UPPMAX Introduction

2024-03-18

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Enabler for Life Sciences

SciLifeLab UPPSALA

Objectives

What is UPPMAX what it provides

Projects at UPPMAX

How to access UPPMAX

Jobs and queuing systems

How to use the resources of UPPMAX

How to use the resources of UPPMAX in a good way!

Efficiency!!!

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UPPMAX

Uppsala Multidisciplinary Center for Advanced Computational Science
http://www.uppmax.uu.se

2 (3) **computer clusters**

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UPPMAX

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2 (3) **computer clusters**

- **Rackham**: ~ 500 nodes à 20 cores (128, 256 & 1024 GB RAM)
  + Snowy (old Milou): ~ 200 nodes à 16 cores (128, 256 & 512 GB RAM)

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>12 PB fast parallel **storage**

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>12 PB fast parallel **storage**

Bioinformatics **software**

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UPPMAX

The basic structure of supercomputer

Login nodes

node = computer

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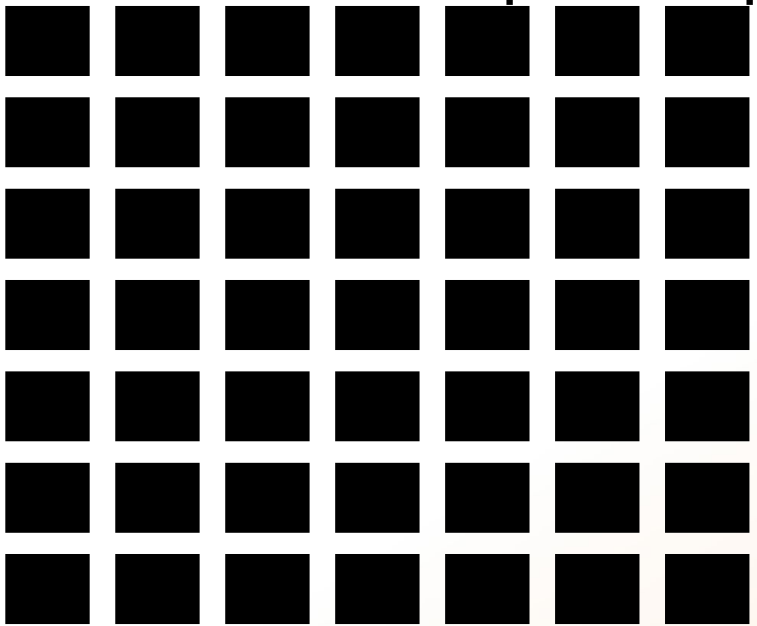
UPPMAX

The basic structure of supercomputer



Calculation nodes

Login nodes

node = computer

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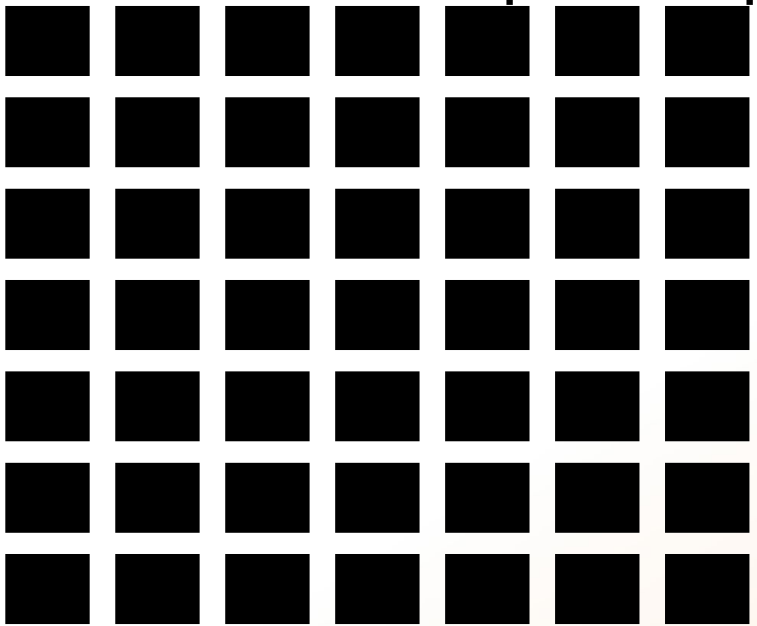
UPPMAX

The basic structure of supercomputer



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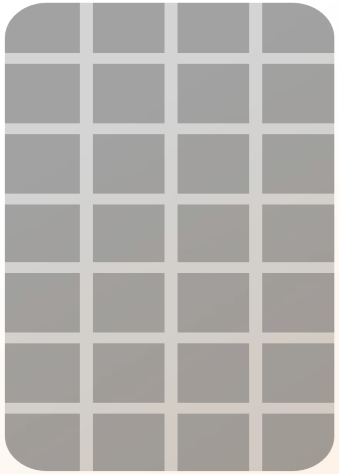

Storage

Login nodes

node = computer

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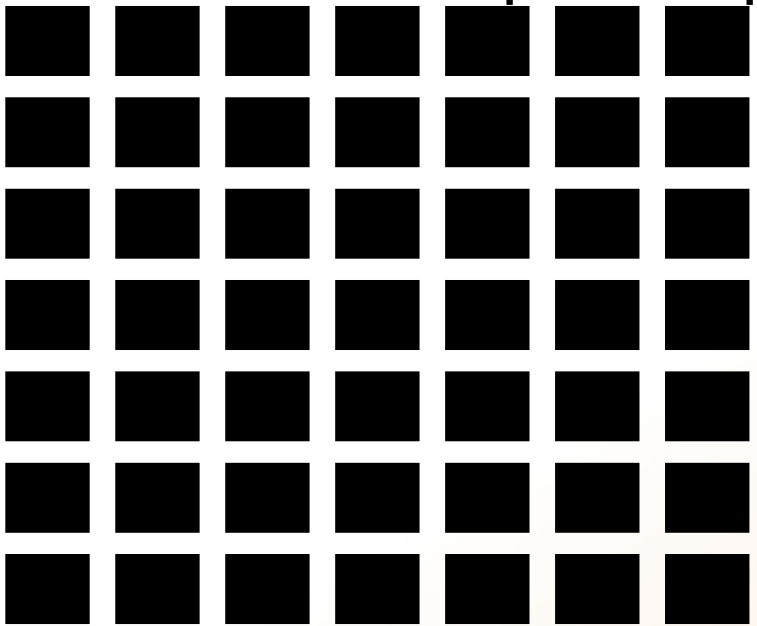
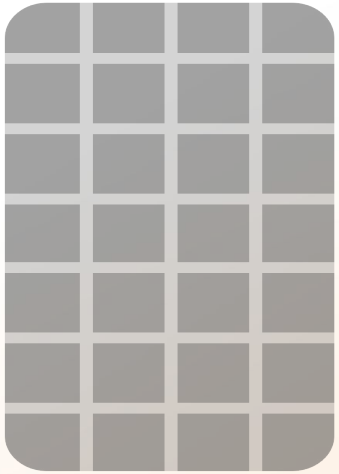
UPPMAX

