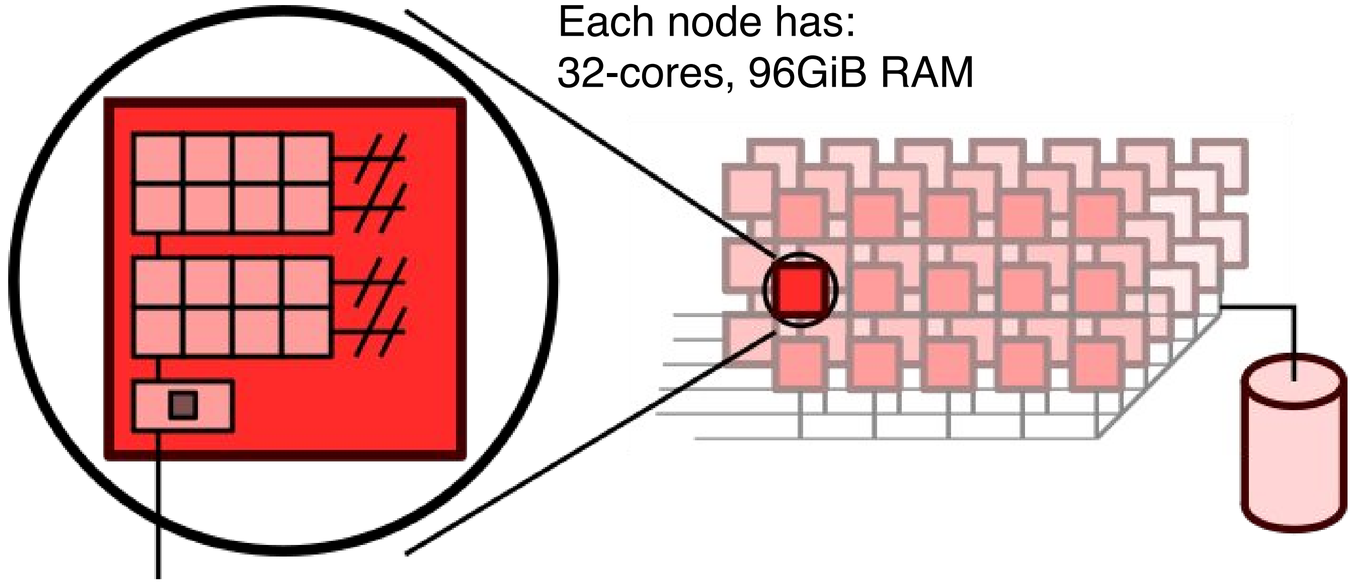
Desktop PC vs HPC: Scale

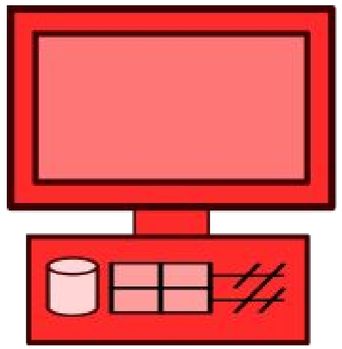


Desktop PC vs HPC: Scale

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

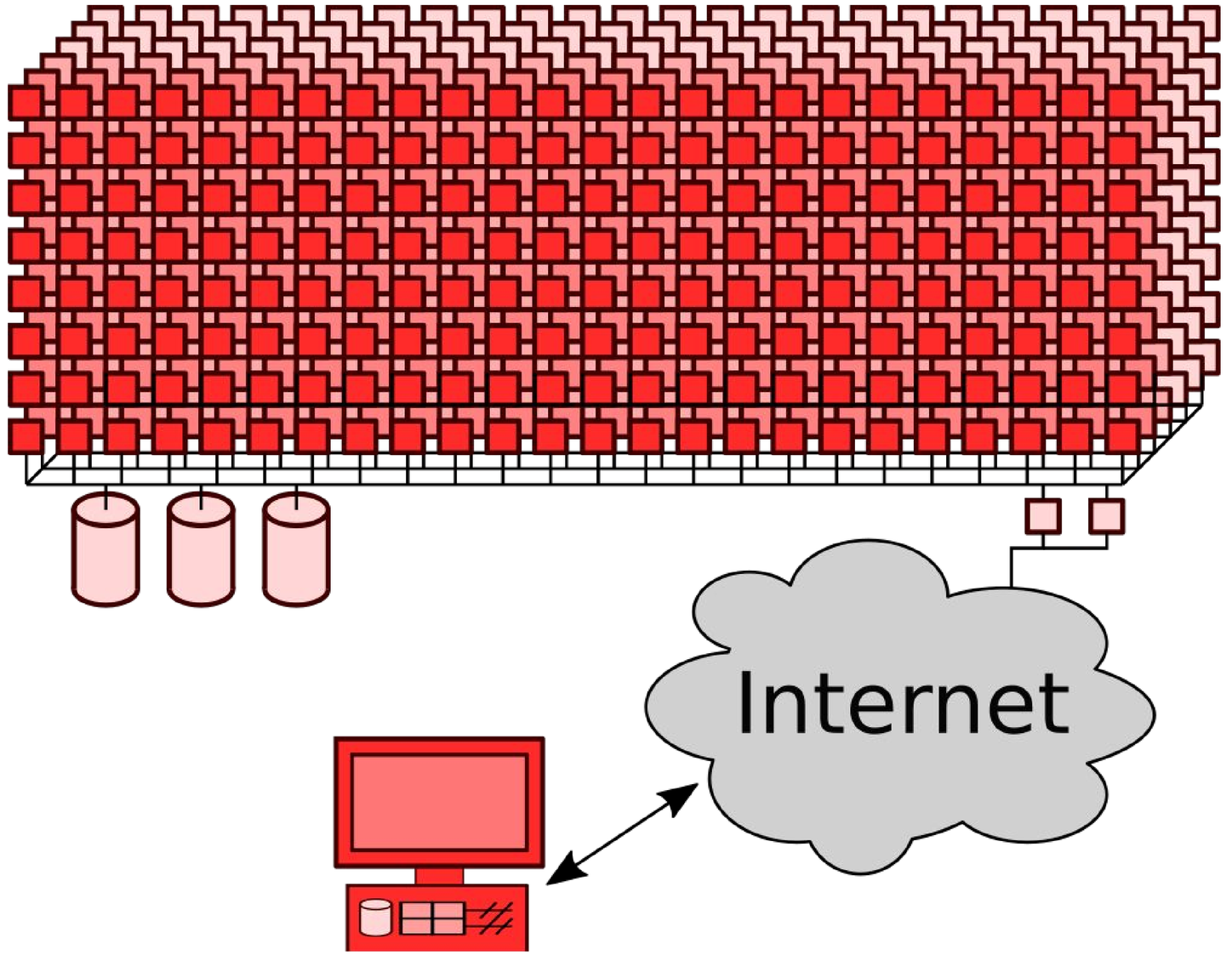
- On a desktop the interfaces are direct and immediate
- On an HPC resource work typically happens in "batch mode". Most work is prepared and queued to run when resources become available

