

# 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

Torben Rasmussen

National Supercomputer Centre (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

# 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

# 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

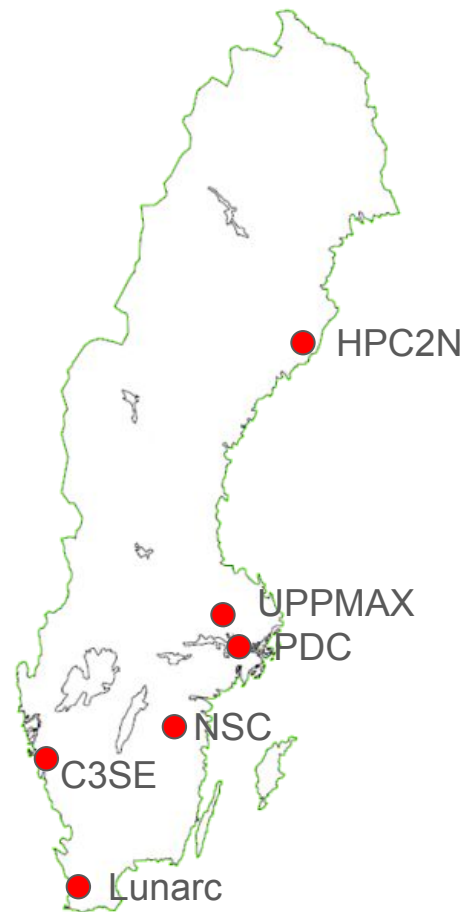
- Triolith (SNIC)
- Gamma (LiU)
- Bi & Frost (SMHI and MET)
- Elvis & Alvin (MET and SMHI)
- Heffa (LiU/SNIC - experimental Hadoop system)

# 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

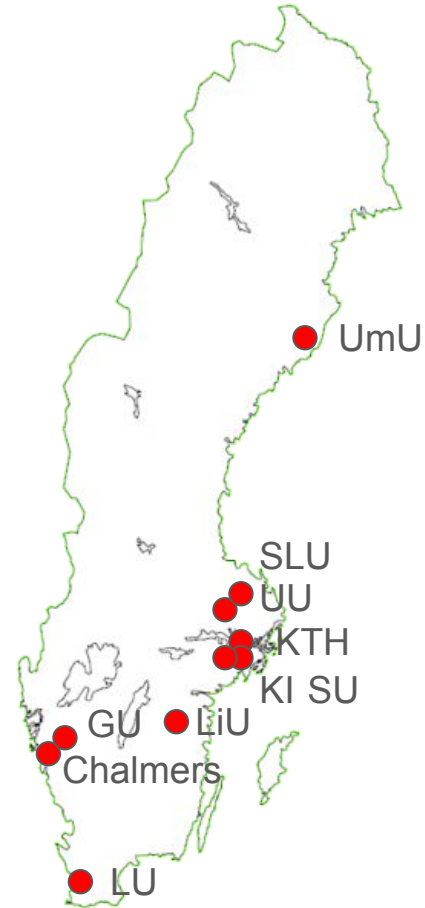
# SNIC is changing in 2018

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

**SUPR - SNIC User and Project Repository**

SUPR is the SNIC database used to keep track of persons, projects, project proposals and more.

To use SUPR you need to be logged in. If you have been a principal investigator for or member in a recent SNAC project you will be present in the system.

to your existing person.

for your existing person.

for your recently registered person.

if you are not present in the system.

### Proposals Rounds

You can view information about proposal rounds without logging in.

