UPPMAX Introduction

2018-02-07

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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!!!

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Efficiency!!!

UPPMAX

Uppsala Multidisciplinary Center for Advanced Computational Science

http://www.uppmax.uu.se

computer clusters:

- Rackham, 334(600) computers à 20 cores (128GB RAM)
- Bianca, 200 nodes à 16 cores (128GB RAM)

  (Milou, 208 computers à 16 cores (128GB RAM) 17 with 256, 17 with 512)

~12 PB fast parallel **storage**

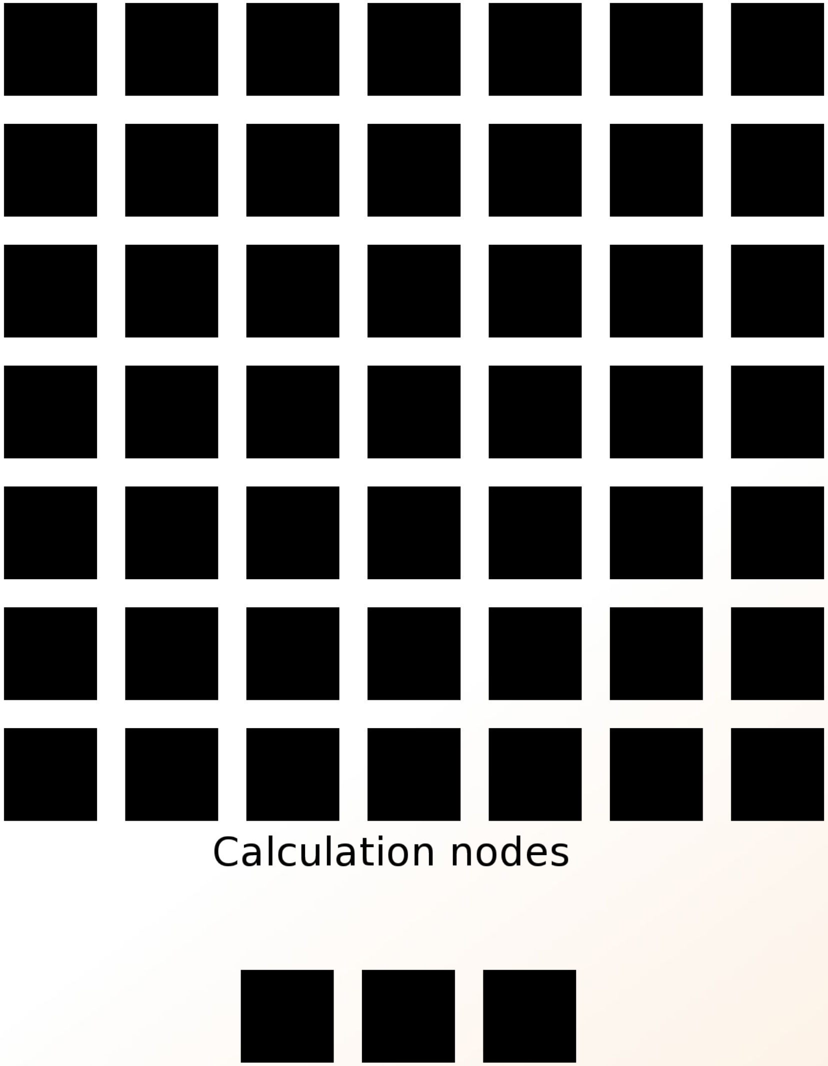
Bioinformatics **software**

The basic structure of supercomputer cluster

node = computer

Login nodes

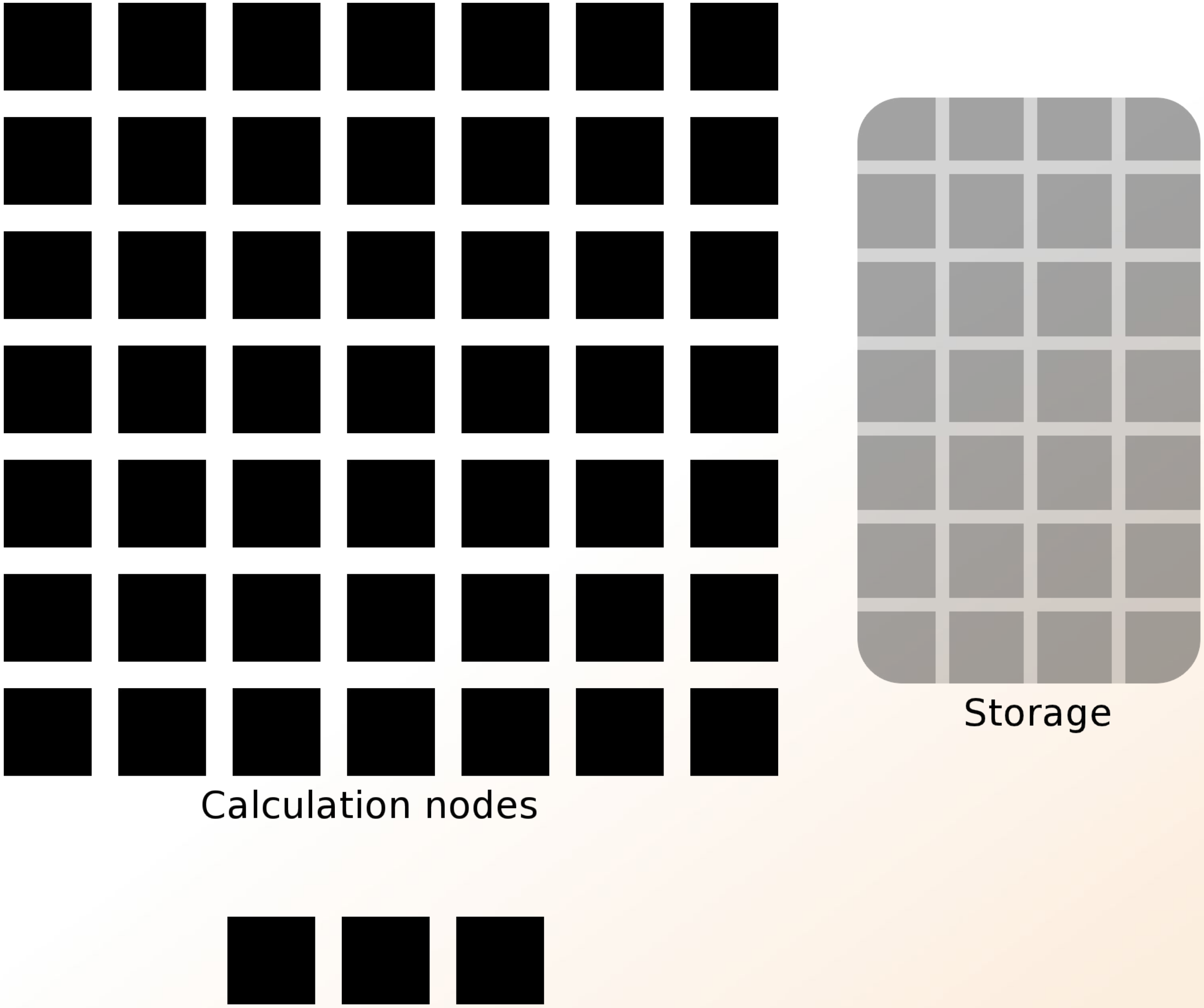
The basic structure of supercomputer



Calculation nodes

Login nodes

