SciLifeLab
UPPSALA

HPC Introduction

High-performance computing

2025-03-24

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Enabler for Life Sciences

SciLifeLab UPPSALA

Objectives

What is PDC, what it provides

Projects at PDC

How to access PDC

Jobs and queuing systems

How to use the resources of PDC

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PDC

Parallell**d**ator**c**entrum
http://www.pdc.kth.se

1 computer cluster, **Dardel**

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PDC

Parallell**d**ator**c**entrum
http://www.pdc.kth.se

1 computer cluster, **Dardel**

- 1 278 nodes
  - 128 cores each, 163 584 in total
  - 128 GB RAM, also 256, 512, 1024, 2048

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- 18 PB fast parallel storage

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PDC

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1 computer cluster, **Dardel**

- 1 278 nodes
  - 128 cores each, 163 584 in total
  - 128 GB RAM, also 256, 512, 1024, 2048
- 18 PB fast parallel storage

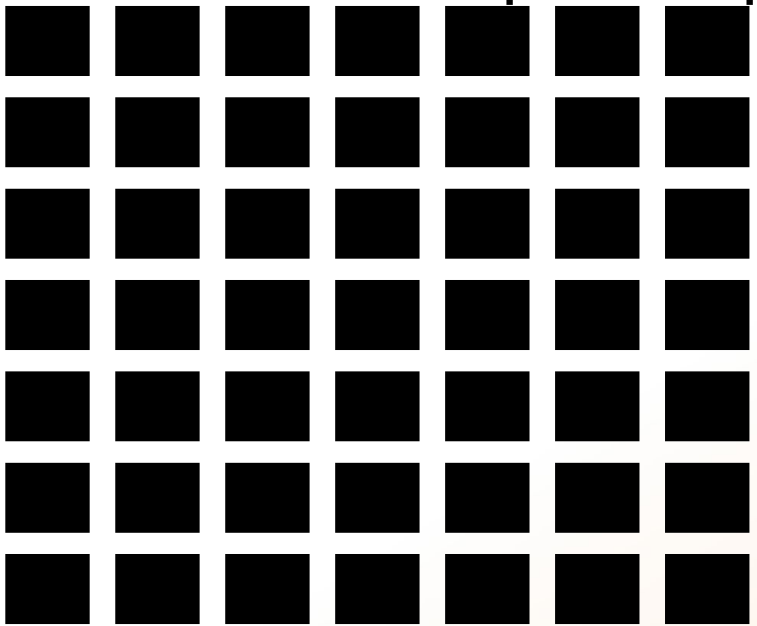
- Bioinformatics **software**

The basic structure of supercomputer

Login nodes

node = computer

The basic structure of supercomputer

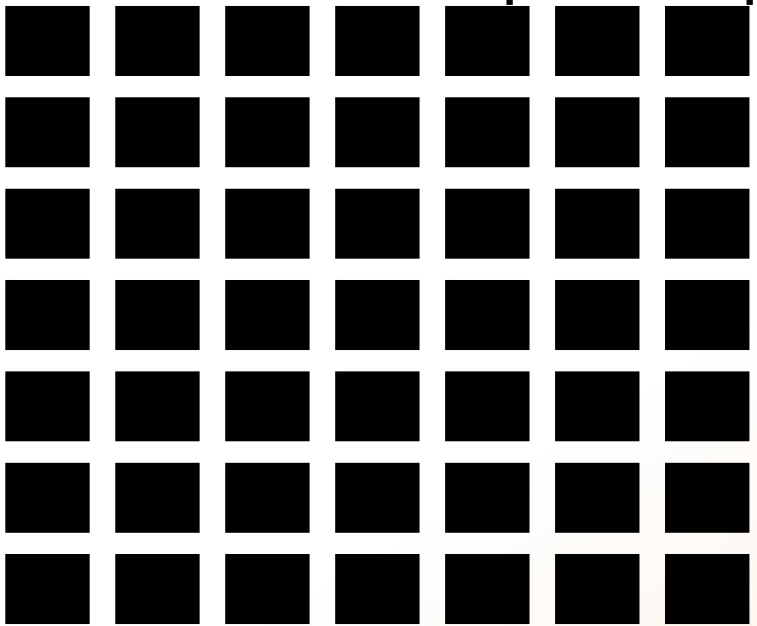


Calculation nodes

Login nodes

node = computer

The basic structure of supercomputer



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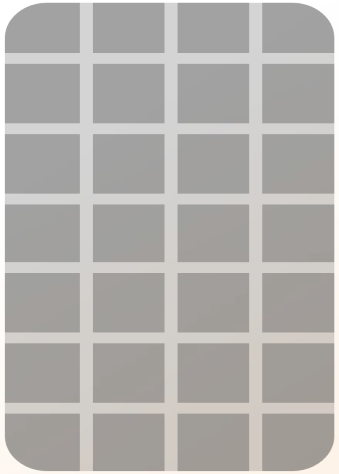

Storage

Login nodes

node = computer

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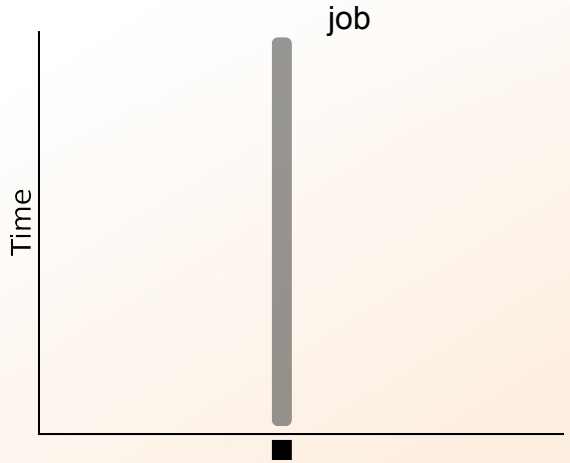
Job