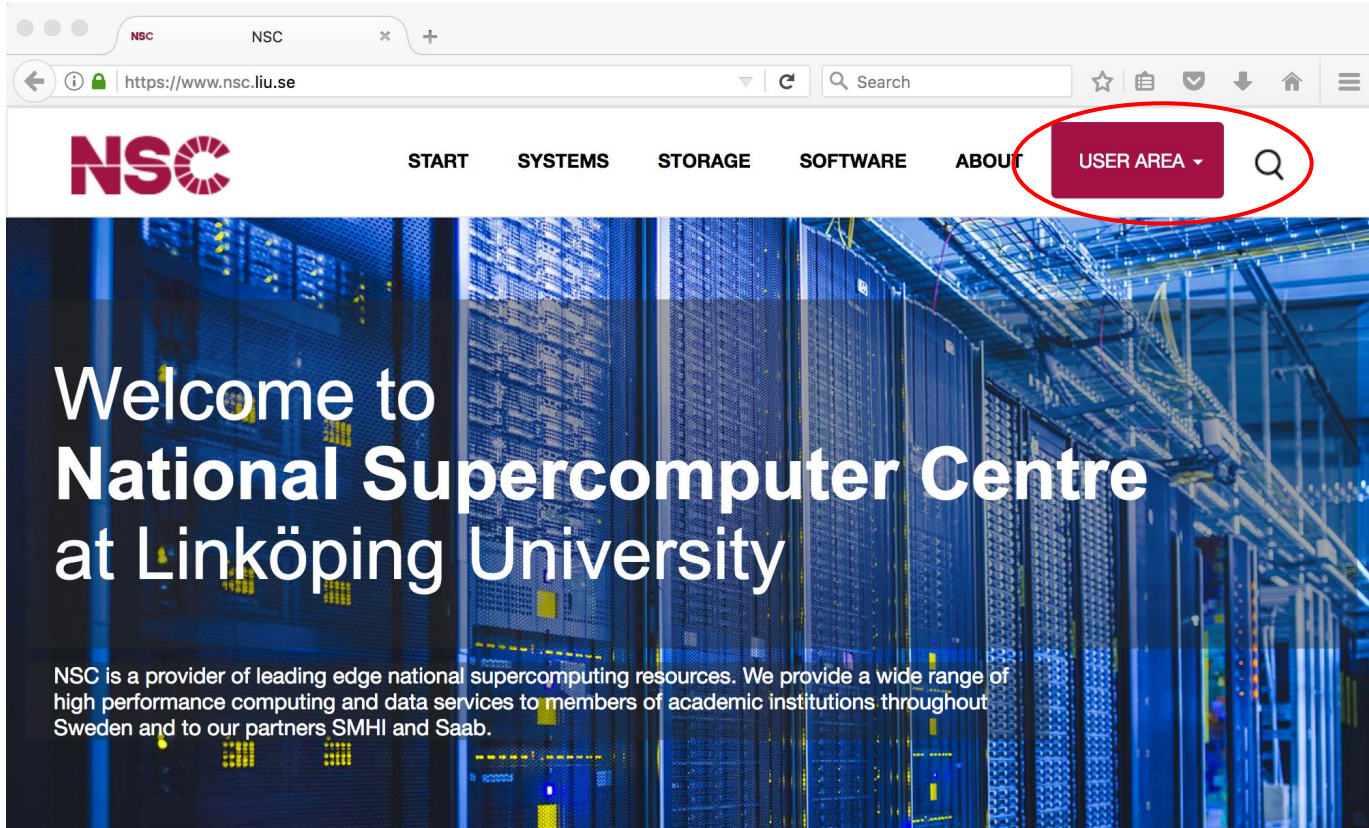
### List of Current SNIC Projects

You can view a list of current SNIC projects without logging in.