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



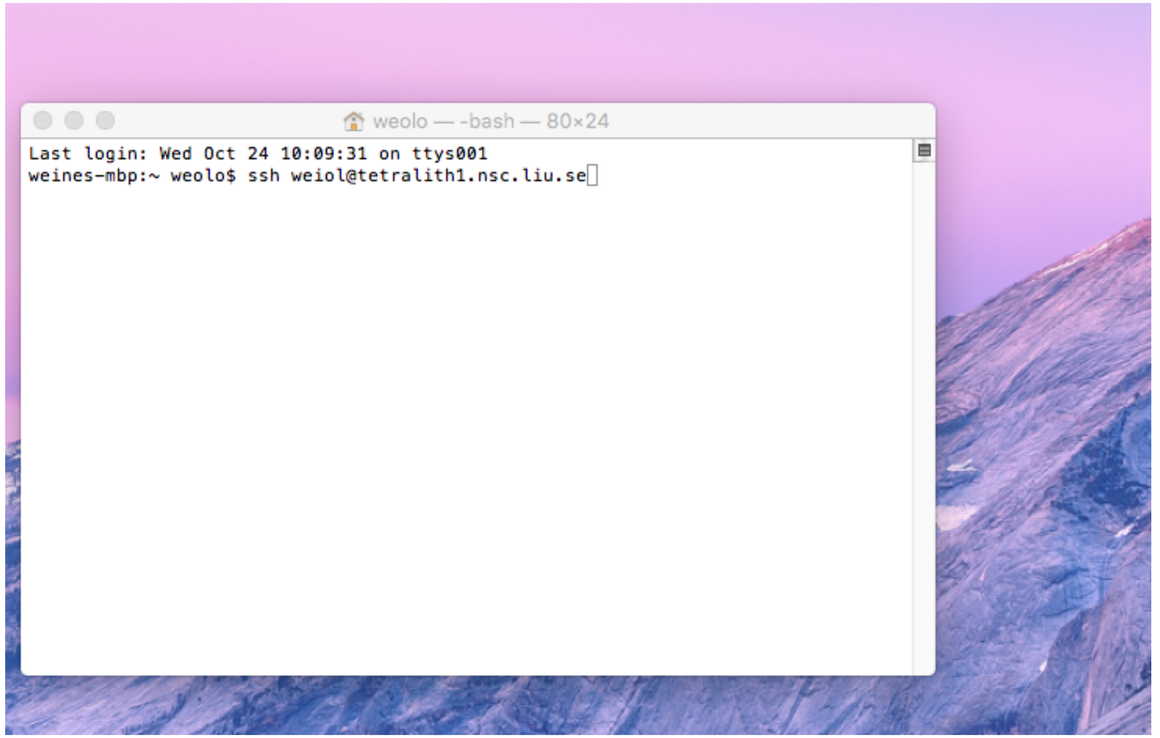
Access to HPC: login, classical way

Typical login via terminal from Linux / Mac:

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

also: `tetralith2`

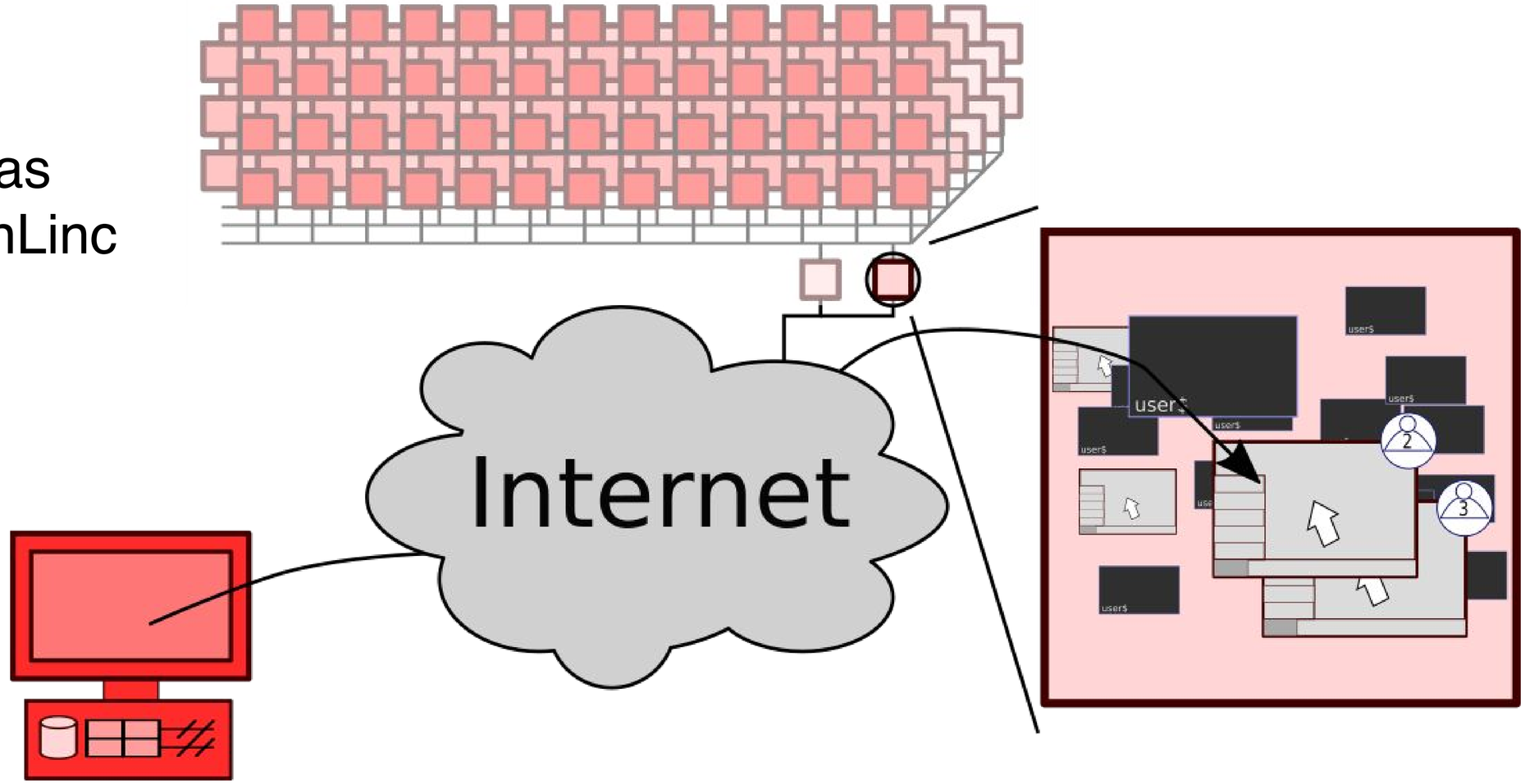
Windows: can use PuTTY



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