The basic structure of a supercomputer

Parallel computing

Not one super fast



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Job

The basic structure of a supercomputer

Parallel computing

Not one super fast

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Objectives

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How to use the resources of PDC

Projects

PDC provides its resources via

projects

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Projects

PDC provides its resources via

projects

compute
(core-hours/month)

storage
(GB)

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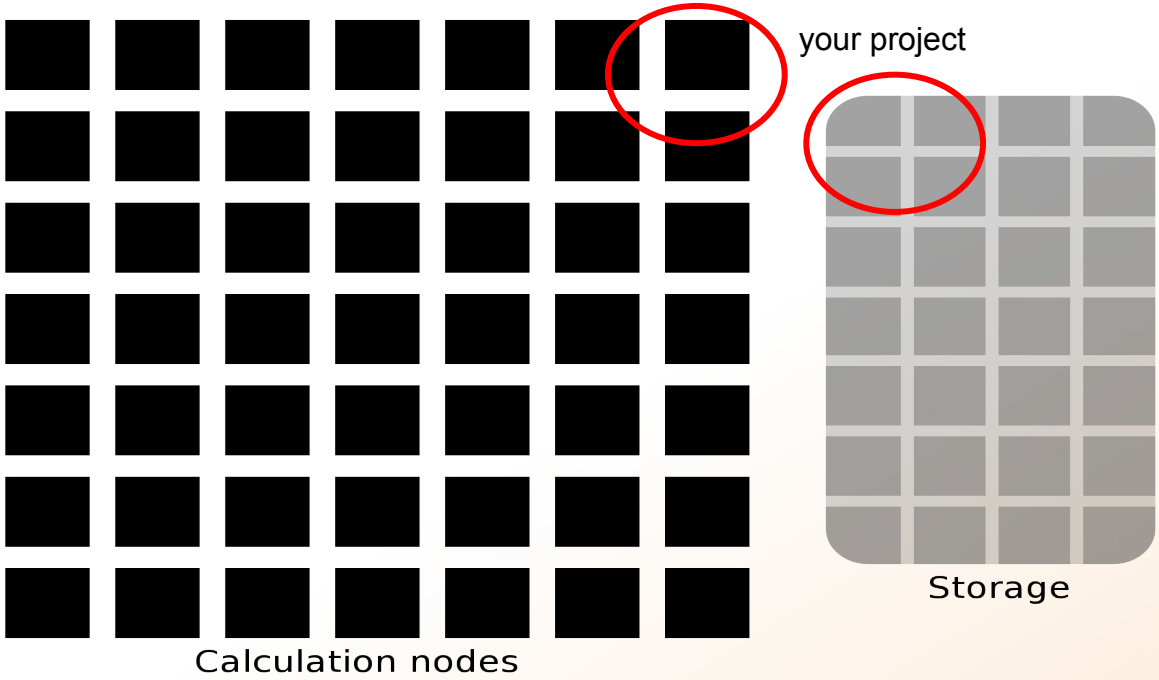
Projects



Projects

Two separate projects:

NAISS compute:

cluster **Dardel**

2000 - 100 000+ core-hours/month

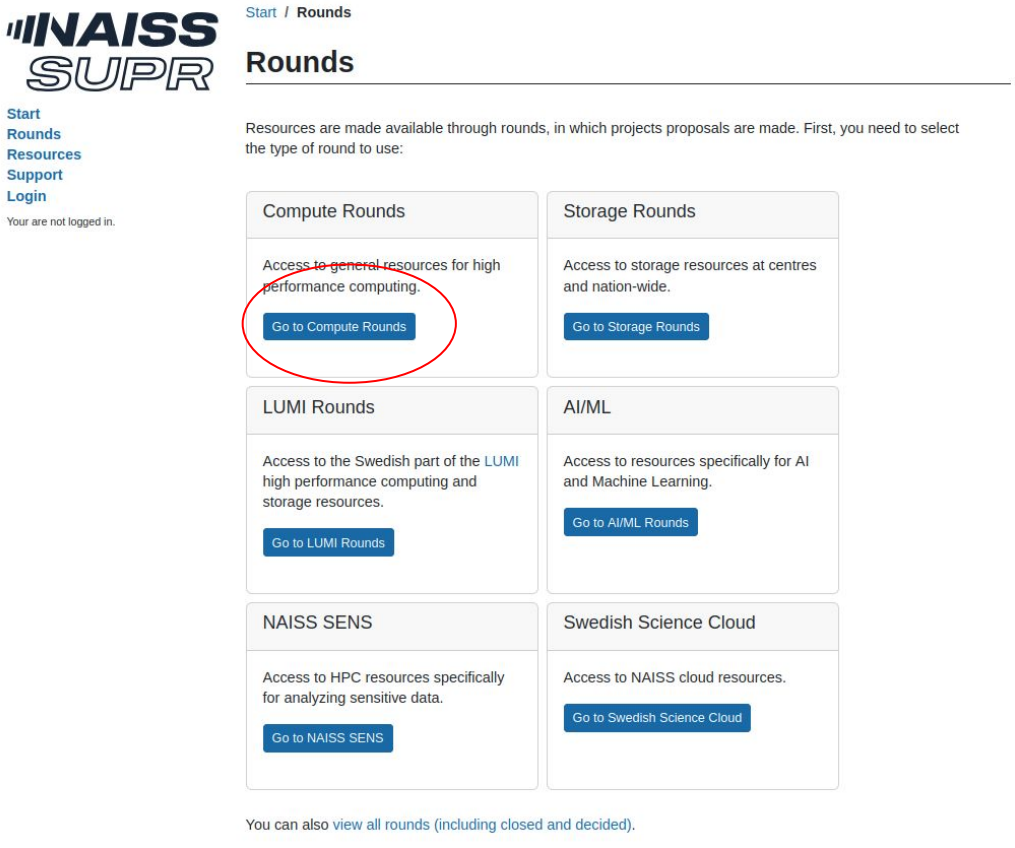
512 GB storage

NAISS Storage:

storage system **Klemming**

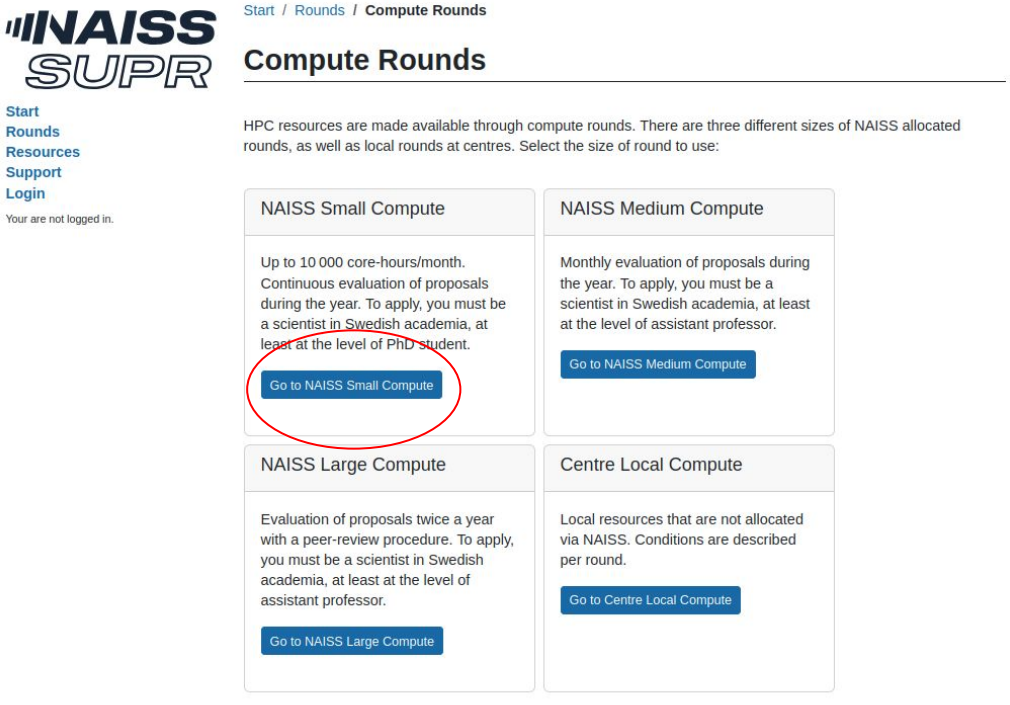
1 - 100+ TB storage

Projects



https://supr.naiss.se/round/

Projects



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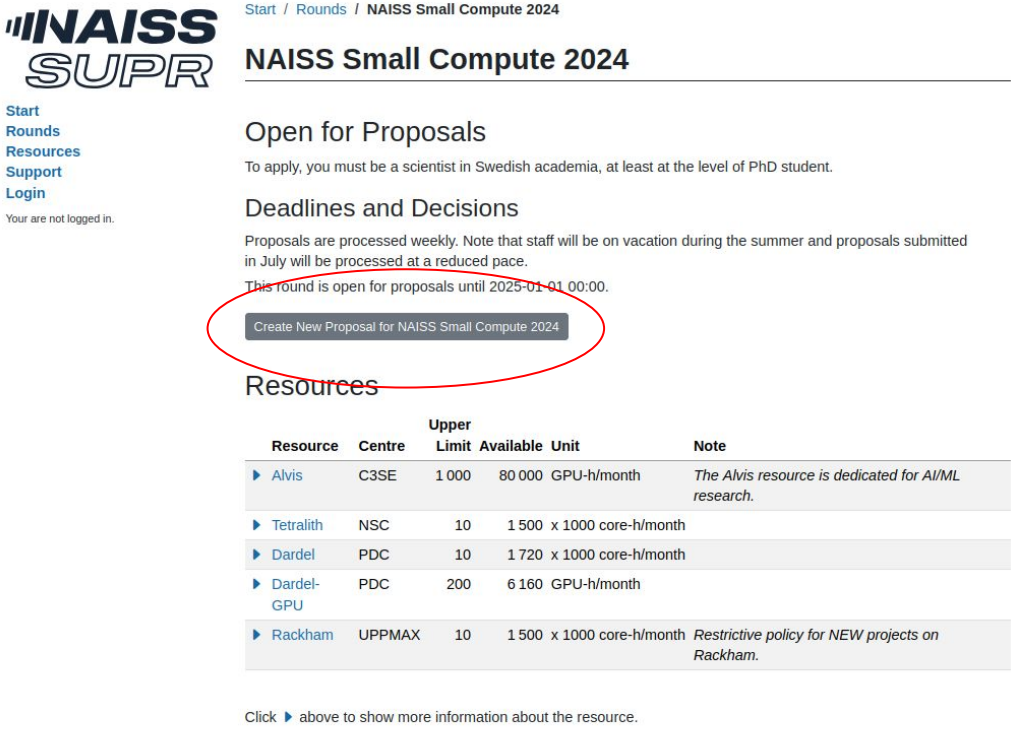
Projects



NAISS SUPR

Start
Rounds
Resources
Support
Login

Your are not logged in.

Start / Rounds / **NAISS Small Compute 2024**

NAISS Small Compute 2024

Open for Proposals

To apply, you must be a scientist in Swedish academia, at least at the level of PhD student.