The basic structure of supercomputer



Calculation nodes



Storage

Login nodes

Compute and **Storage**

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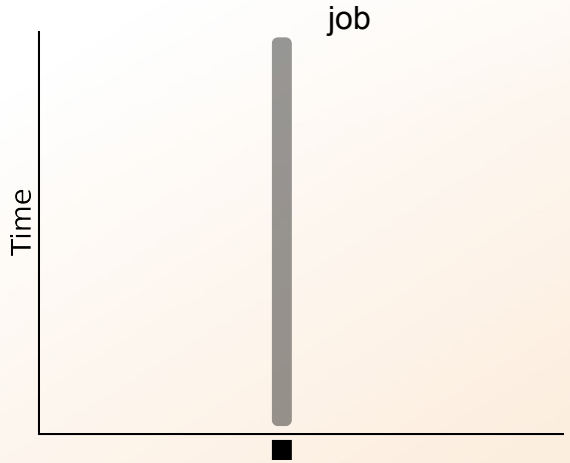
Job

The basic structure of a supercomputer

Parallel computing

Not one super fast



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The basic structure of a supercomputer

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Projects

UPPMAX provides its resources via

projects

Projects

UPPMAX provides its resources via

projects

compute
(core-hours/month)

storage
(GB)

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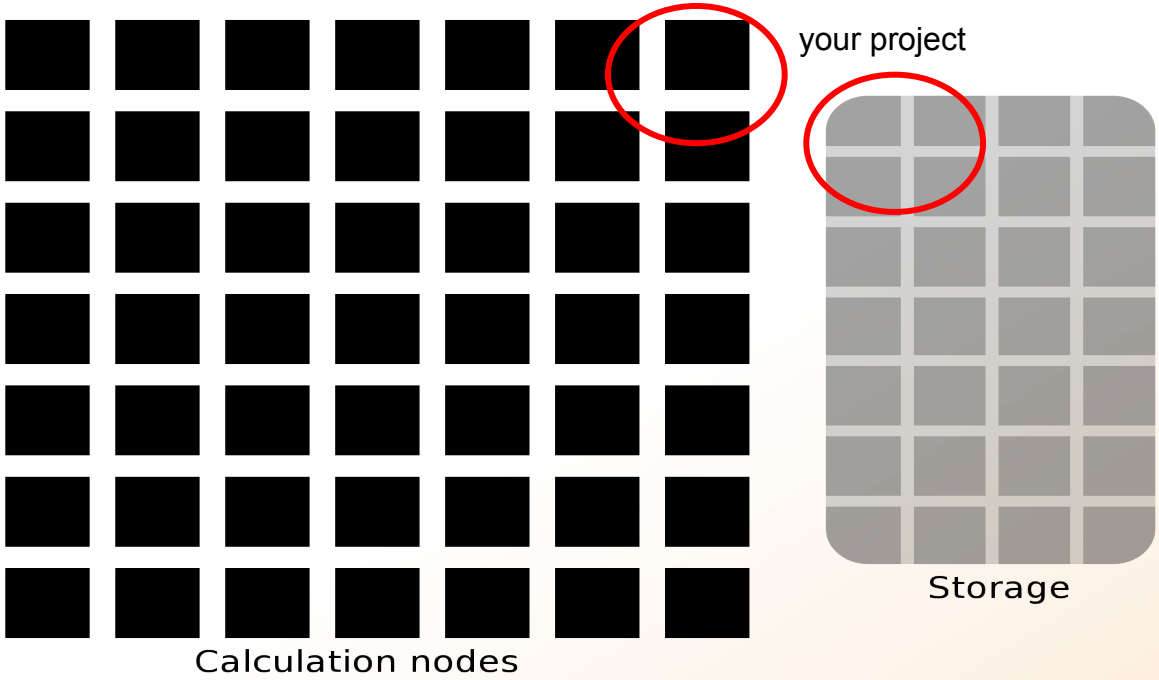
Projects



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Projects

Two separate projects:

SNIC compute:

cluster **Rackham**

2000 - 100 000+ core-hours/month

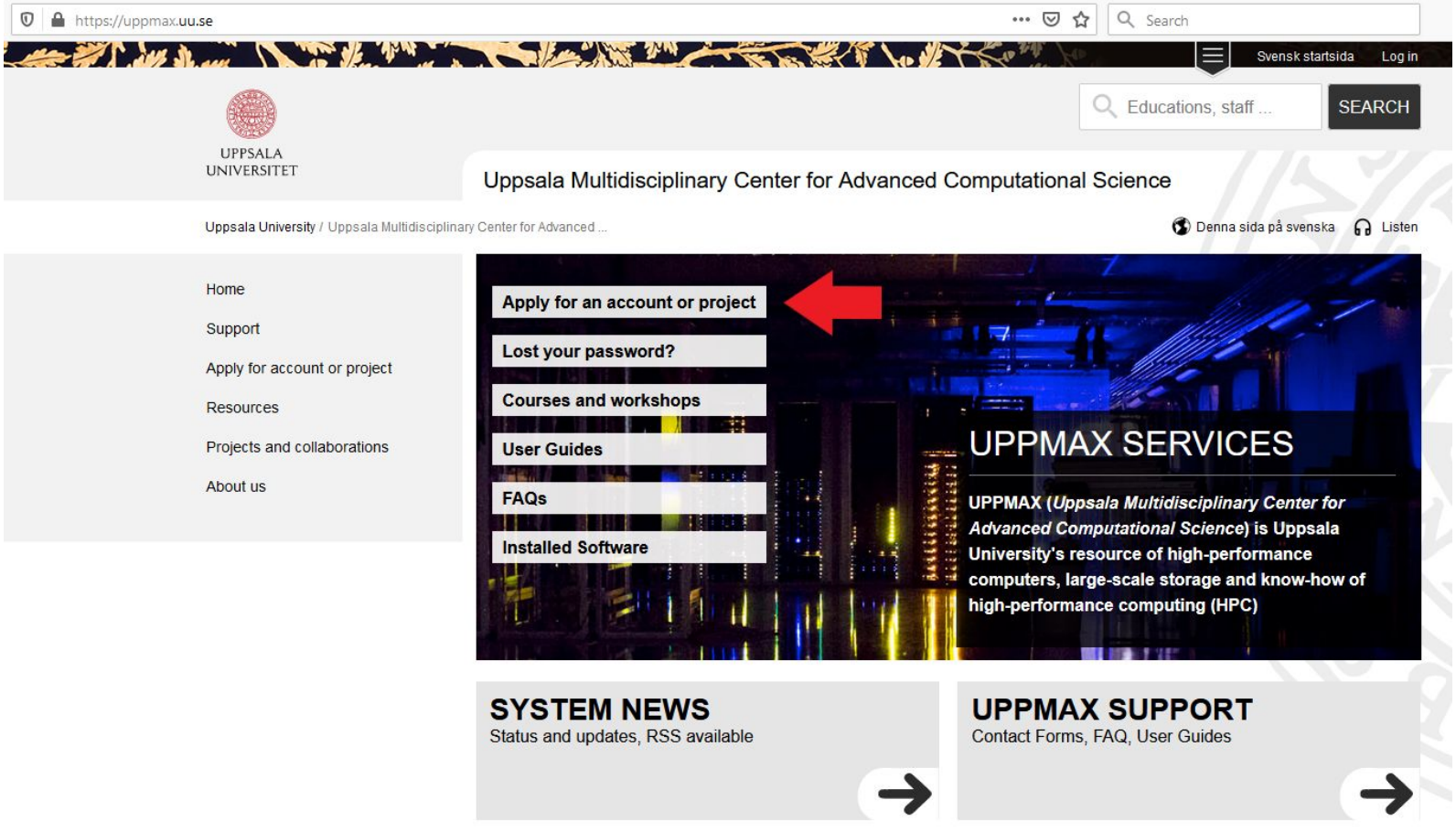
128 GB storage

UPPMAX Storage:

storage system **CREX**

1 - 100+ TB storage

Projects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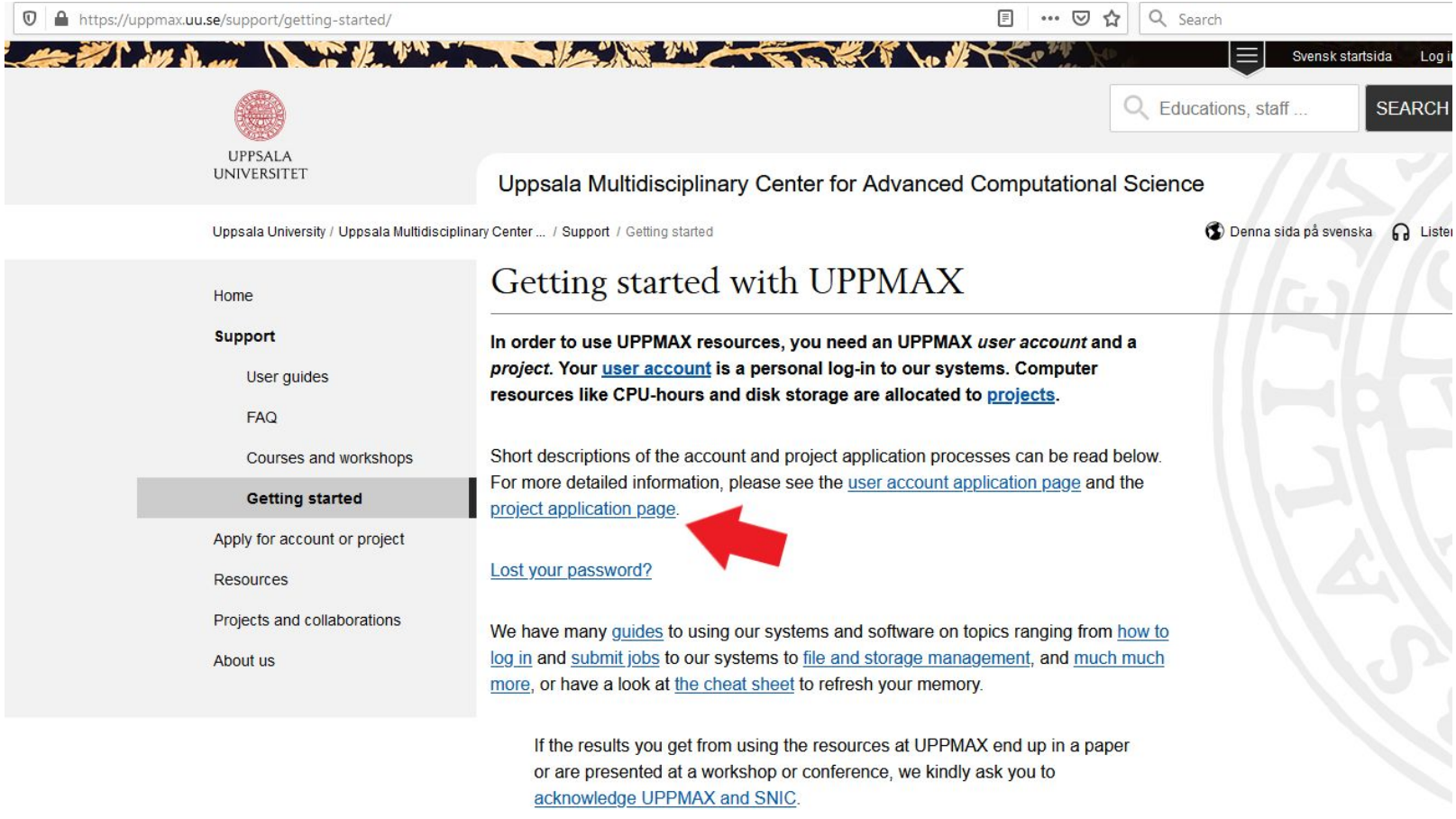
UPPMAX SERVICES
UPPMAX (Uppsala Multidisciplinary Center for Advanced Computational Science) is Uppsala University's resource of high-performance computers, large-scale storage and know-how of high-performance computing (HPC)
SYSTEM NEWS
Status and updates, RSS available
UPPMAX SUPPORT
Contact Forms, FAQ, User Guides

Projects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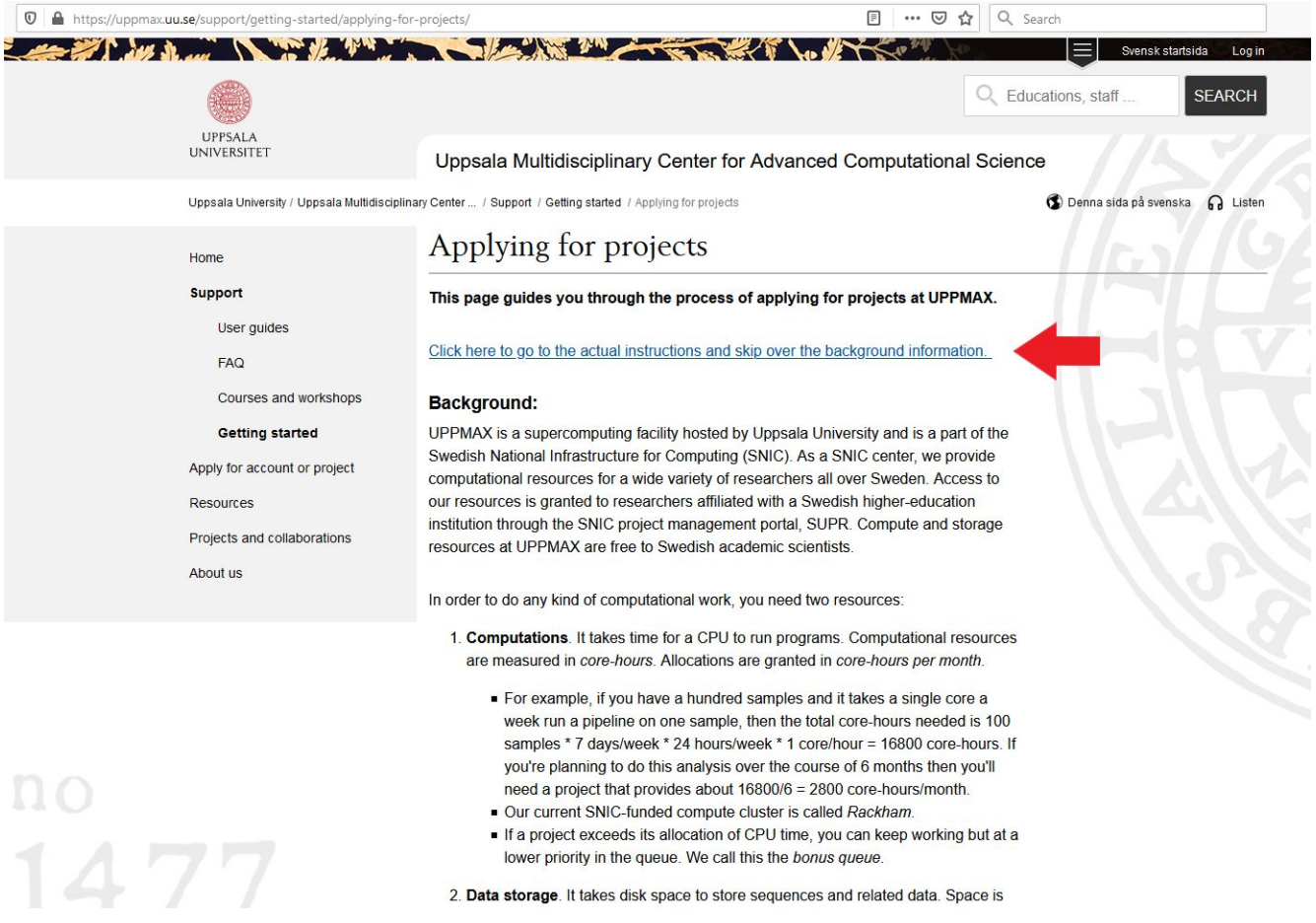
Getting started with UPPMAX
In order to use UPPMAX resources, you need an UPPMAX user account and a project. Your user account is a personal log-in to our systems. Computer resources like CPU-hours and disk storage are allocated to projects.
Short descriptions of the account and project application processes can be read below. For more detailed information, please see the user account application page and the project application page.
Lost your password?
We have many guides to using our systems and software on topics ranging from how to log in and submit jobs to our systems to file and storage management, and much much more, or have a look at the cheat sheet to refresh your memory.
If the results you get from using the resources at UPPMAX end up in a paper or are presented at a workshop or conference, we kindly ask you to acknowledge UPPMAX and SNIC.