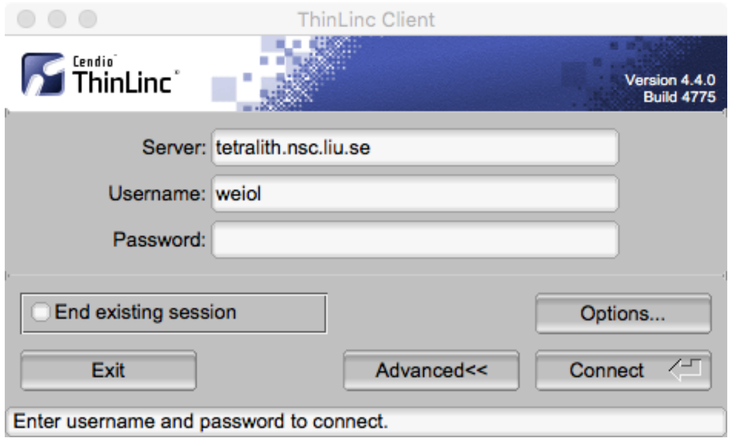
Access to HPC: login, virtual desktop

Each login node has many ssh and ThinLinc users at once



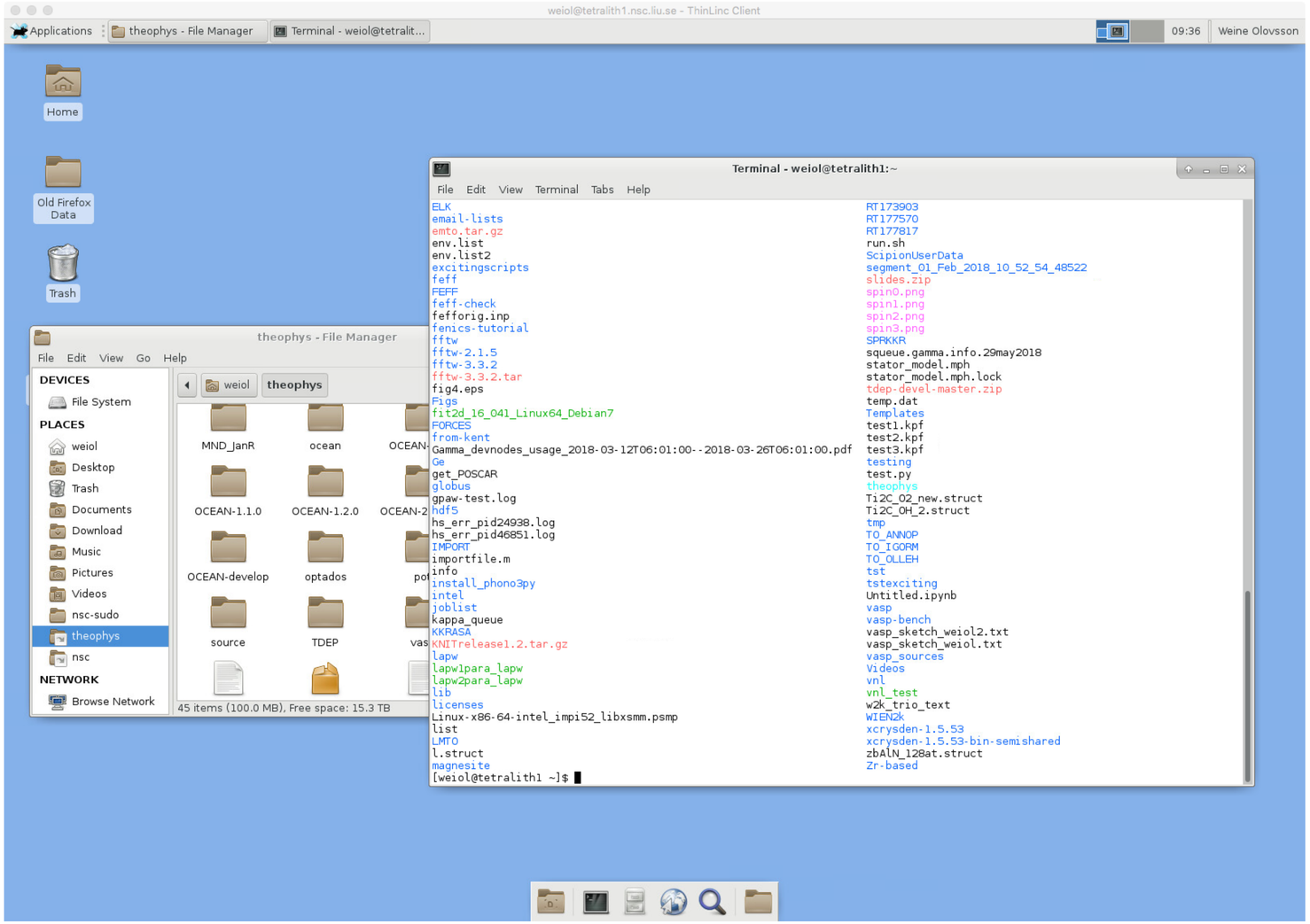