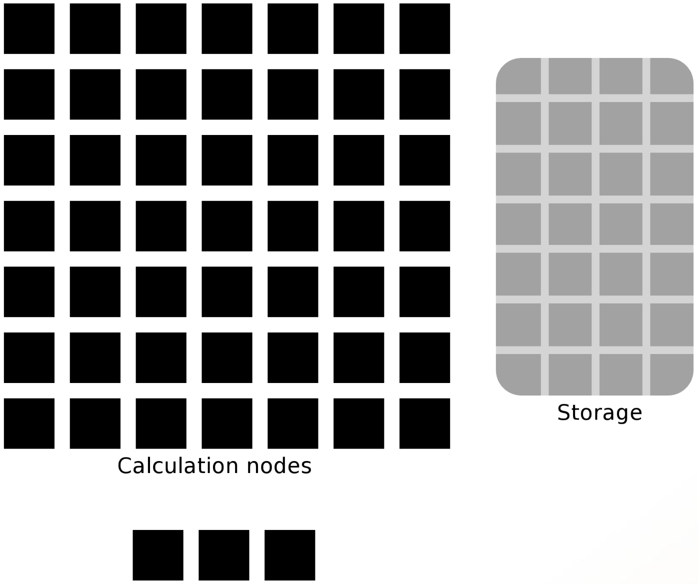
The basic structure of supercomputer



Storage

Calculation nodes

Login nodes



UPPMAX provides

Compute and **Storage**

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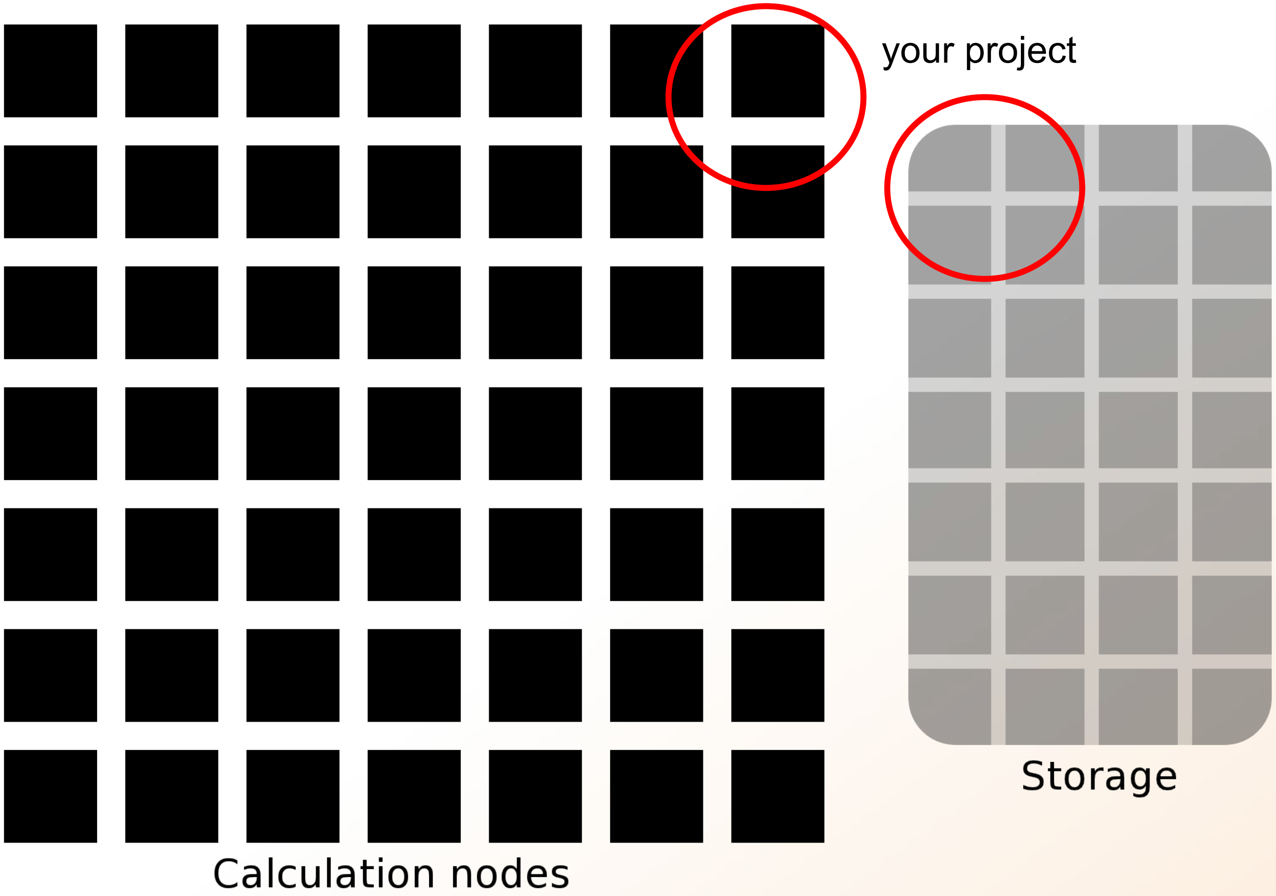
Efficiency!!!

Projects

UPPMAX provides its resources via

projects

Projects



Projects

Resources:

compute
(core-hours/month)

storage
(GB/TB)

