NSC introduction day - 25th Nov 2017

10:00 - 10:45	1. NSC - introduction + *C o f f e e*
10:45 - 12:00	2. HPC: Getting started
L u n c h	
13:00 - 14:20	3. HPC: Further aspects
C o f f e e	
14:40 - 16:00	4. Electronic structure

1. NSC - introduction

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National Supercomputer Centre (NSC)

LINKÖPING UNIVERSITY

NSC

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 (Rektor)

> “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”

About NSC: History

1983

Saab invests 33 MSEK in a Cray 1 computer in connection with the JAS Gripen fighter project. Academic usage is allowed via an agreement with the Research Council

1989

NSC becomes the first supercomputer center in Sweden in connection with the procurement of a Cray X/MP computer for 55 MSEK with means from KAW/SEB. NSC enters into a partnership with Saab

More information: https://www.nsc.liu.se/about/history/

About NSC: History

1996

NSC enters into a partnership with SMHI

2003

The Swedish National Infrastructure for Computing (SNIC) is formed as a meta-center coordinating high-performance computing (HPC) and data storage investments in Sweden.

Monolith becomes the main academic computer resource at NSC

2007

Neolith replaces Monolith as the main academic computer resource at NSC

About NSC: History

2012

Triolith replaces Neolith as the main academic computer resource at NSC

2018

Triolith will be replaced with a new HPC system
(150 MSEK total-cost-of-ownership)

About NSC: Staff

- Currently 37 individuals (not all full-time)
- Mostly system experts and application experts
- Some management and administration

More information: https://www.nsc.liu.se/about/staff/

About NSC: What do we actually do?

“We operate hardware resources and provide day-to-day as well as advanced user support for compute, storage, and analysis”

We don’t really touch the hardware much!

We mostly work with the various layers of software that are needed to make the systems run and be useful for users

About NSC: What do we actually do?

Software layers: (simplified)

- OS - CentOS linux
- System management tools
- User and project setup tools
- Resource sharing and job queuing (e.g. Slurm)
- End-user software and tools

About NSC: Our HPC systems

- Triolith (SNIC)
- Gamma (LiU)
- Bi & Frost (SMHI and MET)
- Elvis & Alvin (MET and SMHI)
- Heffa (LiU/SNIC - experimental Hadoop system)

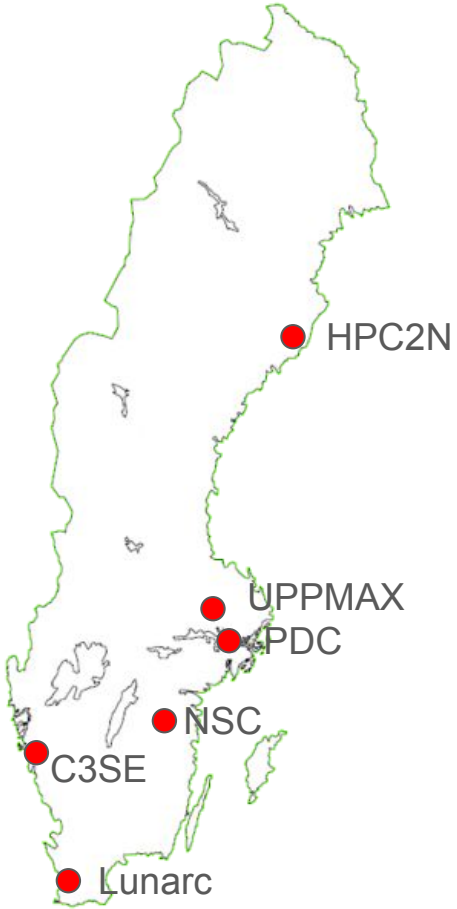
More information: https://www.nsc.liu.se/systems/

About SNIC

SNIC is a meta-center with six partners in terms of supercomputer centres at Chalmers (C3SE), KTH (PDC), LiU (NSC), LU (Lunarc), UmU (HPC2N) and UU (UPPMAX).

The SNIC office (hosted by UU) forms agreements with the partners and organizes the overall partner collaboration and diversity.

Funding comes from VR and the universities that host a HPC center.