### Current SNIC User Agreement

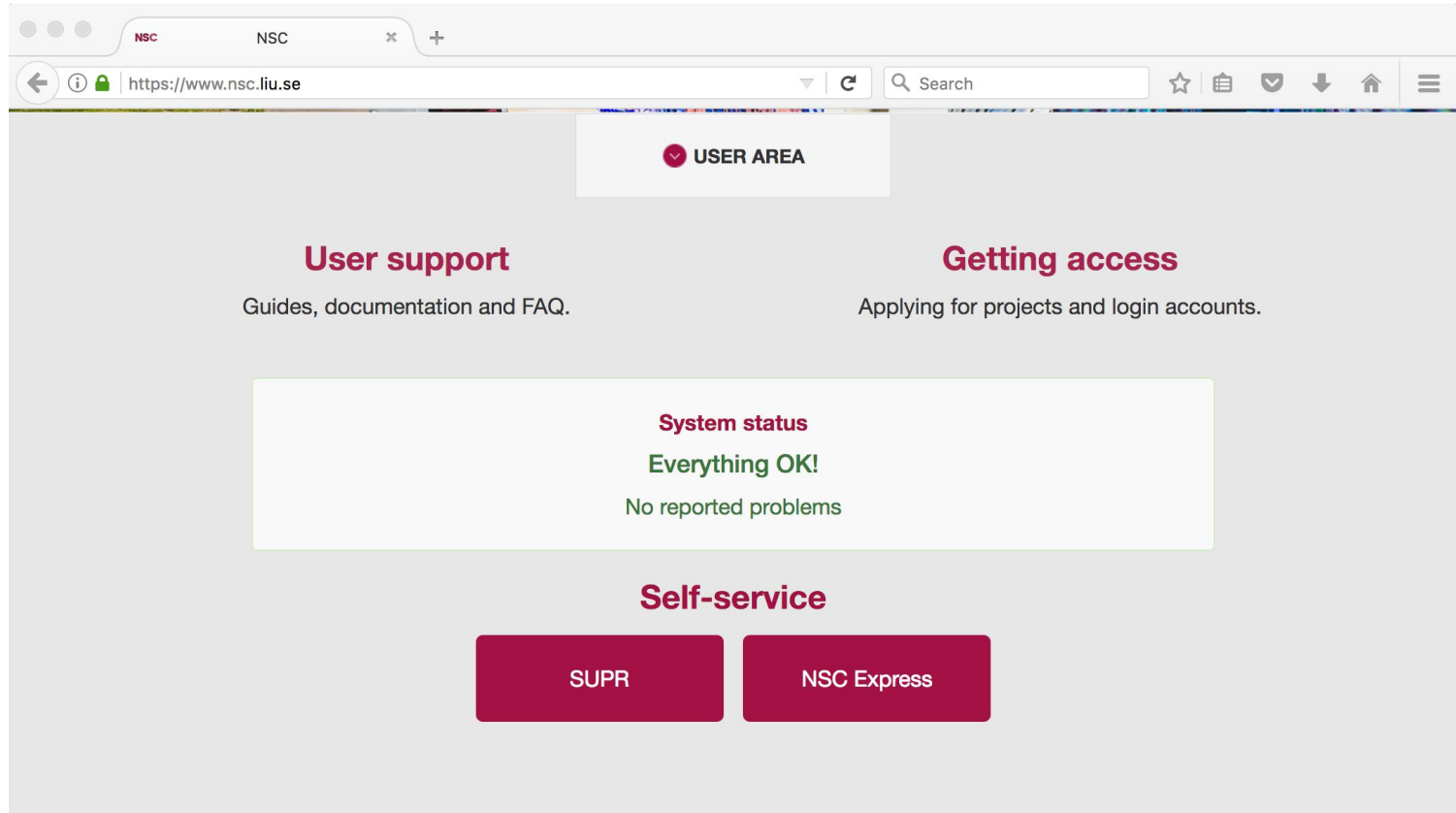
You can view the [current SNIC User Agreement](#) without logging in.

# Documentation & Support



The image shows a web browser window displaying the homepage of the National Supercomputer Centre (NSC) at Linköping University. 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 prominent red button labeled [USER AREA](#) with a dropdown arrow is circled in red. To the right of the navigation menu is a search icon. The main content area features a large blue-tinted image of server racks with the text: "Welcome to National Supercomputer Centre at Linköping University". Below this, a paragraph 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."

# Documentation & Support



The image shows a browser window with the URL <https://www.nsc.liu.se>. The page features a navigation bar with a "USER AREA" button. Below this, there are two main sections: "User support" and "Getting access". A central white box displays the "System status" as "Everything OK!" with "No reported problems". At the bottom, there is a "Self-service" section with two buttons: "SUPR" and "NSC Express".