Projects



https://uppmax.uu.se/support/getting-started/applying-for-projects/

Search

Svensk startsida Log in

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Educations, staff ... SEARCH

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Denna sida på svenska Listen

- Home
- **Support**
  - User guides
  - FAQ
  - Courses and workshops
  - **Getting started**
- Apply for account or project
- Resources
- Projects and collaborations
- About us

Applying for projects

This page guides you through the process of applying for projects at UPPMAX.

Click here to go to the actual instructions and skip over the background information.

Background:

UPPMAX is a supercomputing facility hosted by Uppsala University and is a part of the Swedish National Infrastructure for Computing (SNIC). As a SNIC center, we provide computational resources for a wide variety of researchers all over Sweden. Access to our resources is granted to researchers affiliated with a Swedish higher-education institution through the SNIC project management portal, SUPR. Compute and storage resources at UPPMAX are free to Swedish academic scientists.

In order to do any kind of computational work, you need two resources:

1. **Computations**. It takes time for a CPU to run programs. Computational resources are measured in *core-hours*. Allocations are granted in *core-hours per month*.
   - For example, if you have a hundred samples and it takes a single core a week run a pipeline on one sample, then the total core-hours needed is 100 samples * 7 days/week * 24 hours/week * 1 core/hour = 16800 core-hours. If you're planning to do this analysis over the course of 6 months then you'll need a project that provides about 16800/6 = 2800 core-hours/month.
   - Our current SNIC-funded compute cluster is called *Rackham*.
   - If a project exceeds its allocation of CPU time, you can keep working but at a lower priority in the queue. We call this the *bonus queue*.
2. **Data storage**. It takes disk space to store sequences and related data. Space is

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Efficiency!!!

How to access UPPMAX

SSH to a cluster

```
ssh -Y your_username@cluster_name.uppmax.uu.se
```

How to access UPPMAX

SSH to Rackham

```
VG-MBP:~ valentingeorgiev$ ssh -Y valent@rackham.uppmax.uu.se
Last login: Sun Oct 22 10:14:21 2017 from host-95-195-196-83.mobileonline.telia.com
 _   _ ____  ____  __  __    _    __  __
| | | |  _ \|  _ \|  \/  |  / \   \ \/ /   | System:    rackham1
| | | | |_) | |_) | |\/| | / _ \   \  /    | User:      valent
| |_| |  __/|  __/| |  | |/ ___ \  /  \    | Jobs:      0 running
 \___/|_|   |_|   |_|  |_/_/   \_\/_/\_\   | Queue:     0 pending

###############################################################################

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[valent@rackham1 ~]$
```

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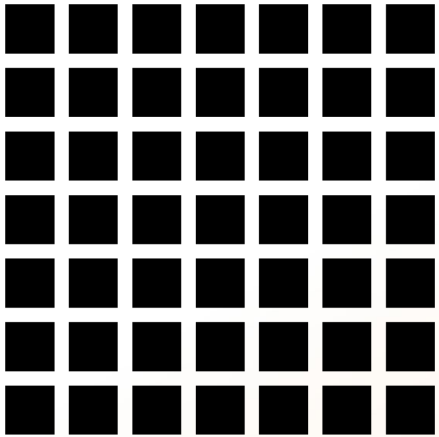
SSH

Local computer

Login nodes



Computation nodes

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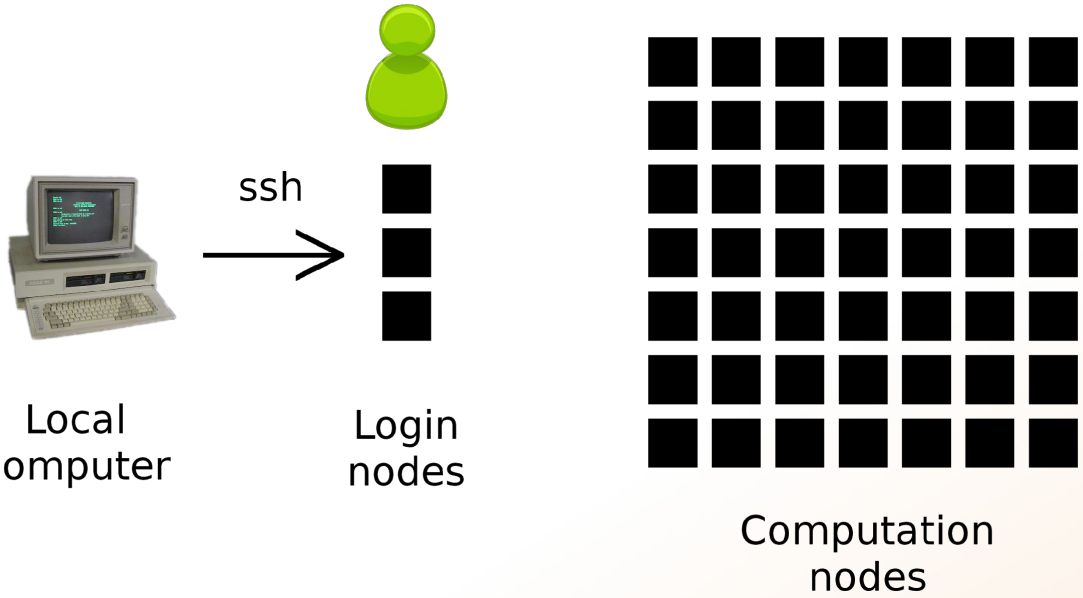
SSH