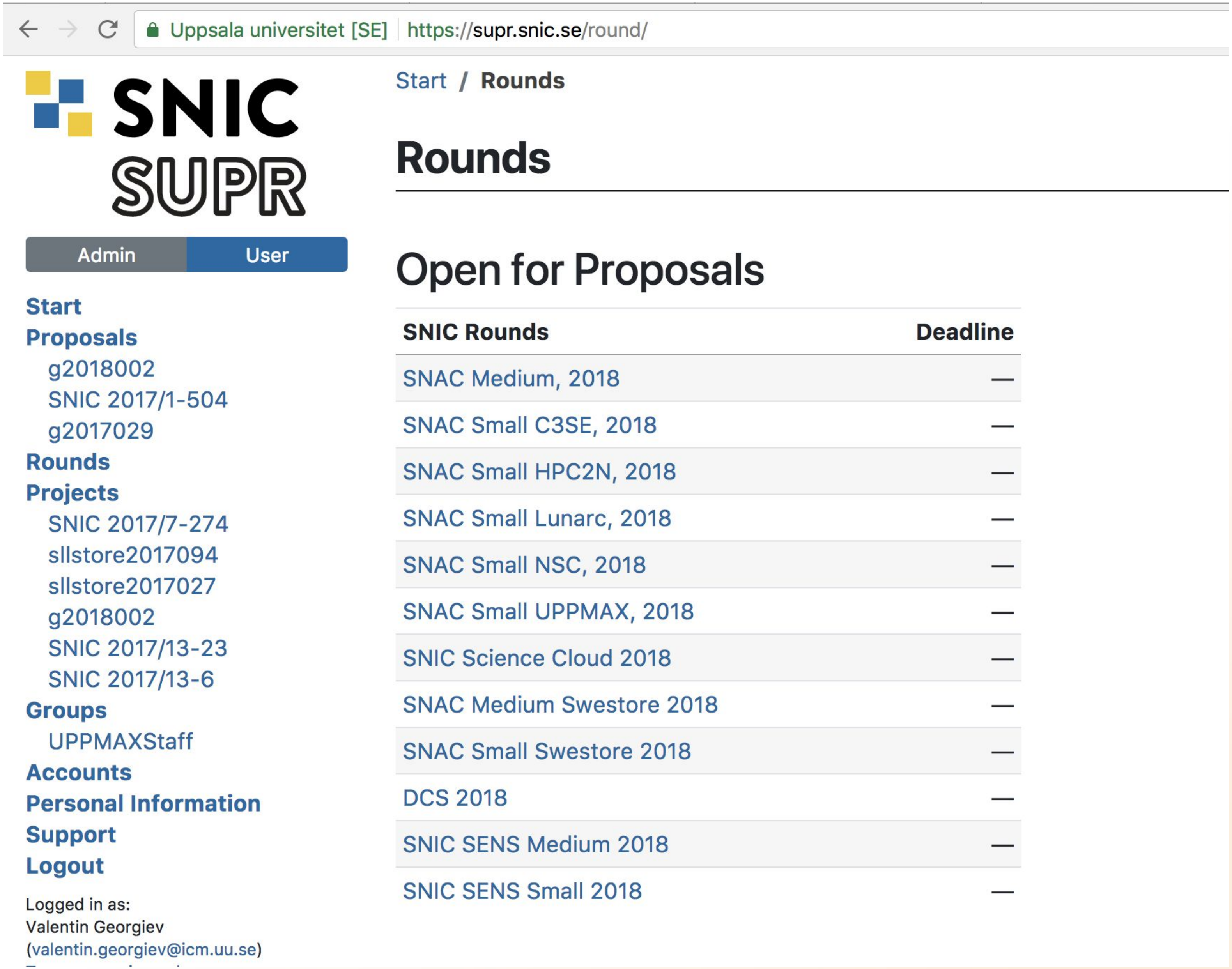
Projects

two separate projects:

SNIC project:
cluster **Rackham**
2000 core-hours/month
128 GB

Uppstore project:
storage system **CREX**
1 - 100 TB

Projects



Uppsala universitet [SE] | https://supr.snic.se/round/

- **Start**
- **Proposals**
  - g2018002
  - SNIC 2017/1-504
  - g2017029
- **Rounds**
- **Projects**
  - SNIC 2017/7-274
  - sllstore2017094
  - sllstore2017027
  - g2018002
  - SNIC 2017/13-23
  - SNIC 2017/13-6
- **Groups**
  - UPPMAXStaff
- **Accounts**
- **Personal Information**
- **Support**
- **Logout**

Logged in as:
Valentin Georgiev
(valentin.georgiev@icm.uu.se)

