Introduction to NSC

National Supercomputer Centre (NSC), Linköping University
SNIC training, online @NSC 17th Nov 2021, 10:00 - ca. 12:00
Information / Schedule

https://www.nsc.liu.se/support/Events/NSC_intro_Nov2021/

- 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 session, questions?
National Supercomputer Centre (NSC)

NSC is part of:

- **SNIC** Swedish National Infrastructure for Computing (10 Univ.)
- **liu.se** LINKÖPING UNIVERSITY

1983 - SAAB buys Cray1

1989 - NSC first supercomputer centre in Sweden / SAAB partner

1996 - SMHI partner

2016 - MET Norway partner

https://www.nsc.liu.se
Swedish National Infrastructure for Computing

10 universities & 6 HPC centers:
Chalmers  C3SE
Göteborg  PDC
Karolinska  NSC
KTH  LUNARC
Linköping  HPC2N
Lund  UPPMAX
SLU
Stockholm
Umeå
Uppsala

Funding: 10 univ. + Vetenskapsrådet (VR)

https://snic.se/
NSC: Quick Overview

Current Director: Björn Alling, Nov 2021 - 
~ 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

**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

Top500 no. 168 (74)
Where to find Information?

https://www.nsc.liu.se
Where to find Information?

New AI Supercomputer at NSC (15 Oct 2020)

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
Where to find Information?

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: esgf-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 modes, interactive jobs, batch jobs.
- Running graphical applications
  Batch jobs and scheduling
  Batch jobs and scheduling, in general and per cluster.
### Where to find Information?

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<th>Getting started</th>
<th>Security</th>
<th>Tutorials</th>
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<td>X11 forwarding and ThinLinc</td>
<td>Batch jobs and scheduling, in general and per cluster.</td>
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<td>Application expert help</td>
<td>Copying data</td>
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<td>Consulting and advanced support for scientists.</td>
<td>Getting data to and from the cluster.</td>
<td>Current events pages</td>
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<td>Getting help</td>
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<tr>
<td>Getting support and help from NSC</td>
<td>Running out of memory. What to do?</td>
<td>Past events pages</td>
</tr>
<tr>
<td>Singularity</td>
<td>Storage</td>
<td>System-specific information</td>
</tr>
<tr>
<td>Run applications in a Linux environment of your own choosing. Allows you to e.g run Ubuntu, different versions of CentOS and Docker containers.</td>
<td>Where and how you can store your data</td>
<td>Getting Started Guide and detailed information about how to use our systems</td>
</tr>
<tr>
<td>PReSTO online documentation</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Getting Access to HPC - 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 most SUPR functions you need to be logged in.

If You Cannot Login

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

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:

<table>
<thead>
<tr>
<th>Project</th>
<th>Project Title</th>
<th>Project Type</th>
<th>End Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>SNIC 2020/13-76</td>
<td>VASP workshop at NSC 19-20th Oct 2020</td>
<td>SNIC Small Compute</td>
<td>2020-12-01</td>
</tr>
</tbody>
</table>

Proposals
You have no proposals in preparation or pending committee decision.

Rounds
View Rounds

Projects and Project Membership Requests
View and Manage

Groups

Personal Information
Support
Logout

Logged in as:
Weine Olovsson
weine@coli.lu.se
Type of machine user:
standard user
Support via SUPR

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.

Repplies will be sent to your registered email address. 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.

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.

Project

If your problem is related to a specific project, select that.

Summary
Projects in SUPR

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 weelo@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
Projects in SUPR

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.

<table>
<thead>
<tr>
<th>Storage Project</th>
<th>Title</th>
<th>PI</th>
</tr>
</thead>
<tbody>
<tr>
<td>SNIC 2020/6-95</td>
<td>Storage for theoretical physics environment</td>
<td>Rickard Arminova</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Resource</th>
<th>Allocation</th>
<th>Unit</th>
<th>Total Usage</th>
<th>Allocation</th>
<th>Percentage</th>
<th>Total Allocation</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beskow @ PDC</td>
<td>1400</td>
<td>x 1000 core/h/month</td>
<td>6792.0</td>
<td>7000.0</td>
<td>97.1%</td>
<td>16800.0</td>
<td>40.5%</td>
</tr>
<tr>
<td>Tetralith @ NSC</td>
<td>900</td>
<td>x 1000 core/h/month</td>
<td>5183.2</td>
<td>4500.0</td>
<td>114.7%</td>
<td>19800.0</td>
<td>47.8%</td>
</tr>
<tr>
<td>Kelbnekaise @ HPC2N</td>
<td>150</td>
<td>x 1000 core/h/month</td>
<td>554.7</td>
<td>750.0</td>
<td>74.0%</td>
<td>1800.0</td>
<td>30.8%</td>
</tr>
<tr>
<td>Tegner @ PDC</td>
<td>23</td>
<td>x 1000 core/h/month</td>
<td>0.0</td>
<td>115.0</td>
<td>115.0%</td>
<td>276.0</td>
<td></td>
</tr>
</tbody>
</table>

Storage

Percentage field to the right, compares Usage with the allocation. Last Updated shows the time at which the usage was last updated.