Deadlines and Decisions

Proposals are processed weekly. Note that staff will be on vacation during the summer and proposals submitted in July will be processed at a reduced pace.

This round is open for proposals until 2025-01-01 00:00.

Create New Proposal for NAISS Small Compute 2024

Resources

Resource	Centre	Upper Limit	Available	Unit	Note
Alvis	C3SE	1 000	80 000	GPU-h/month	*The Alvis resource is dedicated for AI/ML research.*
Tetralith	NSC	10	1 500	x 1000 core-h/month	
Dardel	PDC	10	1 720	x 1000 core-h/month	
Dardel-GPU	PDC	200	6 160	GPU-h/month	
Rackham	UPPMAX	10	1 500	x 1000 core-h/month	*Restrictive policy for NEW projects on Rackham.*

Click ▸ above to show more information about the resource.

https://supr.naiss.se/round/

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How to access PDC

SSH to Dardel

```
ssh -Y your_username@dardel.pdc.kth.se
```

Requires setting up either SSH keys or Kerberos
https://www.pdc.kth.se/support/documents/basics/quickstart.html#how-to-log-in

How to access PDC

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Requires setting up either **SSH keys** or Kerberos
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How to access PDC

SSH to Dardel

```
user@computer ~ $ ssh -Y username@dardel.pdc.kth.se
Last login: Mon Nov 11 10:19:30 2024 from icm-42-29.bmc.uu.se

    --== Welcome to Dardel! ==--

username@login1 ~ $
```

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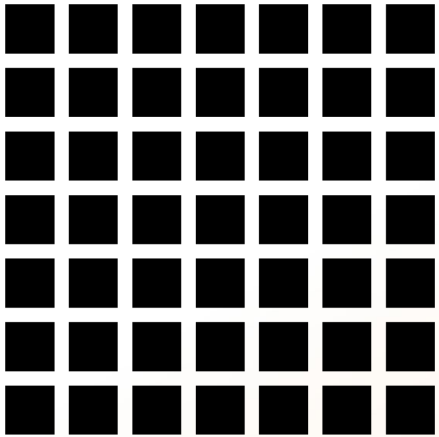
SSH

Local computer

Login nodes



Computation nodes

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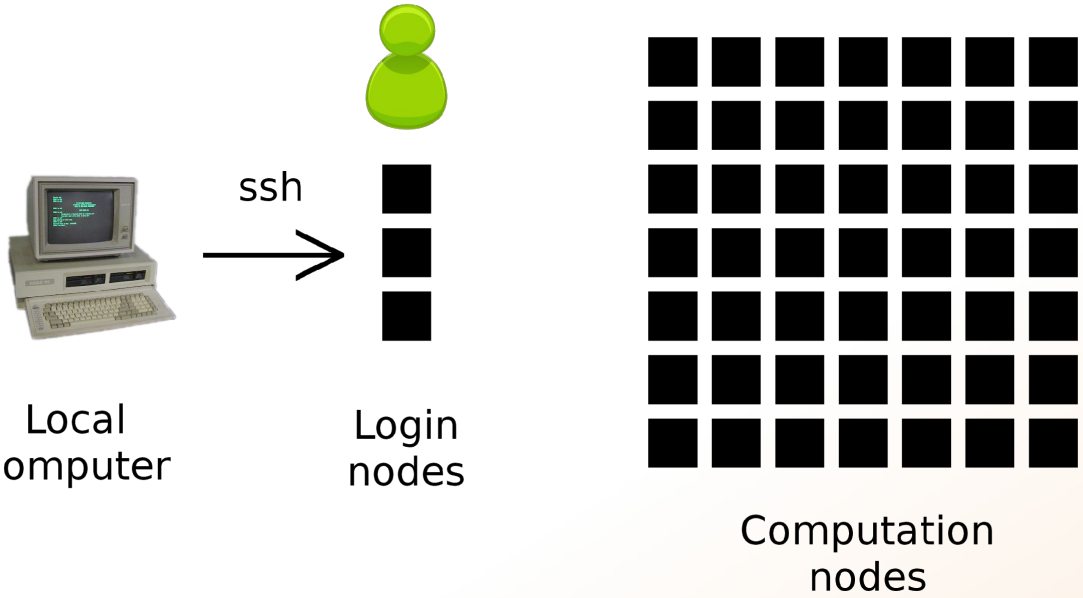
SSH



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How to use PDC

Login nodes

use them to access PDC,
never use them to run **jobs**

Calculation nodes

do your work here - testing and running,
not accessible directly,
SLURM (queueing system) gives you access

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Job

Job (computing)

From Wikipedia, the free encyclopedia

For other uses, see Job (Unix) and Job stream.

In computing, a **job** is a unit of work or unit of execution (that performs said work). A component of a job (as a unit of work) is called a *task* or a *step* (if sequential, as in a job stream). As a unit of execution, a job may be concretely identified with a single process, which may in turn have subprocesses (child processes; the process corresponding to the job being the parent process) which perform the tasks or steps that comprise the work of the job; or with a process group; or with an abstract reference to a process or process group, as in Unix job control.