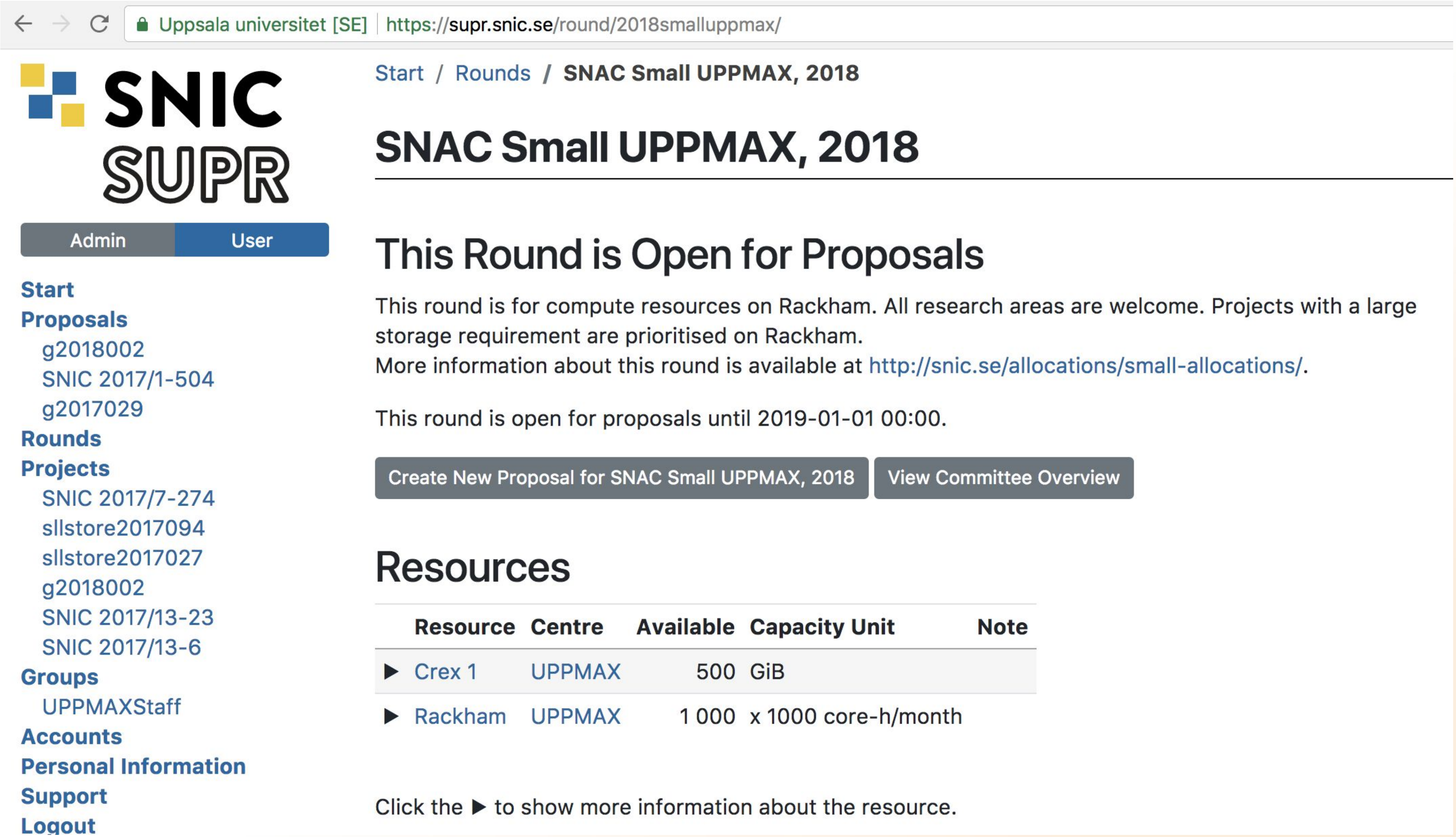
Start / **Rounds**

Rounds

Open for Proposals

SNIC Rounds	Deadline
SNAC Medium, 2018	—
SNAC Small C3SE, 2018	—
SNAC Small HPC2N, 2018	—
SNAC Small Lunarc, 2018	—
SNAC Small NSC, 2018	—
SNAC Small UPPMAX, 2018	—
SNIC Science Cloud 2018	—
SNAC Medium Swestore 2018	—
SNAC Small Swestore 2018	—
DCS 2018	—
SNIC SENS Medium 2018	—
SNIC SENS Small 2018	—

Projects



Start
Proposals
  g2018002
  SNIC 2017/1-504
  g2017029
Rounds
Projects
  SNIC 2017/7-274
  sllstore2017094
  sllstore2017027
  g2018002
  SNIC 2017/13-23
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Start / Rounds / **SNAC Small UPPMAX, 2018**

SNAC Small UPPMAX, 2018

This Round is Open for Proposals

This round is for compute resources on Rackham. All research areas are welcome. Projects with a large storage requirement are prioritised on Rackham.
More information about this round is available at http://snic.se/allocations/small-allocations/.

This round is open for proposals until 2019-01-01 00:00.

Resources

	Resource	Centre	Available	Capacity Unit	Note
▶	Crex 1	UPPMAX	500	GiB	
▶	Rackham	UPPMAX	1 000	x 1000 core-h/month	

Click the ▶ to show more information about the resource.

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Efficiency!!!