ThinLinc: The ThinLinc client

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



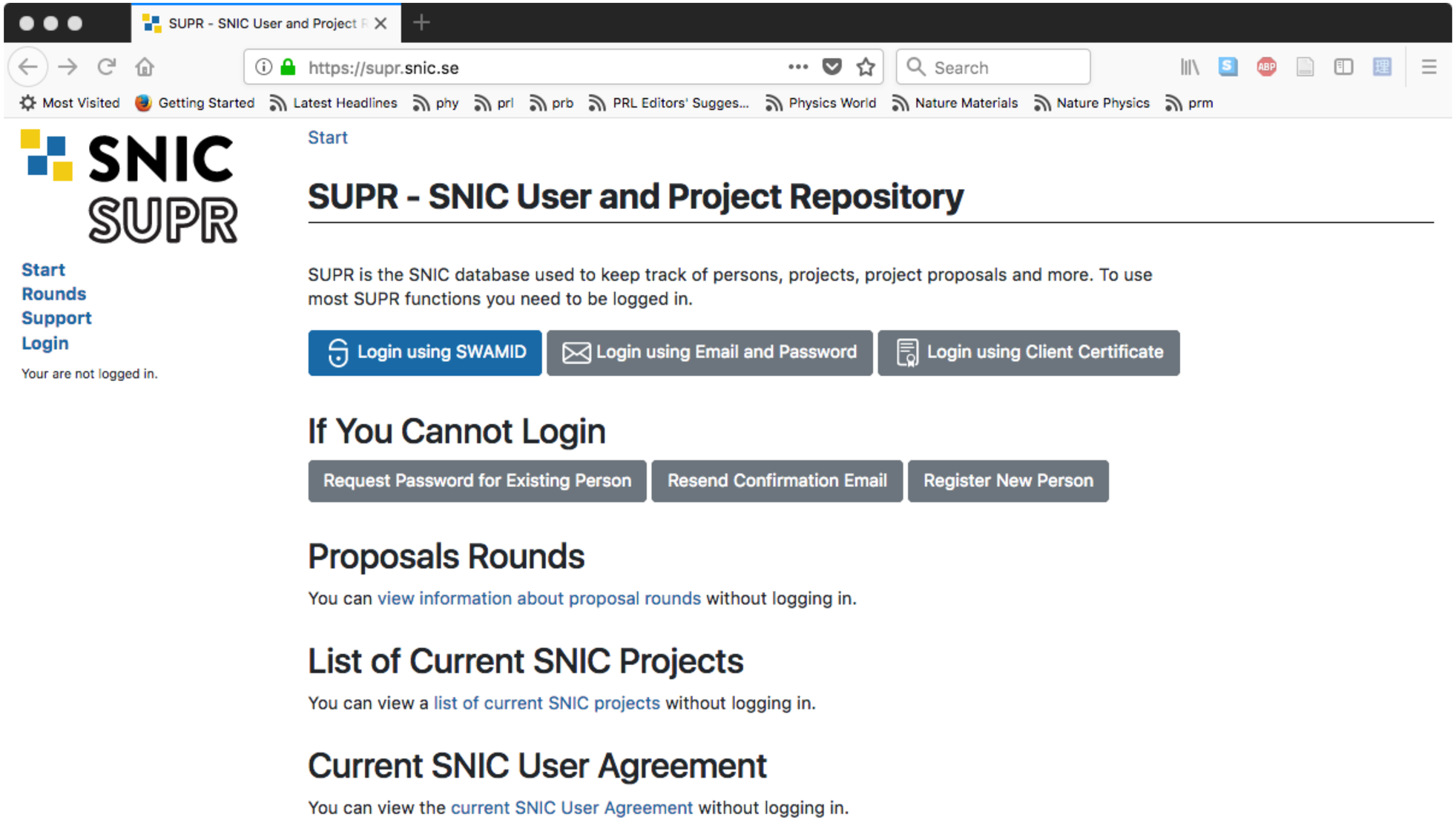
NSC documentation: https://www.nsc.liu.se/support/graphics/