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Job

Read/open files

Do something with the data

Print/save output

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Queue System

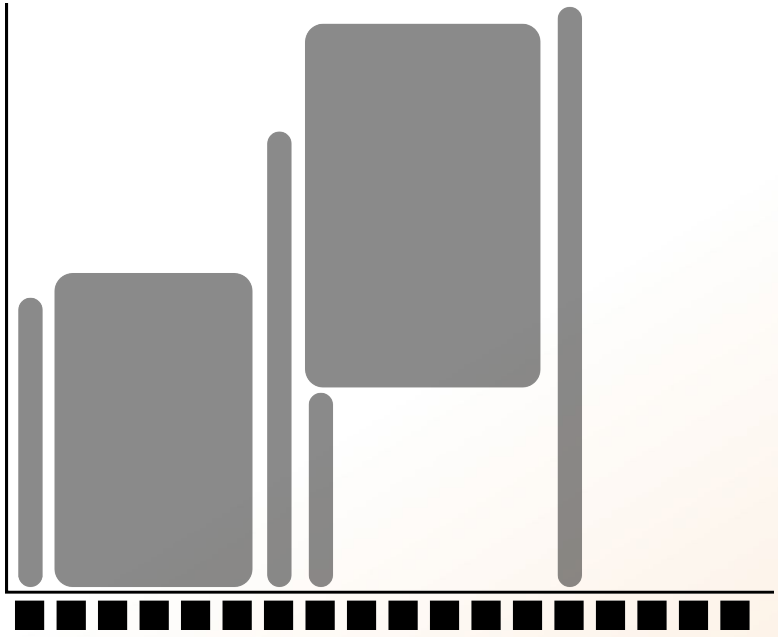
More users than nodes

Need for a queue

Queue System

More users than nodes

Need for a queue



Queue System

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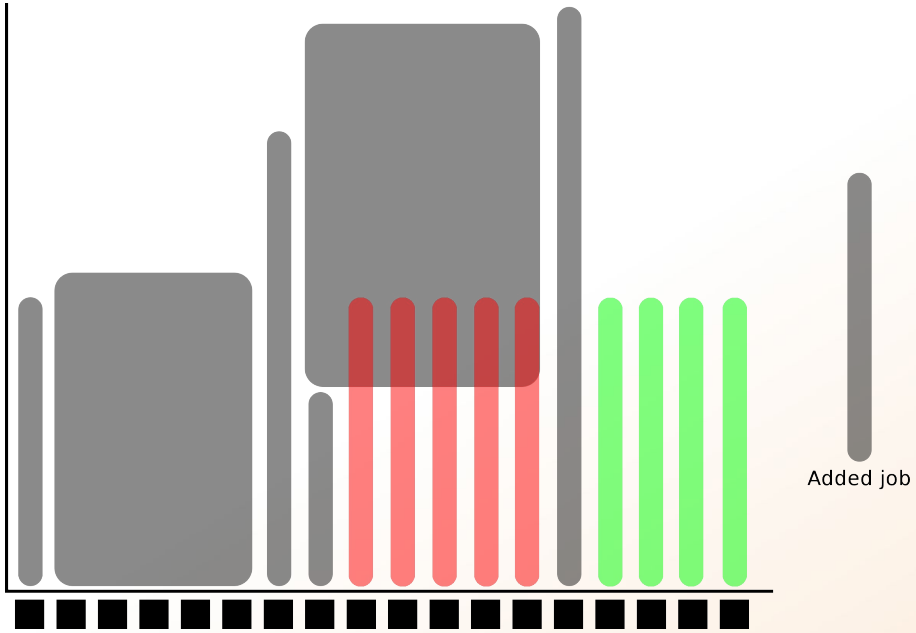

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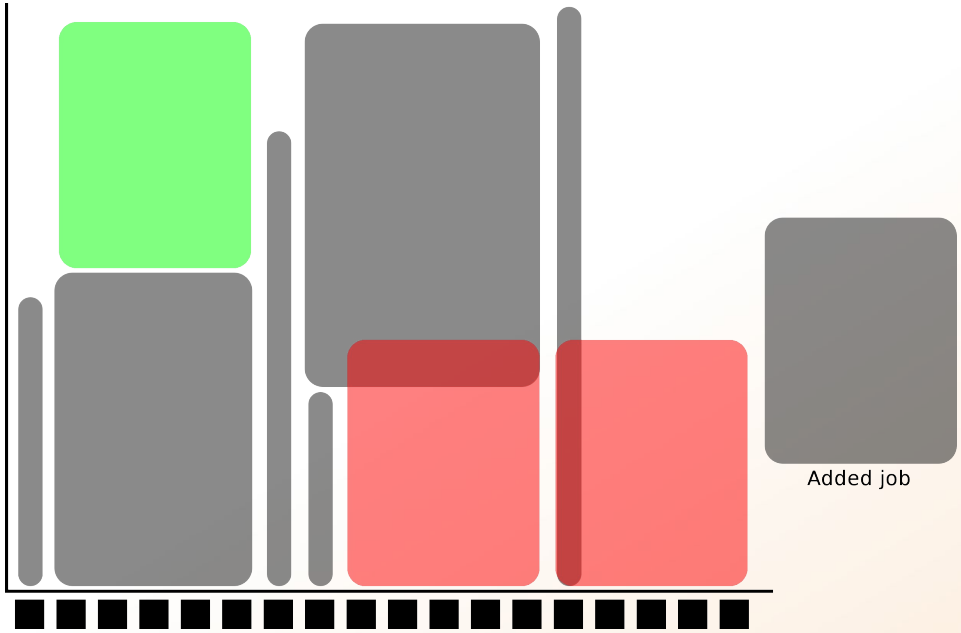

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SLURM

workload manager
job queue
batch queue
job scheduler

SLURM (Simple Linux Utility for Resource Management)

free and open source

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Objectives

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SLURM

1) Ask for resource and run jobs manually

For testing, possibly small jobs, specific programs needing user input while running

2) Write a script and submit it to SLURM

Submits an automated job to the job queue, runs when it’s your turn

1) Ask for resource and run jobs manually

book a node/core

ssh to the node

run programs

1) Ask for resource and run jobs manually

```
salloc -A naiss2099-99-999 -p shared -c 1 -t 00:05:00
```

salloc - command
mandatory job parameters:
-A - project ID (who “pays”)
-p - partition
-c - number of cores
-t - time