About SNIC

The Swedish National Infrastructure for Computing (SNIC) is a national research infrastructure with a threefold mission:

- provide a balanced and cost-efficient set of resources and user support for large scale computation and data storage
- meet the needs of researchers from all scientific disciplines and from all Swedish universities and university colleges
- make the resources available through open application procedures such that the best Swedish research is supported

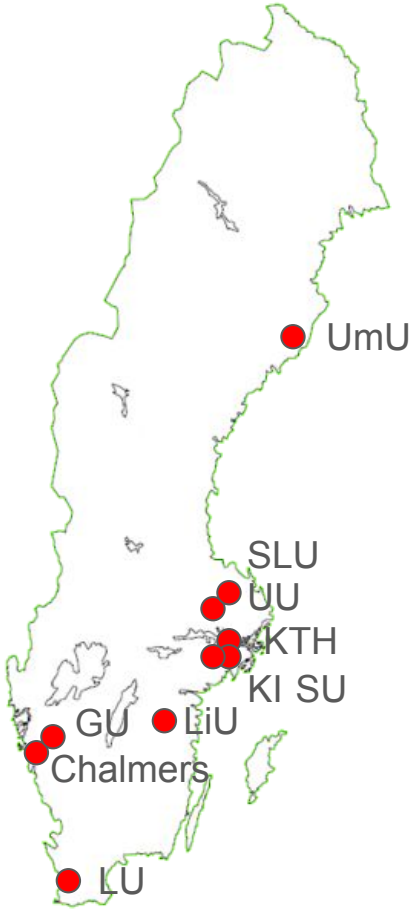
SNIC is changing in 2018

SNIC will be a consortium of 10 universities – Chalmers, GU, KI, KTH, LiU, LU, SLU, SU, UmU, and UU.

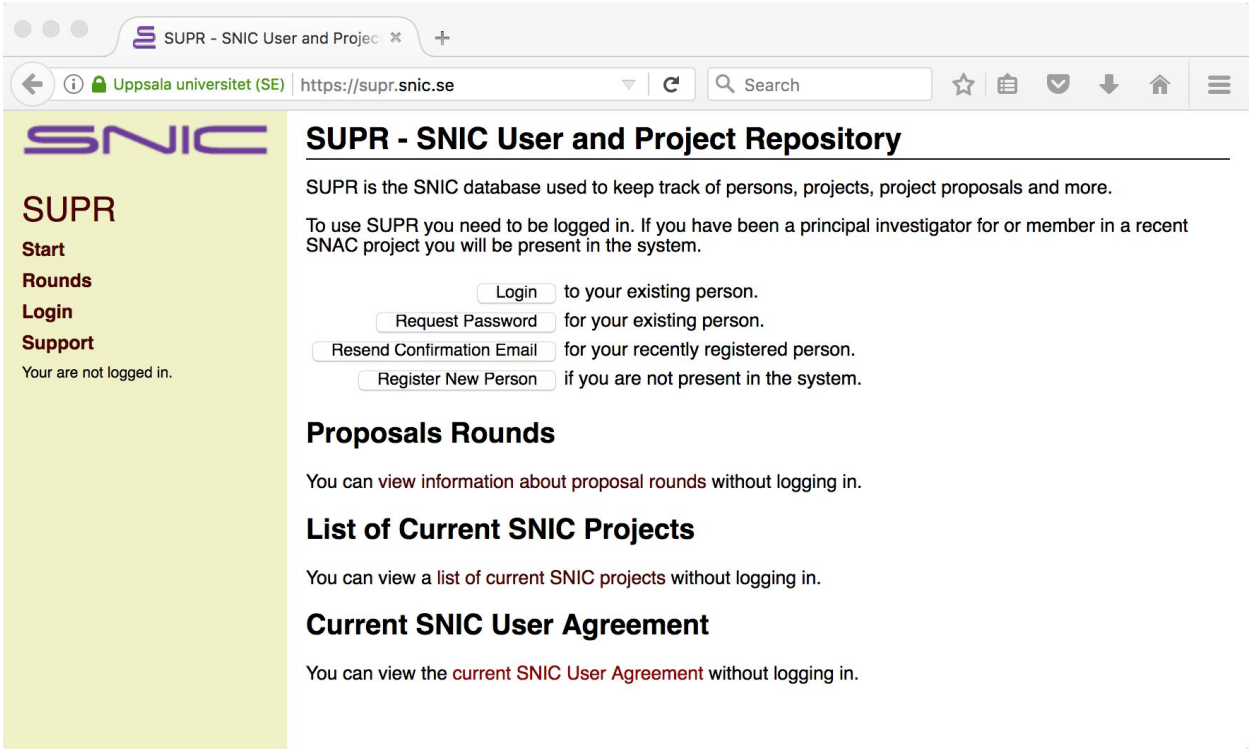
The SNIC office will still be hosted by UU.