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How to use UPPMAX

Login nodes

use them to access UPPMAX,
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

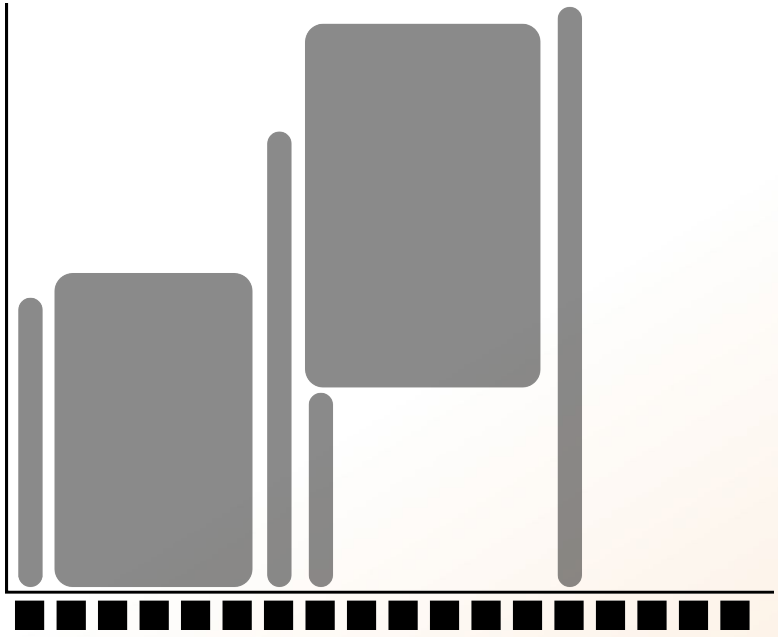
More users than nodes

Need for a queue

Queue System

More users than nodes

Need for a queue



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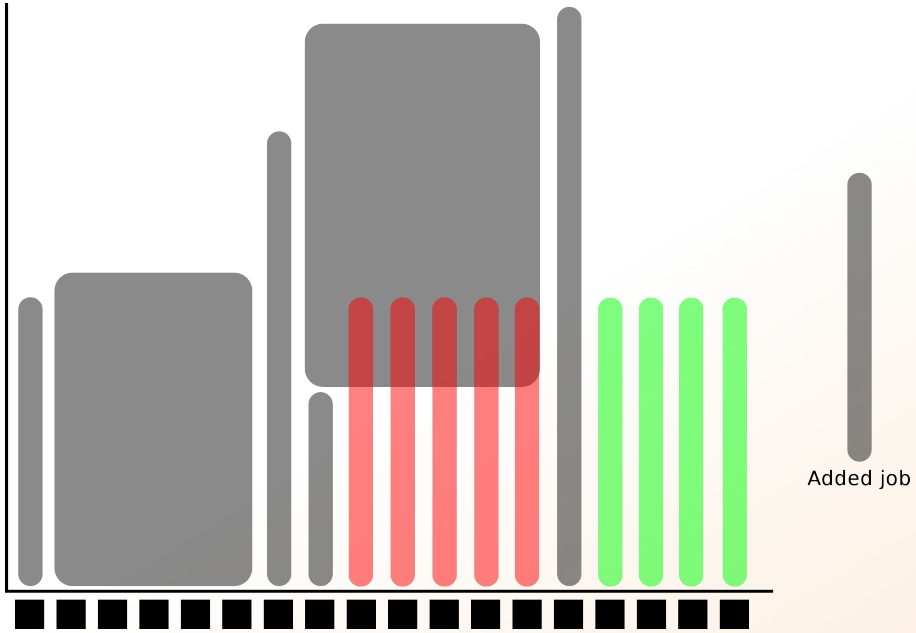

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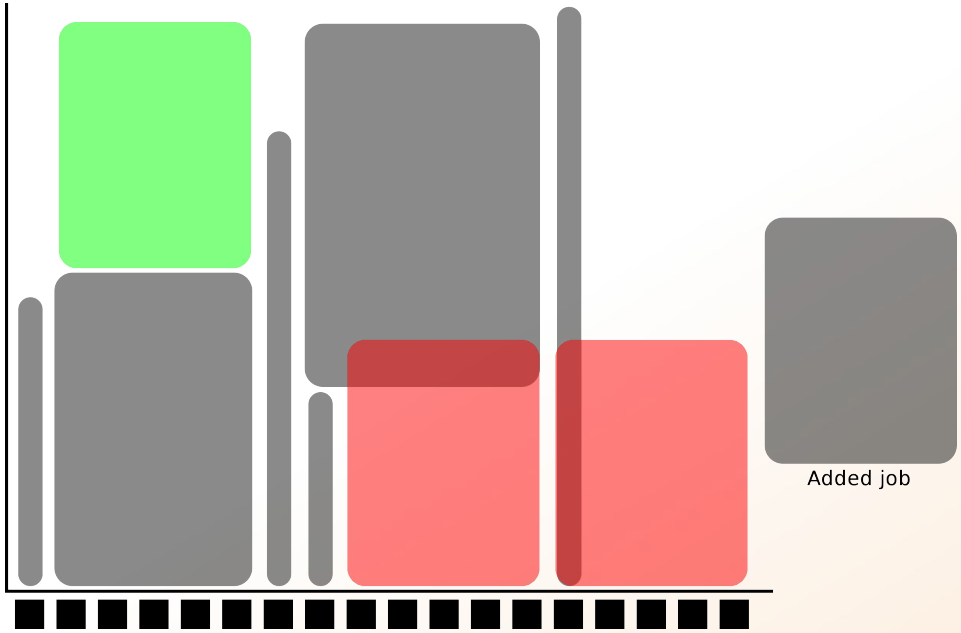

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SLURM

workload manager
job queue
batch queue
job scheduler

SLURM (Simple Linux Utility for Resource Management)

free and open source

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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 snic2022-22-1124 -p core -n 1 -t 00:05:00
```

salloc - command
mandatory job parameters:
-A - project ID (who “pays”)
-p - node or core (the type of resource)
-n - number of nodes/cores
-t - time

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SLURM

```
salloc -A snic2022-22-1124 -p core -n 1 -t 00:05:00
```

-A this course project snic2022-22-769
you have to be a member

-p 1 node = 20 cores
1 hour walltime = 20 core-hours

-n 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>`

```
[valent@milou2 valent]$ squeue -u valent
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          11334919      core       sh   valent  R       0:11      1 m164
```

SSH to a calculation node (from a login node)

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

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SLURM

```
[valent@milou2 valent]$ salloc -A b2015245 -p core -n 1 -t 00:05:00 &
[2] 10994
[valent@milou2 valent]$ salloc: Granted job allocation 11334919

[valent@milou2 valent]$ squeue -u valent
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          11334919      core       sh   valent  R       0:11      1 m164
[valent@milou2 valent]$ ssh -Y m164
  _   _ ____  ____  __  __     _     __  __
 | | | |  _ \|  _ \|  \/  |   / \    \ \/ /    | System:    m164
 | | | | |_) | |_) | |\/| |  / _ \    \  /     | User:      valent
 | |_| |  __/|  __/| |  | | / ___ \   /  \     | Jobs:      1 running
  \___/|_|   |_|   |_|  |_|/_/   \_\/_/\_\    | Queue:     0 pending