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SLURM

```
salloc -A naiss2099-99-999 -p shared -c 1 -t 00:05:00
```

-A example course project naiss2099-99-999
you have to be a member

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SLURM

```
salloc -A naiss2099-99-999 -p shared -c 1 -t 00:05:00
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-A example course project naiss2099-99-999
you have to be a member

-p shared = parts of 1 node 1 node = 128 cores)
main = whole nodes 1 hour walltime = 128 core-hours

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SLURM

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-c number of cores (default value = 1)

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SLURM

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salloc -A naiss2099-99-999 -p shared -c 1 -t 00:05:00
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-A example course project naiss2099-99-999
you have to be a member

-p shared = parts of 1 node 1 node = 128 cores)
main = whole nodes 1 hour walltime = 128 core-hours

-c number of cores (default value = 1)

-t format - hh:mm:ss
or - dd-hh:mm:ss
default value= 7-00:00:00

jobs killed when time limit reaches - always overestimate ~ 50%

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SLURM

Information about your jobs

```
squeue -u <user>
```

```
username@login1 ~ $ squeue -u username
  JOBID  PARTITION     NAME       USER ST     TIME  NODES NODELIST(REASON)
  5236781   shared interact   username  R    20:41      1 nid002582
username@login1 ~ $
```

SSH to a calculation node (from a login node)

```
ssh -Y <node_name>
```

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SLURM

```
username@login1 ~ $ salloc -A naiss2099-99-999 -t 01:00:00 -p shared -c 1
```

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SLURM

```
username@login1 ~ $ salloc -A naiss2099-99-999 -t 01:00:00 -p shared -c 1
salloc: Pending job allocation 5236781
salloc: job 5236781 queued and waiting for resources
salloc: job 5236781 has been allocated resources
salloc: Granted job allocation 5236781
salloc: Nodes nid002582 are ready for job
username@login1 ~ $
```

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SLURM

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username@login1 ~ $ squeue -u username
```

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SLURM

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SLURM

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username@login1 ~ $ ssh -Y nid002582
```

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SLURM

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username@login1 ~ $ ssh -Y nid002582
username@nid002582 ~ $
```

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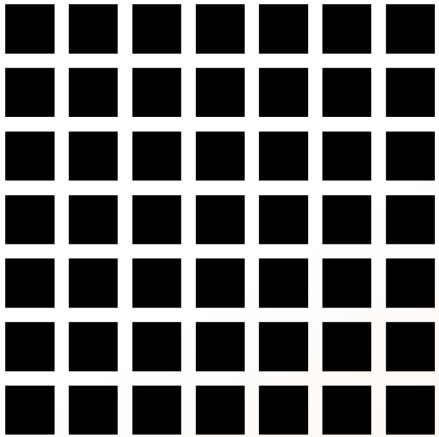
SSH

Local computer

Login nodes



Computation nodes

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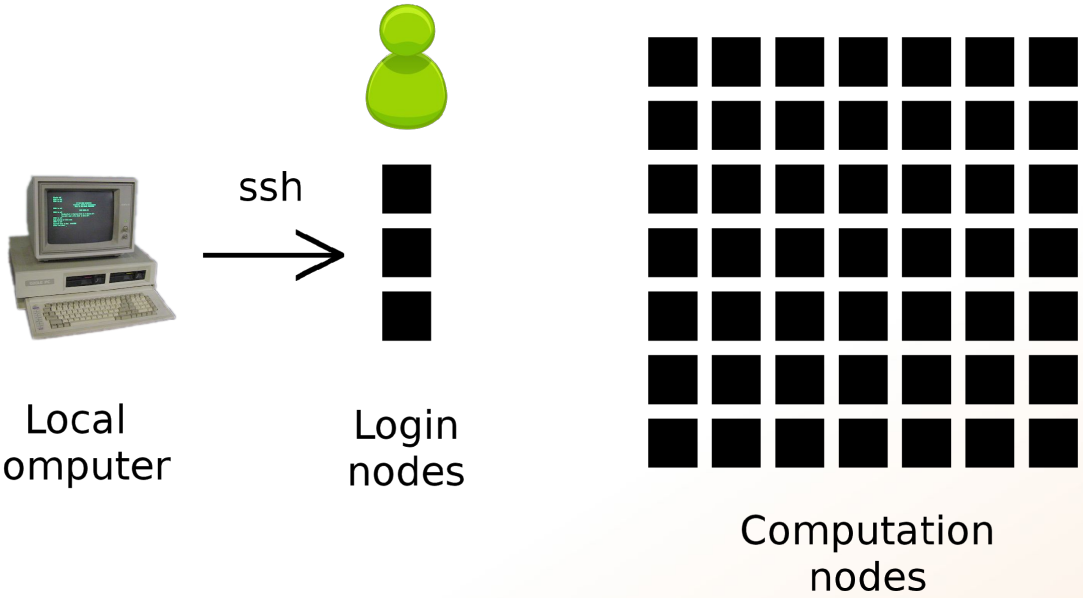
SSH