ThinLinc: Advantages

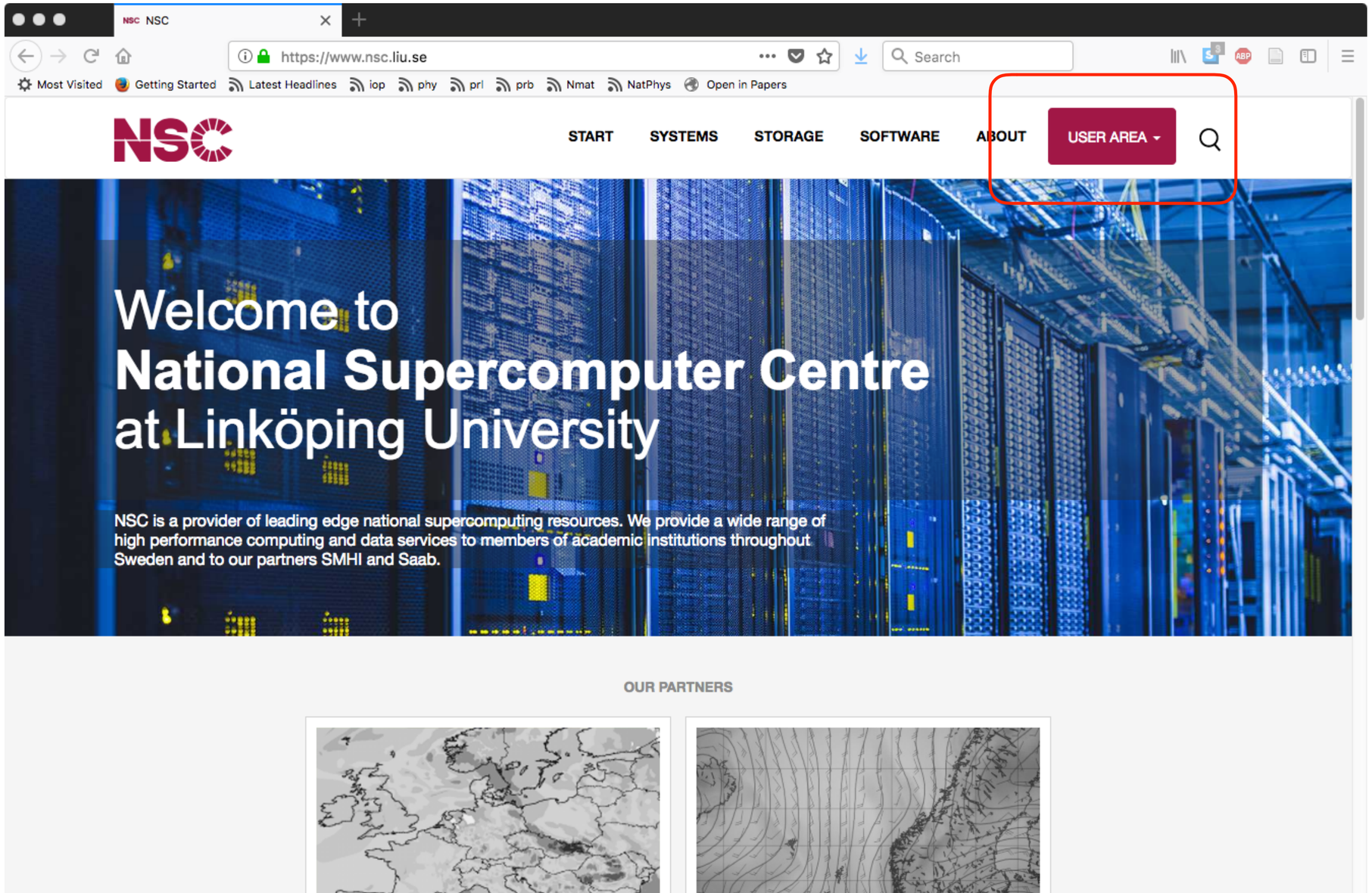
- Provides a desktop interface to the system
- Allows for persistent sessions