################################################################################

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[valent@m164 ~]$
```

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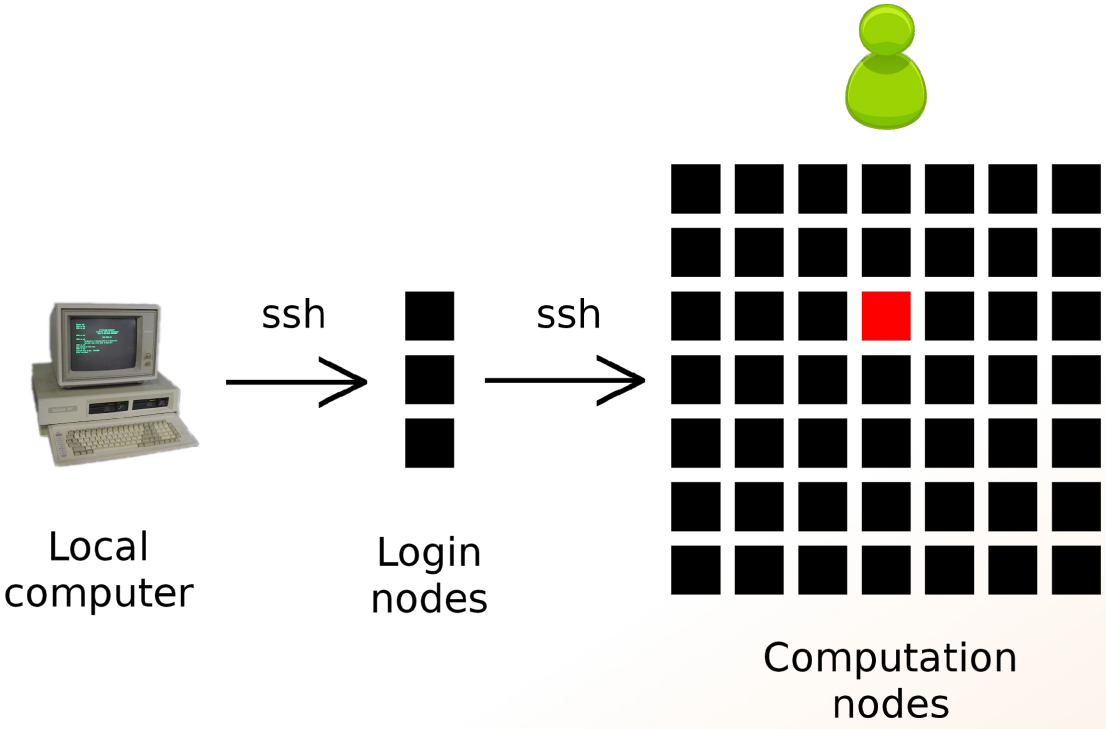
SLURM



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SLURM

1a) Ask for node/core and run jobs manually

Interactive - books a node and connects you to it

```
interactive -A snic2022-22-1124 -p core -n 1 -t 00:05:00
```

```
 _   _ ____  ____  __  __    _    __  __
| | | |  _ \|  _ \|  \/  |  / \   \ \/ /   | System:    m1
| | | | |_) | |_) | |\/| | / _ \   \  /    | User:      valent
| |_| |  __/|  __/| |  | |/ ___ \  /  \    | Jobs:      1 running
 \___/|_|   |_|   |_|  |_/_/   \_\/_/\_\   | Queue:     0 pending

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[valent@m1 valent]$
```

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 g2012157
#SBATCH -p core
#SBATCH -J Template_script
#SBATCH -t 08:00:00

# go to some directory
cd ~/glob

# 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 g2012157
#SBATCH -p core
#SBATCH -J Template_script
#SBATCH -t 08:00:00
```

job parameters

```
# go to some directory
cd ~/glob

# 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 g2012157
#SBATCH -p node
#SBATCH -J Template_script
#SBATCH -t 08:00:00
```

```
# go to the correct directory
cd /home/dahlo/glob/work/uppmaxScripts/misc

# run tophat on the data, using 8 cores
tophat -p 8 /bubo/proj/g2012157/indexes/bowtie/hg19 tophat/input/ad12.fq
```

2) Write a script and submit it to SLURM

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

```
sbatch test.sbatch
```

2) Write a script and submit it to SLURM

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

```
sbatch test.sbatch
```

`sbatch` - command
`test.sbatch` - 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 -A snic2022-22-1124 -p core -n 1 -t 00:05:00 test.sbatch
```

SLURM Output

Prints to a file instead of terminal

`slurm-<job id>.out`

```
[valent@milou2 temp]$ ll
total 32
-rw-rw-r-- 1 valent valent 209 Oct 22 13:34 test.sbatch
[valent@milou2 temp]$ sbatch test.sbatch
Submitted batch job 11334939
[valent@milou2 temp]$ ll
total 64
-rw-rw-r-- 1 valent valent  31 Oct 22 13:35 slurm-11334939.out
-rw-rw-r-- 1 valent valent 209 Oct 22 13:34 test.sbatch
[valent@milou2 temp]$ cat slurm-11334939.out
this goes to slurm-<jobID>.out
[valent@milou2 temp]$ cat test.sbatch
#!/bin/bash -l

#SBATCH -A b2015245
#SBATCH -p core
#SBATCH -n 1
#SBATCH -t 00:05:00


# go to dir work
cd ~/work
# do something useless
echo "this goes to slurm-<jobID>.out"
echo "Hello, world!" > hello.txt
[valent@milou2 temp]$
```

Squeue

Shows information about your jobs

`squeue -u <user>`

```
[valent@milou2 temp]$ sbatch test.sbatch
Submitted batch job 11334948
[valent@milou2 temp]$ squeue -u valent
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          11334948      core test.sba   valent CG       0:01      1 m200
```

`jobinfo -u <user>`

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Queue System

SLURM user guide
go to http://www.uppmax.uu.se/
click User Guides (left-hand side menu)
click Slurm user guide

Queue System

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or just google “uppmax slurm user guide”

link:
http://www.uppmax.uu.se/support/user-guides/slurm-user-guide/

SciLifeLab UPPSALA

UPPMAX Software

100+ programs installed

Managed by a 'module system'

- Installed, but hidden
- Manually loaded before use

UPPMAX Software

100+ programs installed

Managed by a 'module system'

- Installed, but hidden
- Manually loaded before use

`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'

UPPMAX Software

Most bioinfo programs hidden under bioinfo-tools

Load bioinfo-tools first, then program module

```
[dahlo@kalkyl3 work]$ module load cufflinks/1.2.1
ModuleCmd_Load.c(200):ERROR:105: Unable to locate a modulefile for 'cufflinks/1.2.1'
[dahlo@kalkyl3 work]$ module load bioinfo-tools
[dahlo@kalkyl3 work]$ module load cufflinks/1.2.1
[dahlo@kalkyl3 work]$
```

or

```
[dahlo@kalkyl3 work]$ module load samtools
ModuleCmd_Load.c(200):ERROR:105: Unable to locate a modulefile for 'samtools'
[dahlo@kalkyl3 work]$ module load bioinfo-tools samtools
[dahlo@kalkyl3 work]$
```

```
[dahlo@kalkyl4 work]$ module load bioinfo-tools
[dahlo@kalkyl4 work]$ module avail

---------------------------------- /bubo/sw/mf/kalkyl/bioinfo-tools/alignment ----------------------------------
MUMmer/3.22(default)            blast/2.2.24(default)           maq/0.7.1(default)
anfo/0.97                       blast/2.2.24+                   mosaik-aligner/1.0.1388(default)
anfo/0.98(default)              blast/2.2.25                    mosaik-aligner/1.1.0021
blast/2.2.15                    blat/34                         mpiblast/1.6.0(default)
blast/2.2.18                    bwa/0.5.8a                      splitseek/1.3.2
blast/2.2.23                    bwa/0.5.9                       splitseek/1.3.4(default)
blast/2.2.23+                   hmmer/3.0

---------------------------------- /bubo/sw/mf/kalkyl/bioinfo-tools/assembly ----------------------------------
Ray/0.0.4             abyss/1.2.4           abyss/1.3.0           velvet/1.0.03(default)
Ray/0.0.7(default)    abyss/1.2.5(default)  abyss/1.3.2           velvet/1.1.04
Ray/1.6.1             abyss/1.2.7           mira/3.0.0            velvet/1.1.04_K101
abyss/1.2.3           abyss/1.2.7-maxk96    mira/3.2.0(default)   velvet/1.1.07