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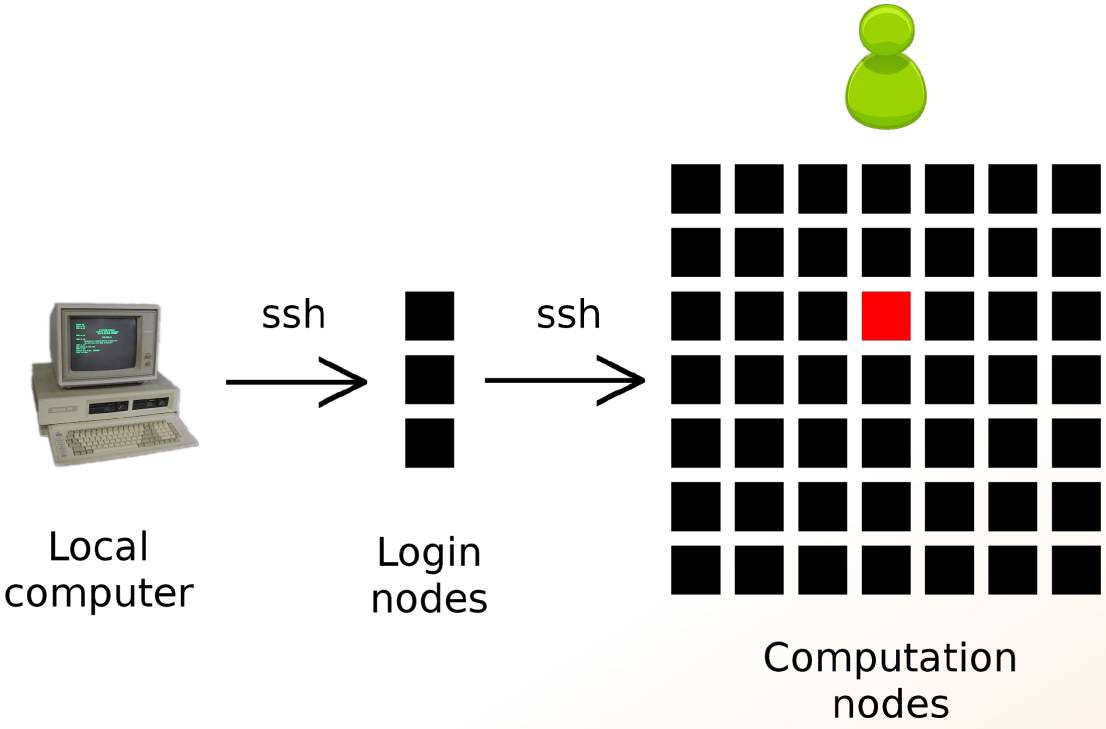
SLURM



2) Write a script and submit it to SLURM

put all commands in a text file - script

tell SLURM to run the script
(use the same job parameters)

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put all commands in a text file - script

```
#! /bin/bash -l
#SBATCH -A XXXXXXX
#SBATCH -p shared
#SBATCH -J Template_script
#SBATCH -t 01:00:00

# load some modules
module load bioinfo-tools

# go to some directory
cd ~/testarea

# do something
echo Hello world!
```

2) Write a script and submit it to SLURM

put all commands in a text file - script

```
#! /bin/bash -l
#SBATCH -A XXXXXXX
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```

job parameters

```
# load some modules
module load bioinfo-tools

# go to some directory
cd ~/testarea

# do something
echo Hello world!
```

tasks to be done

2) Write a script and submit it to SLURM

put all commands in a text file - script

```
#! /bin/bash -l
#SBATCH -A naiss2099-99-999
#SBATCH -p shared
#SBATCH -J sample_001.fq_alignment
#SBATCH -t 7-00:00:00

# load some modules
module load bioinfo-tools bwa

# go to project directory
cd /cfs/klemming/projects/supr/naiss2099-99-999/

# align reads
bwa mem ref/human_reference.fa raw/sample_001.fq | samtools sort -o results/sample_001.aligned.sorted.bam
```

2) Write a script and submit it to SLURM

tell SLURM to run the script
(use the same job parameters)

```
sbatch test.sh
```

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tell SLURM to run the script
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```
sbatch test.sh
```

`sbatch` - command
`test.sh` - name of the script file

2) Write a script and submit it to SLURM

tell SLURM to run the script
(use the same job parameters)

```
sbatch test.sh
```

```
sbatch -A naiss2099-99-999 -p main -c 8 -t 60:00:00 test.sh
```

SLURM Output

Prints to a file instead of terminal

```
username@login1 ~/test $ ll
-rw-------   1 username username  209 Nov 11 13:43 test.sh
username@login1 ~/test $
```

SLURM Output

Prints to a file instead of terminal

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username@login1 ~/test $ ll
-rw-------   1 username username  209 Nov 11 13:43 test.sh
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SLURM Output

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username@login1 ~/test $ ll
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username@login1 ~/test $ cat test.sh
#! /bin/bash -l
#SBATCH -A naiss2099-99-999
#SBATCH -p shared
#SBATCH -J echo_test
#SBATCH -t 00:01:00

# go to home directory
cd ~/test

# print stuff
echo "Hello, this will be printed to the slurm-<jobID>.out"

username@login1 ~/test $
```

SLURM Output

Prints to a file instead of terminal

```
username@login1 ~/test $ ll
-rw-------   1 username username  209 Nov 11 13:43 test.sh
username@login1 ~/test $ cat test.sh
#! /bin/bash -l
#SBATCH -A naiss2099-99-999
#SBATCH -p shared
#SBATCH -J echo_test
#SBATCH -t 00:01:00

# go to home directory
cd ~/test

# print stuff
echo "Hello, this will be printed to the slurm-<jobID>.out"

username@login1 ~/test $ sbatch test.sh
```

SLURM Output

Prints to a file instead of terminal

```
username@login1 ~/test $ ll
-rw-------   1 username username  209 Nov 11 13:43 test.sh
username@login1 ~/test $ cat test.sh
#! /bin/bash -l
#SBATCH -A naiss2099-99-999
#SBATCH -p shared
#SBATCH -J echo_test
#SBATCH -t 00:01:00