**USER AREA**

**User support**  
Guides, documentation and FAQ.

**Getting access**  
Applying for projects and login accounts.

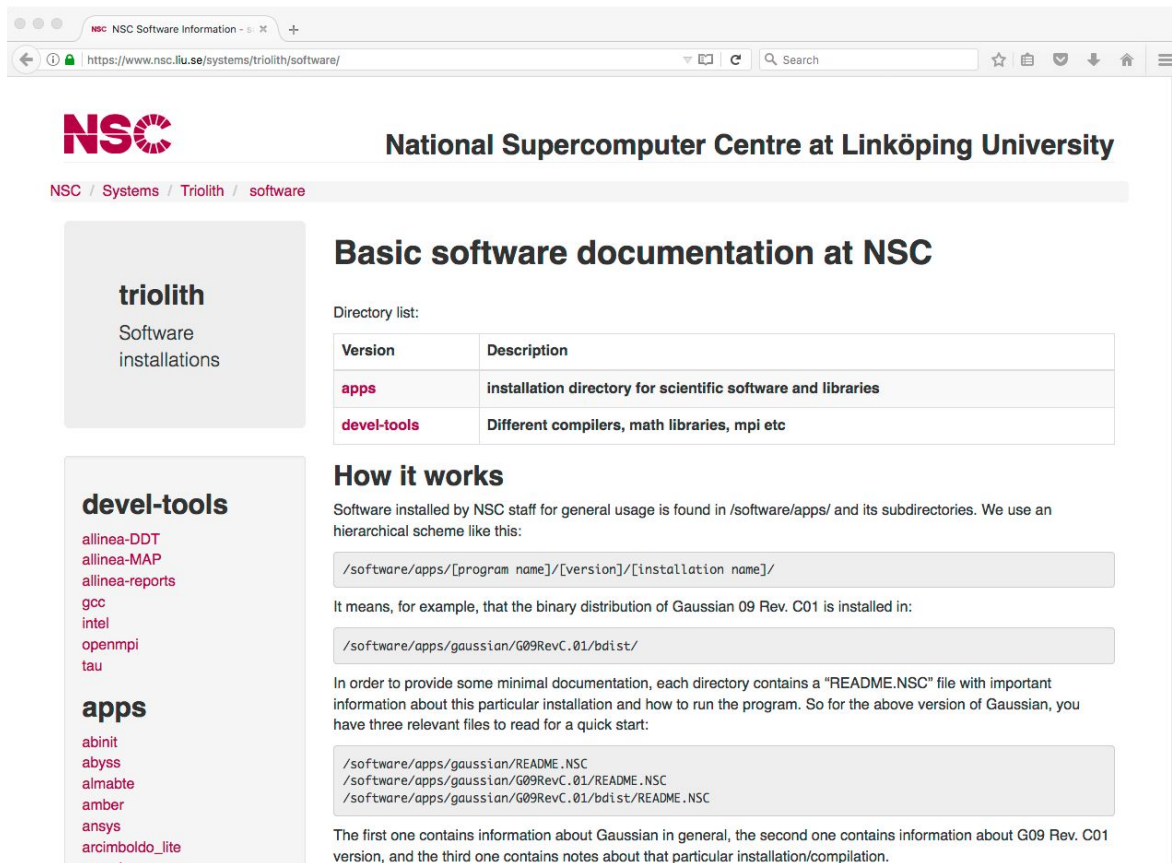
**System status**  
**Everything OK!**  
No reported problems

**Self-service**

SUPR      NSC Express



# Documentation & Support



The screenshot shows a web browser window with the URL `https://www.nsc.liu.se/systems/triolith/software/`. The page header features the NSC logo and the text "National Supercomputer Centre at Linköping University". A breadcrumb trail reads "NSC / Systems / Triolith / software".

The main content area is titled "Basic software documentation at NSC". It includes a "Directory list:" section with a table:

Version	Description
<b>apps</b>	installation directory for scientific software and libraries
<b>devel-tools</b>	Different compilers, math libraries, mpi etc

Below the table is a "How it works" section. It explains that software is installed in `/software/apps/` and its subdirectories. A code block shows the directory structure: `/software/apps/[program name]/[version]/[installation name]/`. An example is given: the binary distribution of Gaussian 09 Rev. C01 is installed in `/software/apps/gaussian/G09RevC.01/bdist/`.

The section further states that each directory contains a "README.NSC" file. A code block lists the files: `/software/apps/gaussian/README.NSC`, `/software/apps/gaussian/G09RevC.01/README.NSC`, and `/software/apps/gaussian/G09RevC.01/bdist/README.NSC`. The text concludes that the first file contains general information about Gaussian, the second contains information about the G09 Rev. C01 version, and the third contains notes about the particular installation/compilation.

On the left side, there are two sidebar sections:

- triolith**  
Software installations
- devel-tools**
  - allinea-DDT
  - allinea-MAP
  - allinea-reports
  - gcc
  - intel
  - openmpi
  - tau
- apps**
  - abinit
  - abyss
  - almabte
  - amber
  - ansys
  - arcimboldo\_lite

# 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!