----------------------------------- /bubo/sw/mf/kalkyl/bioinfo-tools/misc -----------------------------------
BclConverter/1.7.1                freebayes/0.8.9                   samtools/0.1.12-10(default)
BioPerl/1.6.1                     freebayes/0.9.4                   samtools/0.1.16
BioPerl/1.6.1_PERL5.10.1(default) gcta/0.92.0                       samtools/0.1.18
BioPerl/1.6.1_PERL5.12.3          gcta/0.92.6                       samtools/0.1.7a
FastQC/0.6.1                      genometools/1.3.5(default)        samtools/0.1.8
FastQC/0.7.2(default)             htseq/0.4.6                       samtools/0.1.9
Fastx/0.0.13(default)             htseq/0.5.1                       snpEff/2.0.3
IGV/1.5.51                        matrix2png/1.2.1                  trinity/2011-05-13
biopython/1.56                    picard/1.40                       trinity/2011-10-29
cellprofiler/20111024             picard/1.41
emmax/beta-07Mar2010              plink/1.07

---------------------------------- /bubo/sw/mf/kalkyl/bioinfo-tools/phylogeny ----------------------------------
concaterpillar/1.4    garli/2.0             raxml/7.0.4(default)  raxml/7.2.8
garli/0.96b8(default) mrbayes/3.1.2-mpi     raxml/7.2.7

---------------------------------- /bubo/sw/mf/kalkyl/bioinfo-tools/pipelines ----------------------------------
ab_wtp/1.1(default)      cufflinks/0.9.2          cufflinks/1.1.0          tophat/1.2.0
bowtie/0.12.6(default)   cufflinks/0.9.3          cufflinks/1.2.1          tophat/1.3.3
```

UPPMAX Commands

uquota

```
[dahlo@biologin work]$ uquota
Your File Area                  Usage (GB)   Quota Limit (GB)     Over Quota     Grace Time
--------------                  ----------   ----------------     ----------     ----------
dahlo glob                             196              2048                             -
dahlo home                               4                32                             -
/proj/b2010015                         229               256
/proj/b2010015/nobackup                  0               512                             -
/proj/b2010033                         132              6348
/proj/b2010033/nobackup                 27               512                             -
```

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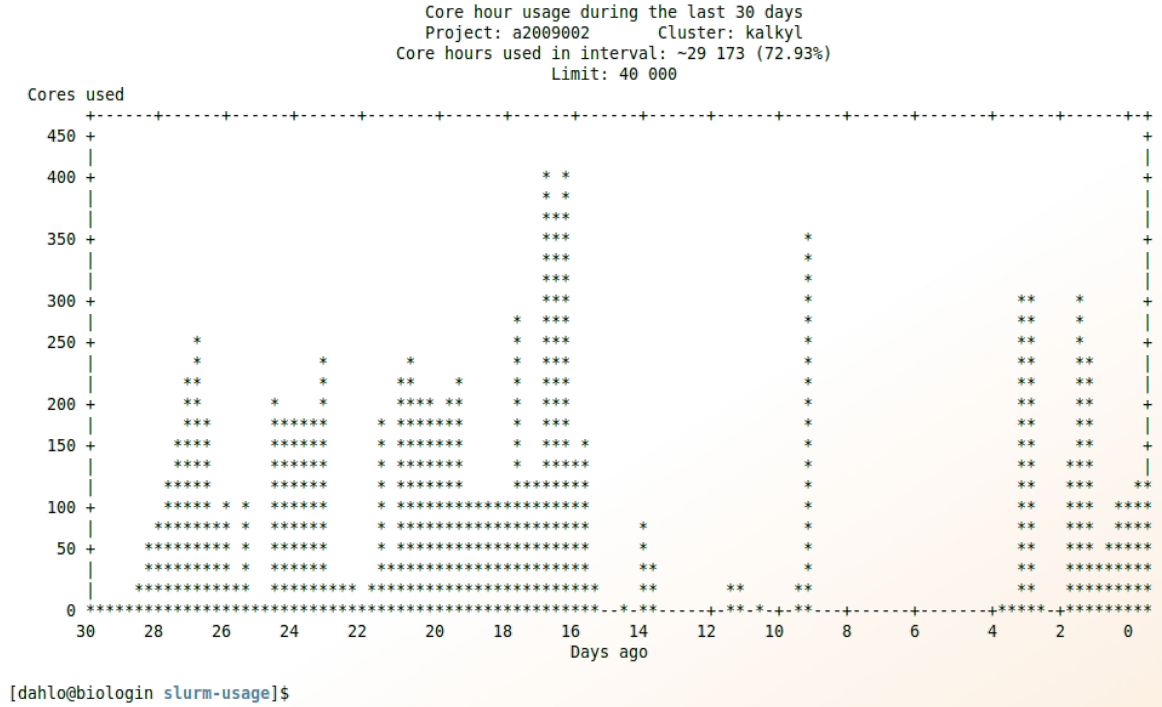
UPPMAX Commands

`projinfo`

```
[dahlo@kalkyl4 work]$ projinfo
(Counting the number of core hours used since 2012-08-19/00:00:00 until now.)

Project             Used[h]   Current allocation [h/month]
   User
-------------------------------------------------------
b2010015            1257.20               2000
   ameur            1257.20

-------------------------------------------------------
b2010069               0.00               2000

-------------------------------------------------------
b2010074             110.98               2000
   dahlo               1.01
   seba              109.97

-------------------------------------------------------
b2012044               0.00               2000

-------------------------------------------------------
g2012005               0.00               2000

-------------------------------------------------------
g2012083               0.00               2000

-------------------------------------------------------
g2012157               0.12               2000
   dahlo               0.12

[dahlo@kalkyl4 work]$
```

UPPMAX Commands

`projplot -A <proj-id>` (-h for more options)



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Objectives

What is UPPMAX what it provides

Projects at UPPMAX

How to access UPPMAX

Jobs and queuing systems

How to use the resources of UPPMAX

How to use the resources of UPPMAX in a good way!

Efficiency!!!

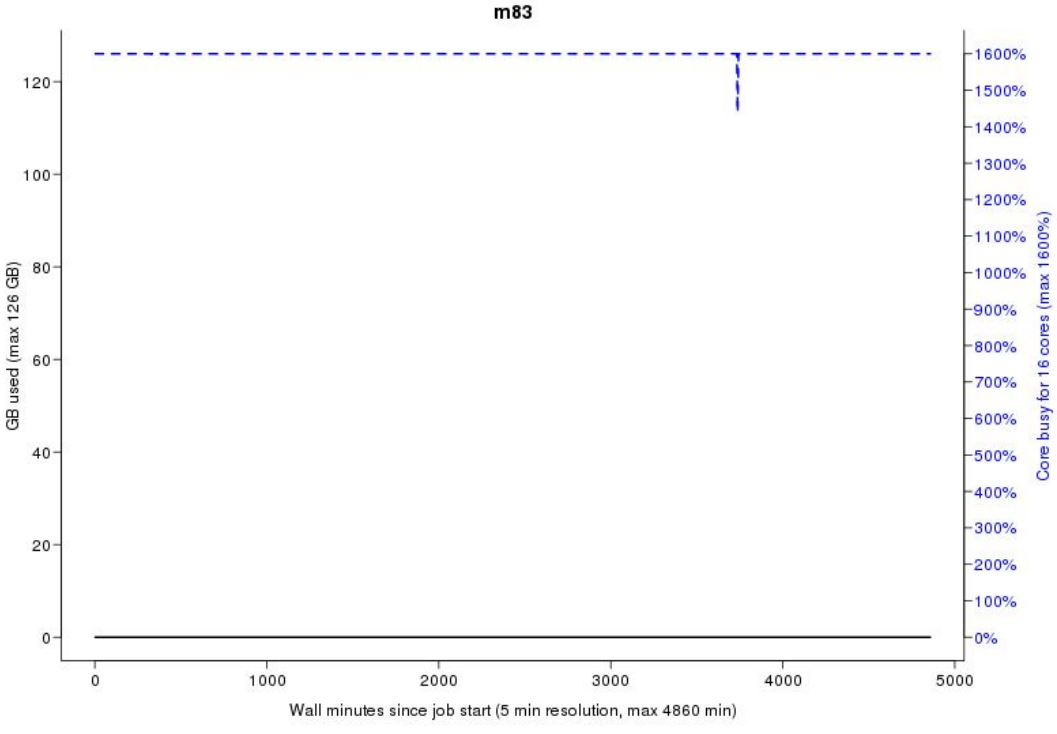
UPPMAX Commands

Plot efficiency