# go to home directory
cd ~/test

# print stuff
echo "Hello, this will be printed to the slurm-<jobID>.out"

username@login1 ~/test $ sbatch test.sh
Submitted batch job 5831681
username@login1 ~/test $
```

SLURM Output

Prints to a file instead of terminal

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username@login1 ~/test $ ll
-rw-------   1 username username  209 Nov 11 13:43 test.sh
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# go to home directory
cd ~/test

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username@login1 ~/test $ ll
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# go to home directory
cd ~/test

# print stuff
echo "Hello, this will be printed to the slurm-<jobID>.out"

username@login1 ~/test $ sbatch test.sh
Submitted batch job 5831681
username@login1 ~/test $ ll
-rw-------   1 username username  252 Nov 11 13:43 slurm-5831681.out
-rw-------   1 username username  209 Nov 11 13:43 test.sh
username@login1 ~/test $
```

SLURM Output

Prints to a file instead of terminal

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username@login1 ~/test $ ll
-rw-------   1 username username  209 Nov 11 13:43 test.sh
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-rw-------   1 username username  209 Nov 11 13:43 test.sh
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Submitted batch job 5831681
username@login1 ~/test $ ll
-rw-------   1 username username  252 Nov 11 13:43 slurm-5831681.out
-rw-------   1 username username  209 Nov 11 13:43 test.sh
username@login1 ~/test $ cat slurm-5831681.out
Hello, this will be printed to the slurm-<jobID>.out
username@login1 ~/test $
```

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Software

100+ programs installed

Managed by a 'module system'

- Installed, but hidden
- Manually loaded before use

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`module avail`	- Lists all available modules
`module load <module name>`	- Loads the module
`module unload <module name>`	- Unloads the module
`module list`	- Lists loaded modules
`module spider <word>`	- Searches all modules after 'word'

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Software

Most bioinfo programs hidden under bioinfo-tools

Load bioinfo-tools first, then program module

```
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username@login1 ~ $ module load cufflinks
```

or

```
username@login1 ~ $ module load bioinfo-tools cufflinks
```

```
username@login1 ~ $ module avail

------------------------------------------------- /pdc/software/eb/modules/all
   angsd/0.940                          googletest/1.8.1            ncurses/6.4             (L,D)
   ant/1.10.14                          gperf/3.0.4                 nextflow/24.04.2
   apr/1.7.0                            gperf/3.1             (D)   ninja/1.10.2
   argtable/2.13                        groff/1.23.0                ninja/1.11.0
   autoconf-archive/2022.02.11          gsl/2.3                     ninja/1.11.1
   autoconf/2.69                        gsl/2.7.1             (D)   ninja/1.12.1              (D)
   autoconf/2.71                 (D)    guile/2.0.14                ntcard/1.2.1
   autodiff/0.5.10                      gzip/1.10                   onetbb/2021.5.0
   autodiff/0.6.5                (D)    gzip/1.12                   opari2/2.0.6
   automake/1.16.1                      gzip/1.13             (D)   openexr/3.2.0
   automake/1.16.4                      haploeagle/2.4.1            openjpeg/2.5.0
   automake/1.16.5               (D)    harfbuzz/8.2.2              osmesa/21.3.7
   autotools/20220317                   hdf/4.2.16-2                ospray/2.4.0
   bamm/2.5.0                           help2man/1.49.2             otf2/2.3
   bamsifter/2.15.0                     hifiasm/0.19.7              otf2/3.0.3                (D)
   bamtools/2.5.2                       highway/1.2.0               paml/4.9j
   barrnap/0.9                          hisat2/2.2.1                pango/1.50.14
   bazel/6.3.1                          htslib/1.15.1               parafly/0.1.0
   bbmap/38.61b                         htslib/1.20           (L,D) parallel/20230422
   bbmap/39.01                          hwloc/2.6.0                 parasail/2.6.2
   bbmap/39.06                   (D)    hwloc/2.9.0                 patchelf/0.14.5
   bcftools/1.15.1                      hwloc/2.11.1          (D)   pbbam/1.0.7
   bcftools/1.20                 (D)    icu/69.1                    pbcopper/1.8.0
   bcl2fastq2/2.20.0                    icu/74.1              (D)   pblat/2.5.1
   bedtools/2.31.0                      imagemagick/7.1.0-32        pcre/8.45
   bifrost/1.0.6.4                      imath/3.1.9                 pcre2/10.40
```

PDC Commands

projinfo

```
username@login1 ~ $ projinfo
$HOME folder
Path: /cfs/klemming/home/u/username
Storage: 12.34 GiB
Number of files: 83135

Project info for all projects for user: username

Information for compute project: uppmax.staff (PI: username)
Test allocation for UPPMAX
Active from 2023-10-01 00:00:00 to 2027-01-01 00:00:00
Members: username, username01, username02
dardel: 10000 corehours/month, used 12.52% (1252 corehours) during the past 30 days

Information for compute project: naiss2024-5-11 (PI: username)
SNIC systems access for application experts
Active from 2024-01-09 00:00:00 to 2025-02-01 00:00:00
Members: username, username01
dardel: 2000 corehours/month, used 0.00% (0 corehours) during the past 30 days
```

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PDC Commands

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Members: username, username01, username02
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Take-home messages

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- Do not ask for more cores/nodes than your job can actually use

Take-home messages

- The difference between **user account** and **project**
- **Login nodes** are not for running jobs
- SLURM gives you access to the **compute nodes** when you specify a project that you are member of
- Do not ask for more cores/nodes than your job can actually use
- A job script usually consists of:
  - Job settings (-A, -p, -c, -t)
  - Modules to be loaded
  - Bash code to perform actions
  - Run a program, or multiple programs

SciLifeLab UPPSALA

Laboratory time! (again)

https://nbisweden.github.io/workshop-ngsintro/2503/topics/hpc/intro/lab_intro.html