University co-funding will no longer be by way of hosting a HPC center.

The current HPC centers are expected to still be the ones that operate SNIC HPC systems.

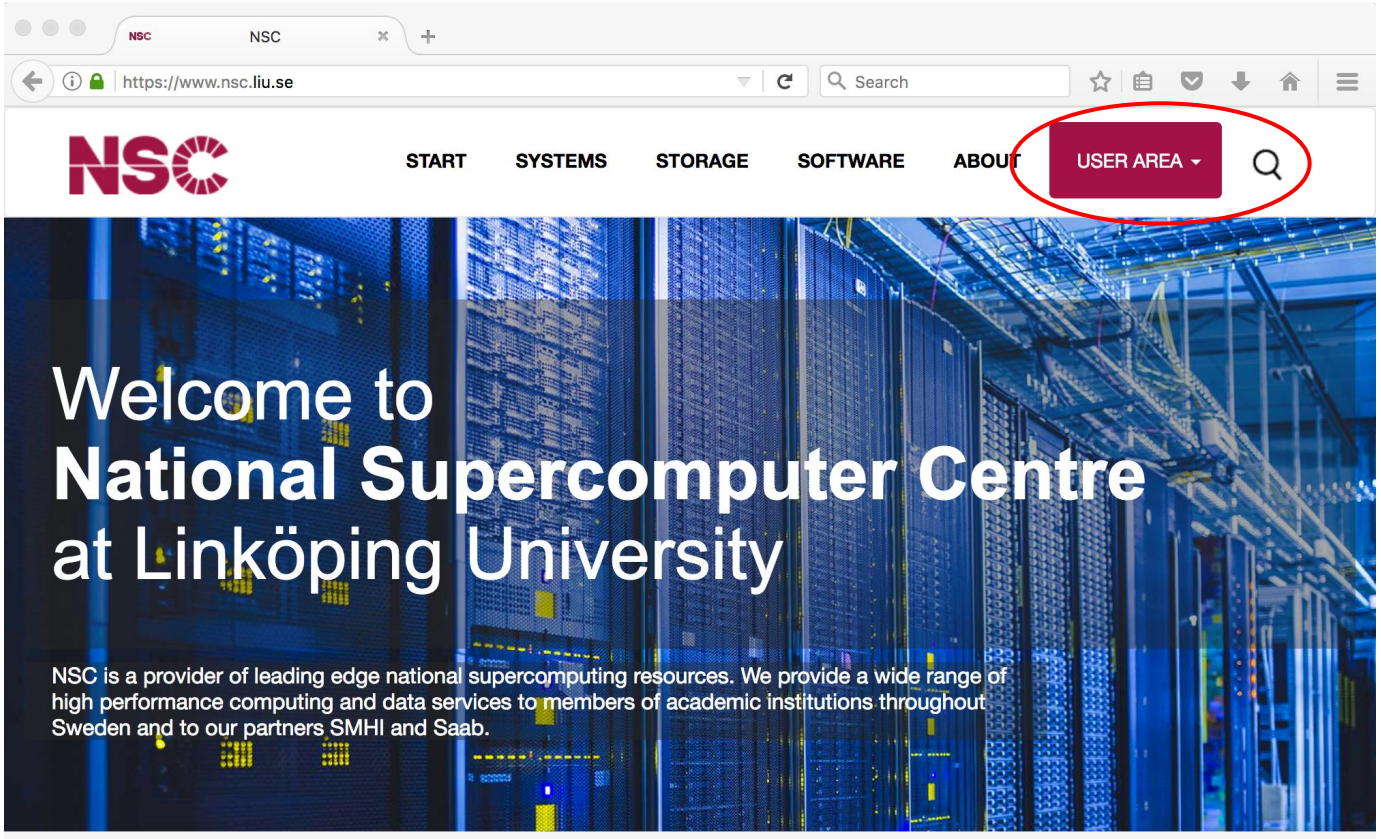


How to get access to an HPC system - SUPR

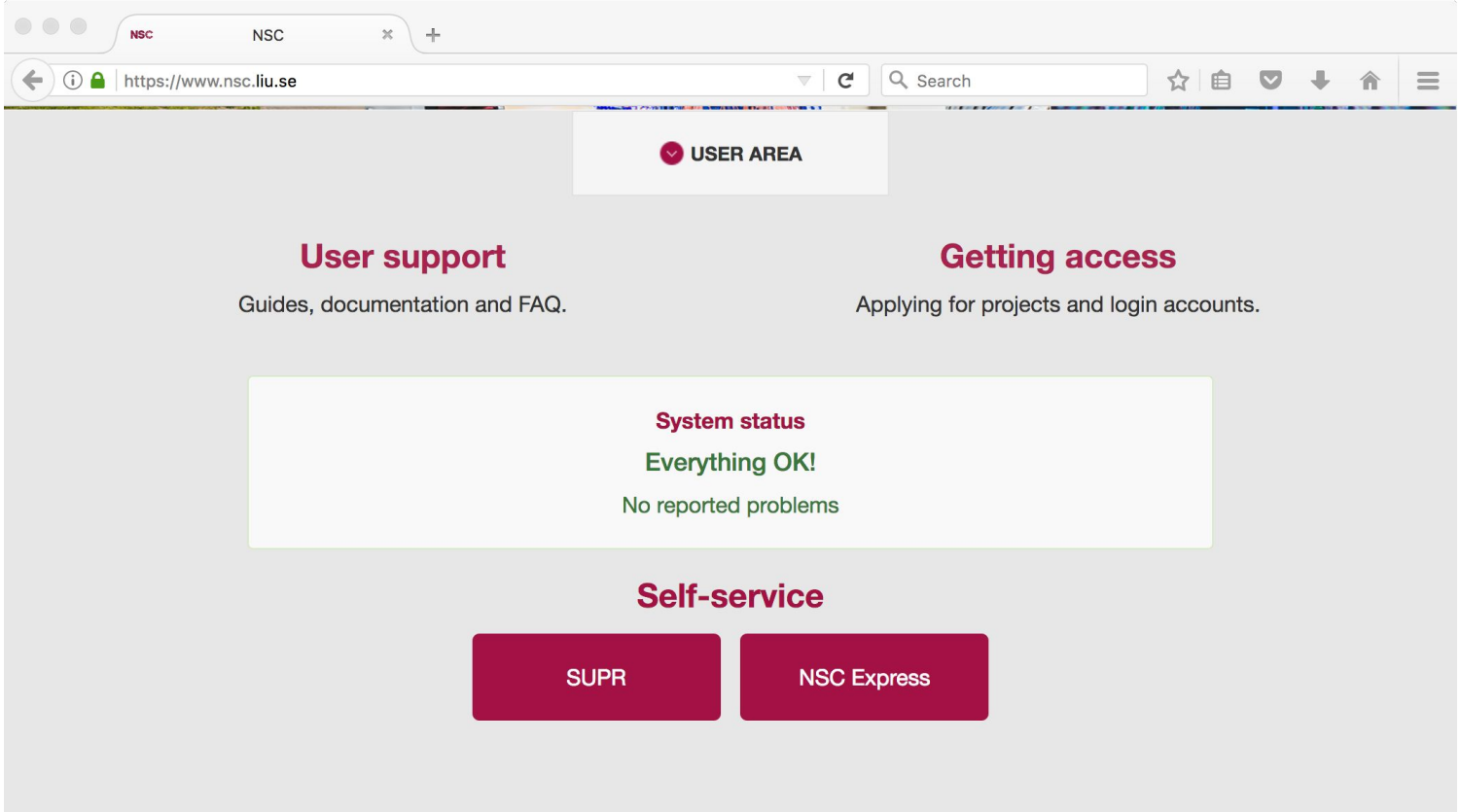


More information: https://www.nsc.liu.se/access/

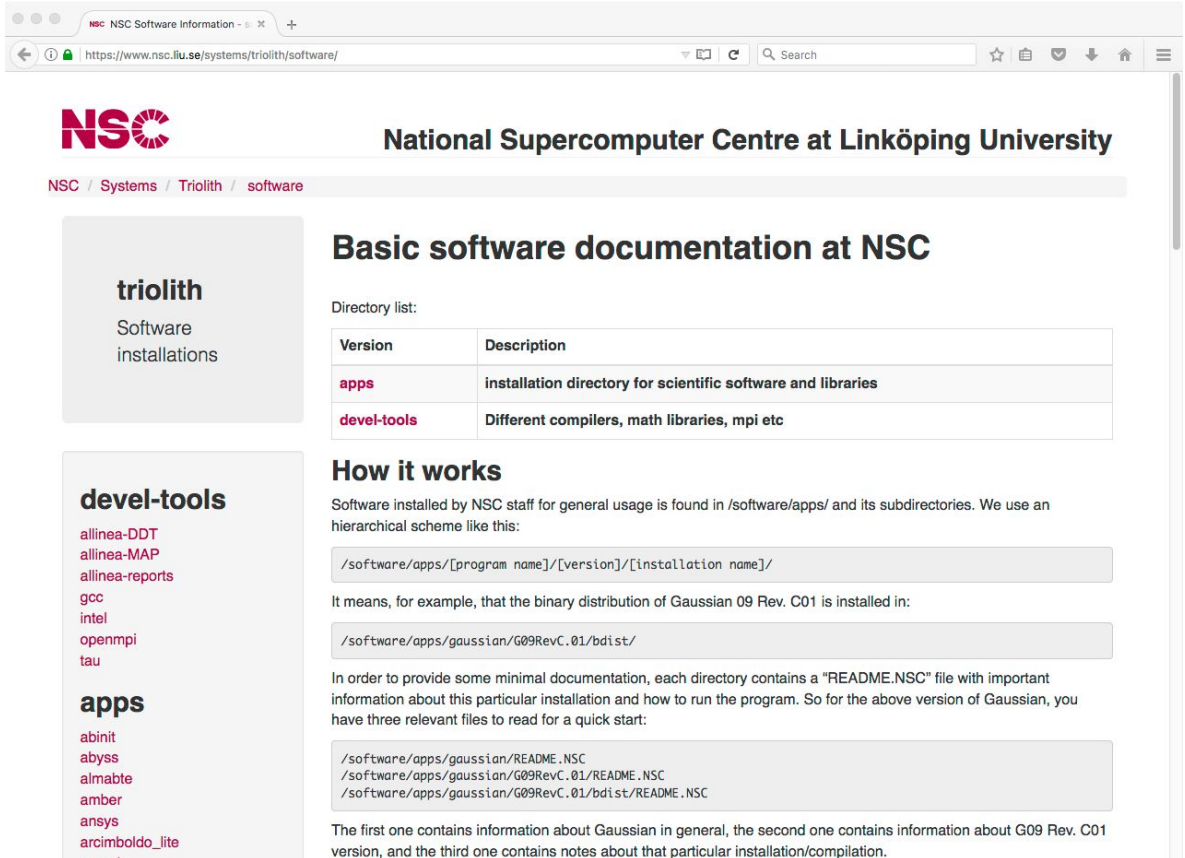
Documentation & Support



Documentation & Support



Documentation & Support



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 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.

What is HPC used for?

- Numerical weather prediction simulations - weather forecasts
- Climate simulations
- Flow simulations - car, truck, train, aeroplane etc. construction
- Materials science
- Many disciplines within chemistry, physics, and biology
- …

When to use HPC?

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

Important to think about

Most HPC clusters contain **the same components** as regular desktop computers. Just more of them!

And, each individual component **need not** be more powerful (or faster) than the same component in a desktop.

For example, one cpu-core in Triolith is probably not faster than one cpu-core in your laptop.

Hence, your jobs won't **automatically** run faster on a HPC system!