<table>
<thead>
<tr>
<th>Resource</th>
<th>Allocation</th>
<th>Usage</th>
<th>Unit</th>
<th>Percentage</th>
<th>Allocation</th>
<th>Usage</th>
<th>Unit</th>
<th>Percentage</th>
<th>Last Updated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Centre Storage @ NSC</td>
<td>0</td>
<td>GIB</td>
<td>files</td>
<td></td>
<td>0</td>
<td>files</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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)

Login nodes:
2 nodes
Linux
Many users

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

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

Three types of storage areas available:
1. Personal home directory, e.g. /home/x_user
2. Project storage, owned by PI, e.g. /proj/ourstuff
3. Work node local disk (during runs)

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

Backup? Snapshot?
yes! yes!
no! yes!
no! no!

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

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

Also, on how to use key-pair authentication
Software: How do I get Code X?

1. Check installed software webpage
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

Global installation: wide or not usage, license?

Special wrappers/rec. e.g.: Gaussian

Testing, benchmarking, optimization

https://www.nsc.liu.se/software/installed/tetralith/
https://www.nsc.liu.se/software/installation-policy/
Software: Installation Webpage

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”)

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

https://www.nsc.liu.se/software/modules/
Software: Module System

[weiol@tetralith1 ~]$ module avail vasp

<table>
<thead>
<tr>
<th>Module Path</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>p4vasp/recommendation</td>
<td>VASP/5.4.4.16052018-nsc1-intel-2018b-eb</td>
</tr>
<tr>
<td>p4vasp/tmp1</td>
<td>VASP/5.4.4.16052018-nsc2-intel-2018a-eb</td>
</tr>
<tr>
<td>p4vasp/0.3.30-nsc1</td>
<td>VASP/5.4.4.16052018-vanilla-nsc1-intel-2018a-eb</td>
</tr>
<tr>
<td>VASP-OMC/5.4.4.16052018-nsc1-intel-2018a-eb</td>
<td>VASP/5.4.4.16052018-wannier90-nsc1-intel-2018a-eb</td>
</tr>
<tr>
<td>VASP-VTST/3.2-sol-5.4.4.16052018-nsc2-intel-2018a-eb</td>
<td>VASP/6.1.0.28012020-nsc1-intel-2018a-eb</td>
</tr>
<tr>
<td>VASP-VTST/3.2-sol-5.4.4.16052018-vanilla-nsc1-intel-2018a-eb</td>
<td>VASP/6.1.2.25082020-nsc1-intel-2018a-eb</td>
</tr>
<tr>
<td>VASP/recommendation</td>
<td>VASP/6.1.2.25082020-omp-nsc1-intel-2018a-eb</td>
</tr>
<tr>
<td>VASP/5.4.4.16052018-nsc1-intel-2018a-eb</td>
<td>vasptools/0.3</td>
</tr>
</tbody>
</table>

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 ~]$
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

https://www.nsc.liu.se/software/index.html
# Software: Build Environment

[weiol@tetralith1 ~]$ module avail buildenv

<table>
<thead>
<tr>
<th>buildenv-gcc/recommendation   (D)</th>
<th>buildenv-intel/recommendation (D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>buildenv-gcc/7.3.0-bare</td>
<td>buildenv-intel/2015.1.133-impi-2018.1.163-eb</td>
</tr>
<tr>
<td>buildenv-gcc/2016b-eb</td>
<td>buildenv-intel/2016b-eb</td>
</tr>
<tr>
<td>buildenv-gcc/2018a-eb</td>
<td>buildenv-intel/2017.u7-bare</td>
</tr>
<tr>
<td>buildenv-gcccuda/recommendation (D)</td>
<td>buildenv-intel/2018a-eb</td>
</tr>
<tr>
<td>buildenv-gcccuda/10.2-7.3.0-bare</td>
<td>buildenv-intel/2018b-eb</td>
</tr>
<tr>
<td>buildenv-impi-gcc/recommendation (D)</td>
<td>buildenv-intel/2018.u1-bare</td>
</tr>
<tr>
<td>buildenv-impi-gcc/2018a-eb</td>
<td></td>
</tr>
</tbody>
</table>

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 buildenv-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                        6) GCCcore/6.4.0                        10) impi/.2018.1.163 (H)
        (H,S)                      7) binutils/2.28                     11) imkl/.2018.1.163 (H)
3) EasyBuild/4.3.0-nscde3532a      8) icc/.2018.1.163-GCC-6.4.0-2.28  12) intel/2018a
4) nsc-eb-scripts/1.2             9) GCCcore/6.4.0                        (H)

Where:
S: Module is Sticky, requires --force to unload or purge
H: Hidden Module
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

https://www.nsc.liu.se/support/batch-jobs/tetralith/
Slurm: Running Batch Job

- Regular production runs
- Output to files
  slurm-JOBID.out

Example: a job script called “run.sh”

```bash
#!/bin/bash
#SBATCH -A snic2020-13-76
#SBATCH -t 1:00:00
#SBATCH -n 32
#SBATCH -J vasptst
module load VASP/6.2.1.29042021-omp-nsc1-intel-2018a-eb
mpirun vasp_std
```

NSC MPI job launching tool

Submit job: sbatch run.sh
Check queue: squeue -u USERNAME
Checking jobs:
  jobload JOBID
  jobsh NODE
  seff JOBID
  lastjobs

https://www.nsc.liu.se/support/batch-jobs/introduction/
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

https://www.nsc.liu.se/support/batch-jobs/tetralith/
Best Practices & Suggestions

In general:

- Be careful how you use Tetralith/Sigma login nodes
- Use SUPR to follow project usage
- Use the NSC documentation
- 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

https://www.nsc.liu.se/support/getting-help/
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)

- Presentations available at webpage!
- Working effectively with HPC systems