  (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/



Documentation & Support



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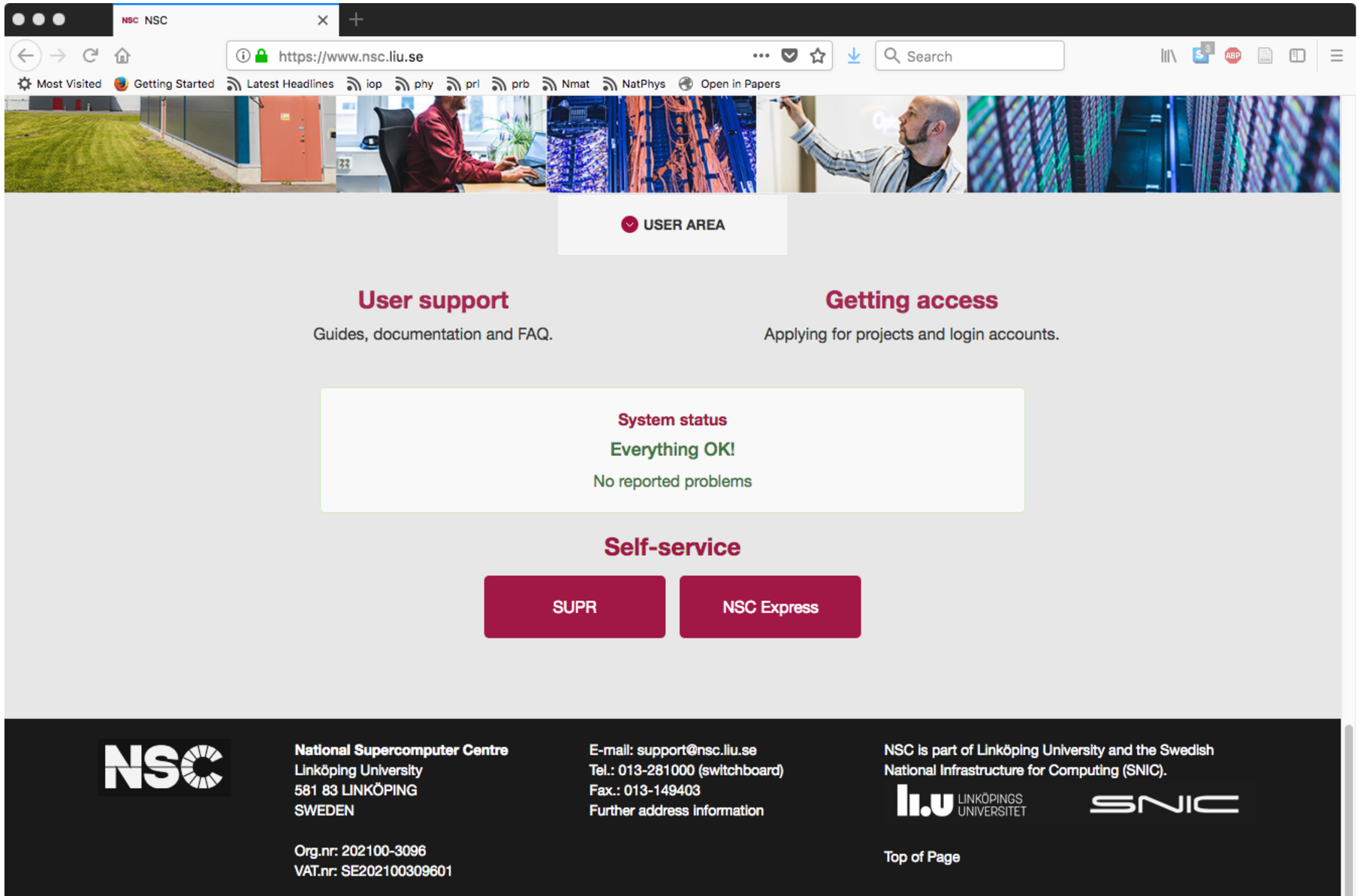