```
$ jobstats -p -A <projid>
```

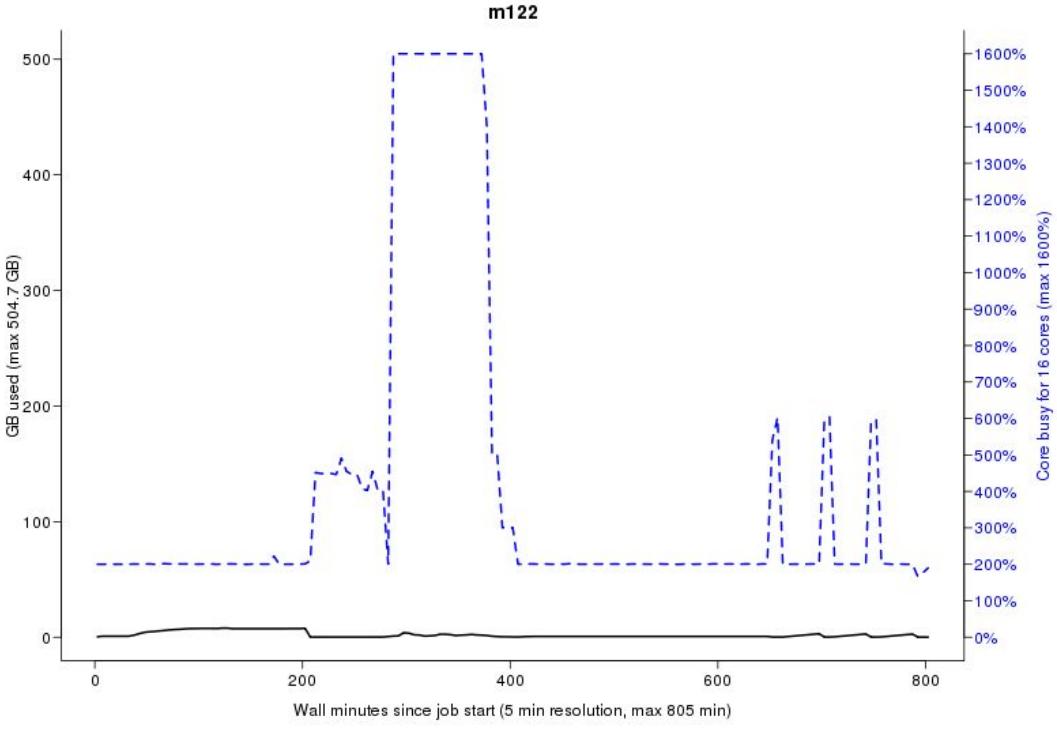
2719328 on 'milou' end: 2014-09-09T08:26:34 runtime: 03-08:59:53

Flags: mem_underused:126:0



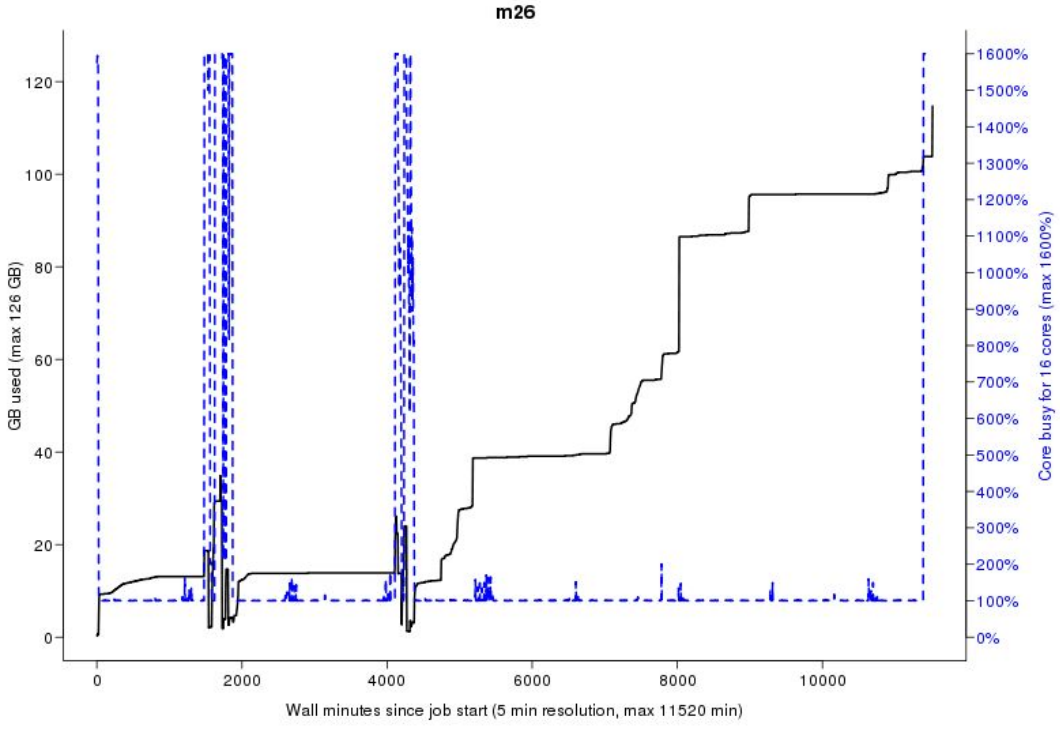
2934193 on 'milou' end: 2014-09-26T01:40:23 runtime: 13:30:23

Flags: mem_underused:504.7:7.9 node_type_misbooked:mem512GB:mem128GB



2799665 on 'milou' end: 2014-09-18T07:36:54 runtime: 07-23:56:23

Flags: none



Take-home messages

- The difference between **user account** and **project**

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- **Login nodes** are not for running jobs

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Take-home messages

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- **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
- Use **interactive** for quick jobs and for testing
- Do not ask for more cores/nodes than your job can actually use
- A job script usually consists of:
  - Job settings (-A, -p, -n, -t)
  - Modules to be loaded
  - Bash code to perform actions
  - Run a program, or multiple programs

Laboratory time! (again)

https://nbisweden.github.io/workshop-ngsintro/2403/topics/uppmax/intro/lab_uppmax_intro.html