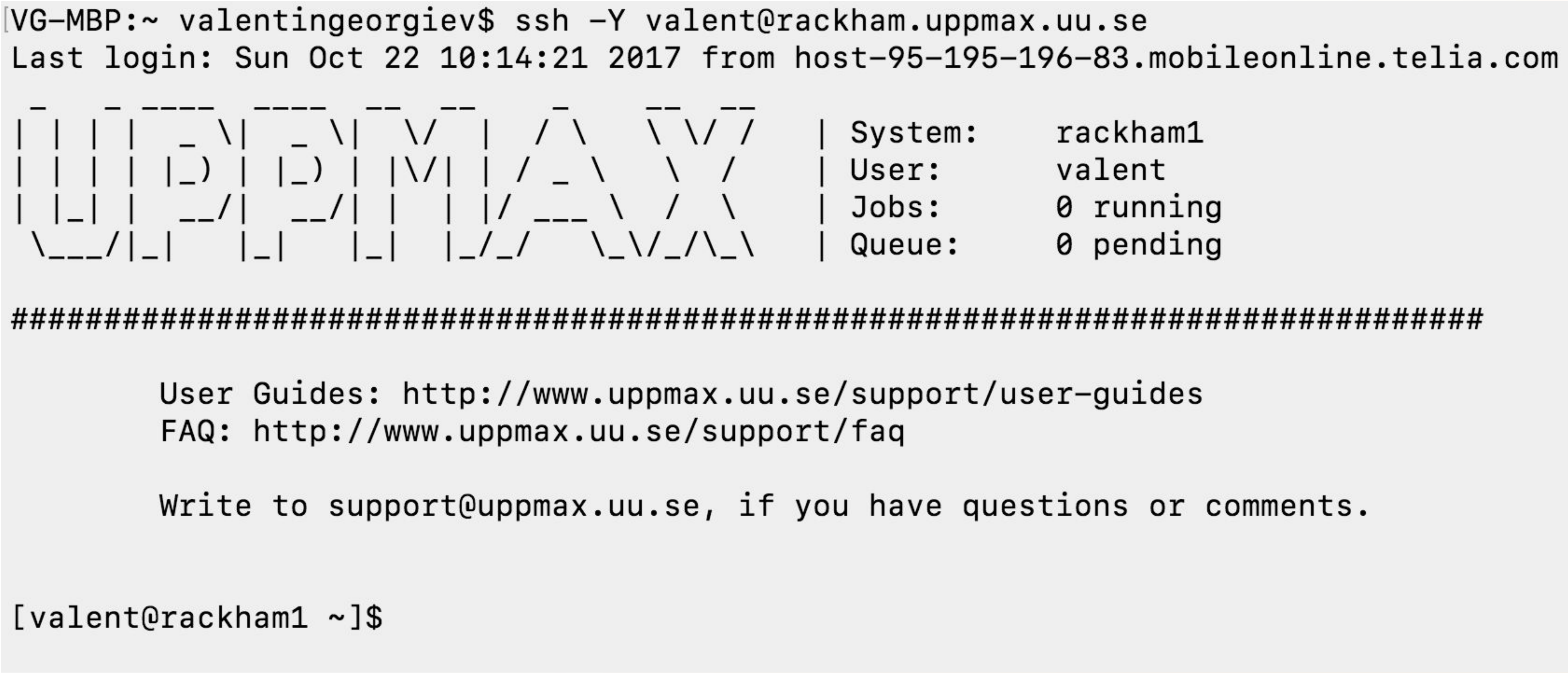
How to access UPPMAX

SSH to a cluster

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

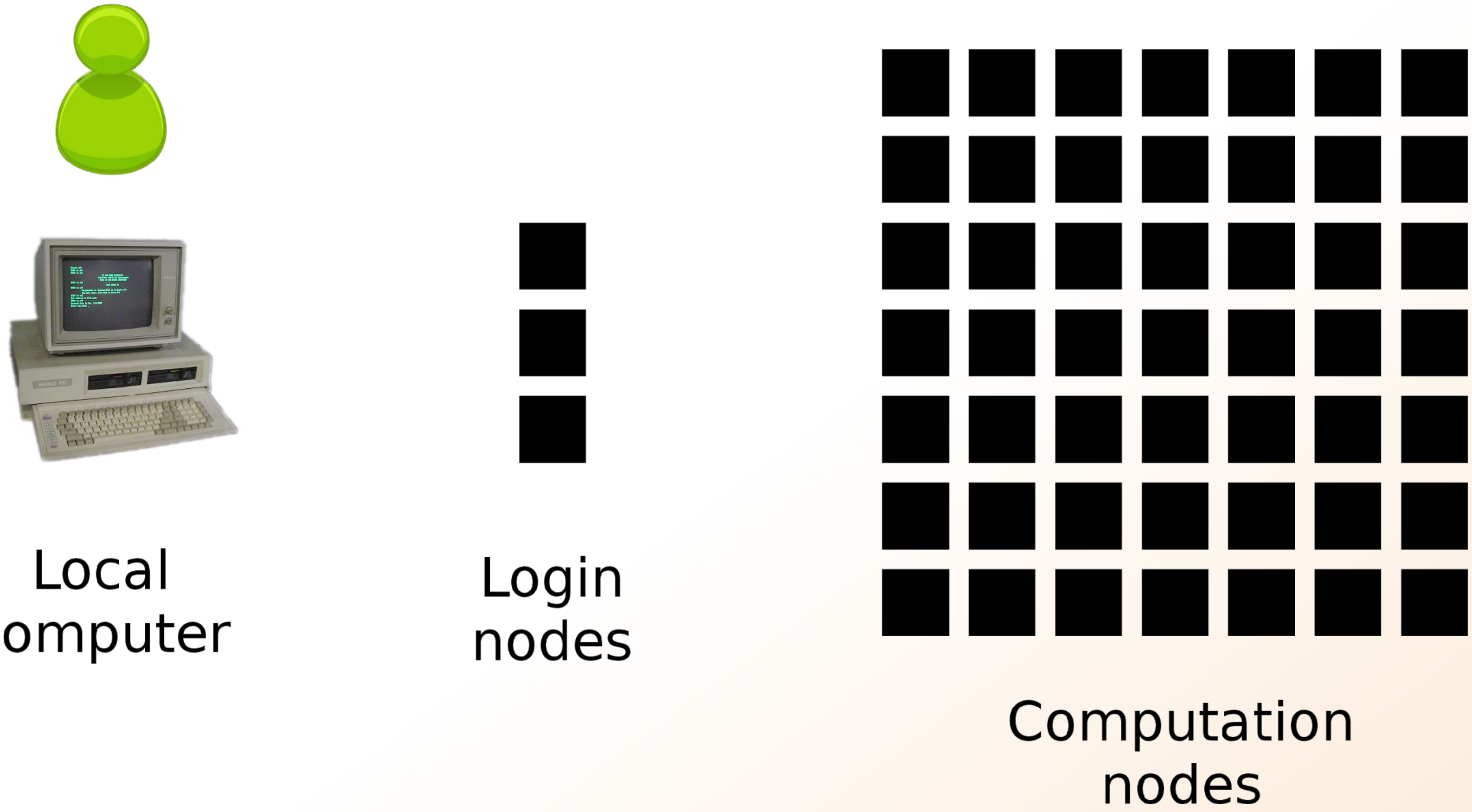
How to access UPPMAX

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

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

        User Guides: http://www.uppmax.uu.se/support/user-guides
        FAQ: http://www.uppmax.uu.se/support/faq

        Write to support@uppmax.uu.se, if you have questions or comments.