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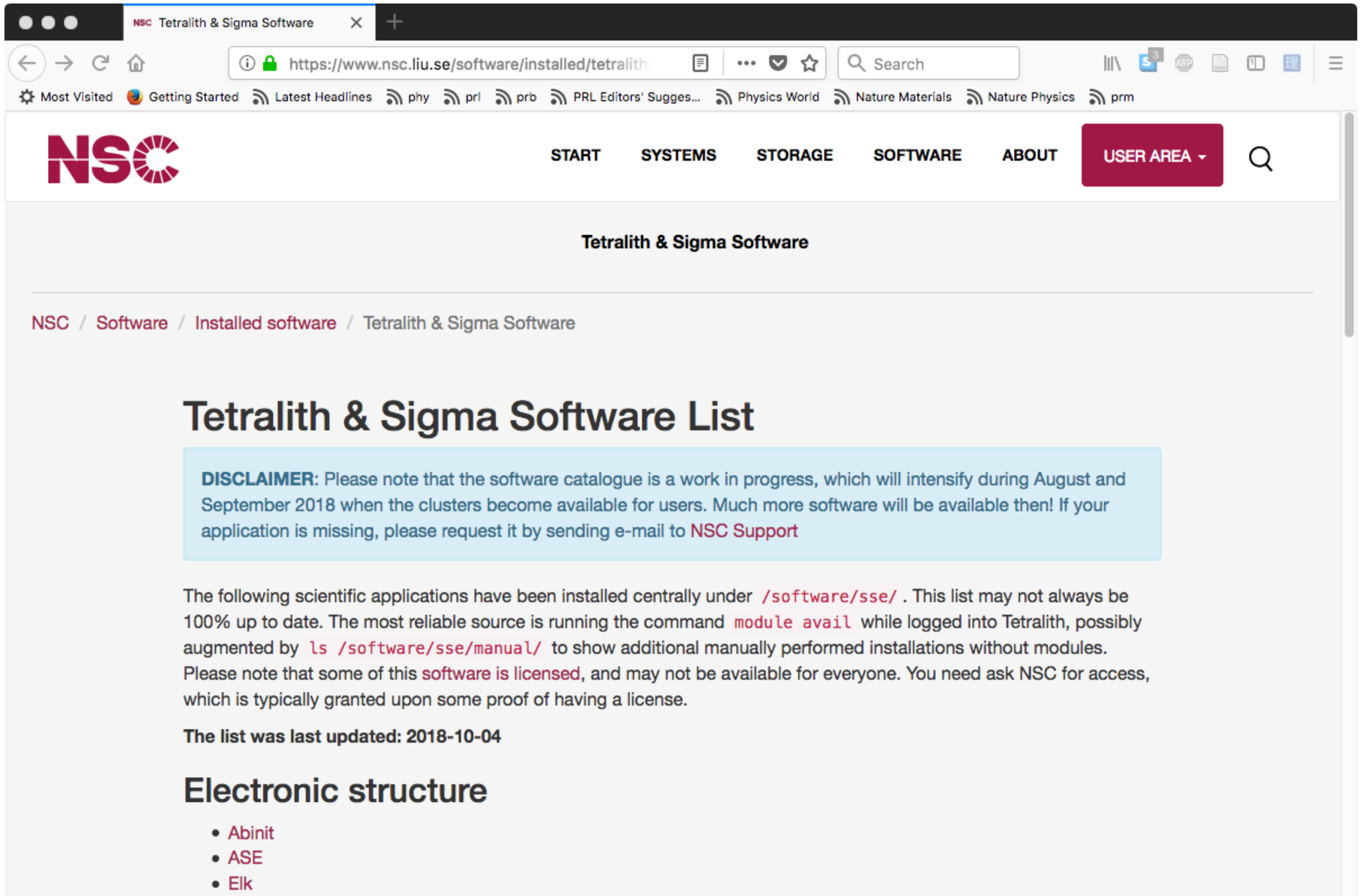


About NSC: Staff

- 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:	**PhD:**	**Work at NSC:**
Rickard Armiento (30%)	Physics	Hadoop/EasyBuild
Chandan Basu	Cond. mat. physics	Comp. sci.
Frank Bramkamp	Mechanics	Comp. fluid dynamics
Martin Moche (20%)	Str. biology	Str. biology
Weine Olovsson (90%)	Physics	Comp. materials sci.
Johan Raber	Chemistry	Comp. chemistry
Torben Rasmussen	Chemistry	Comp. chemistry
Hamish Struthers	Chemical physics	Climate research
Wei Zhang	HPC	Comp. sci.

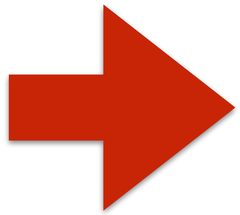
How NSC can help

- 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

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