[valent@rackham1 ~]$
```

SSH

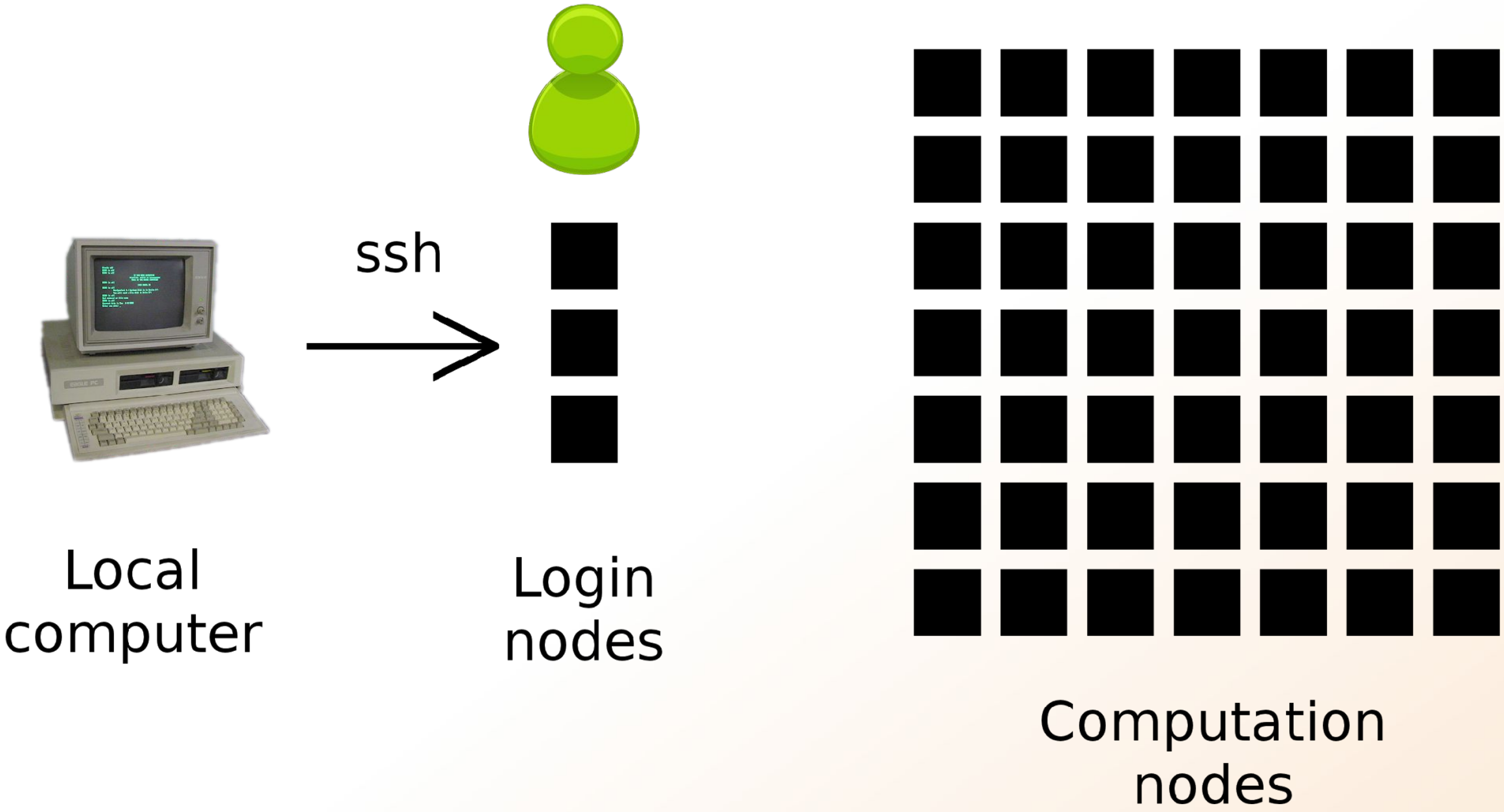


Local computer

Login nodes

Computation nodes

SSH



ssh

Local
computer

Login
nodes

Computation
nodes

How to use UPPMAX

Login nodes

use them to access UPPMAX
never use them to run **jobs**
don’t even use them to do “quick stuff”

Calculation nodes

do your work here - testing and running

How to use UPPMAX

Calculation nodes

not accessible directly

SLURM (queueing system) gives you access

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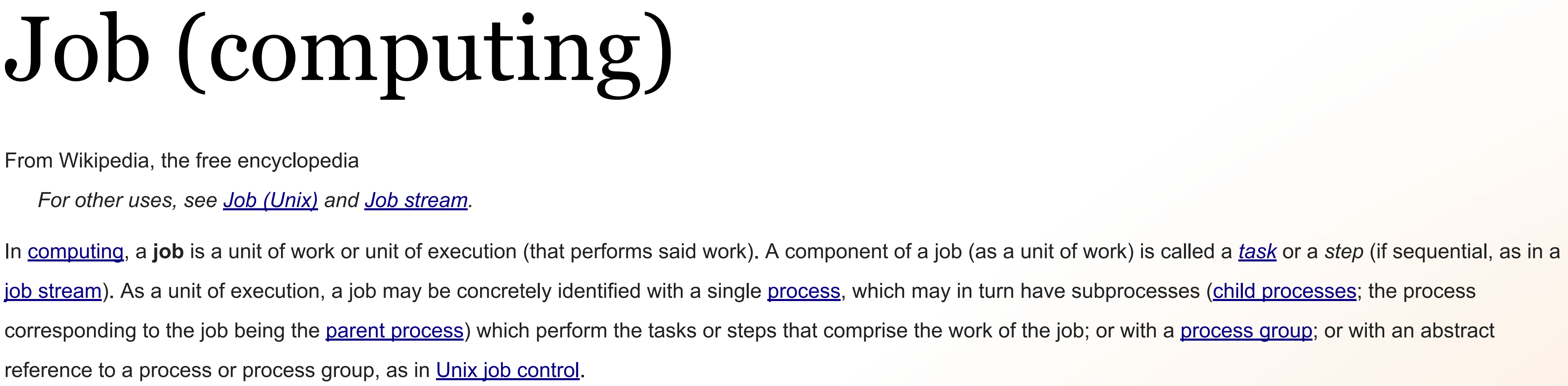
Job



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.

Job

Read/open files

Do something with the data

Print/save output

Job

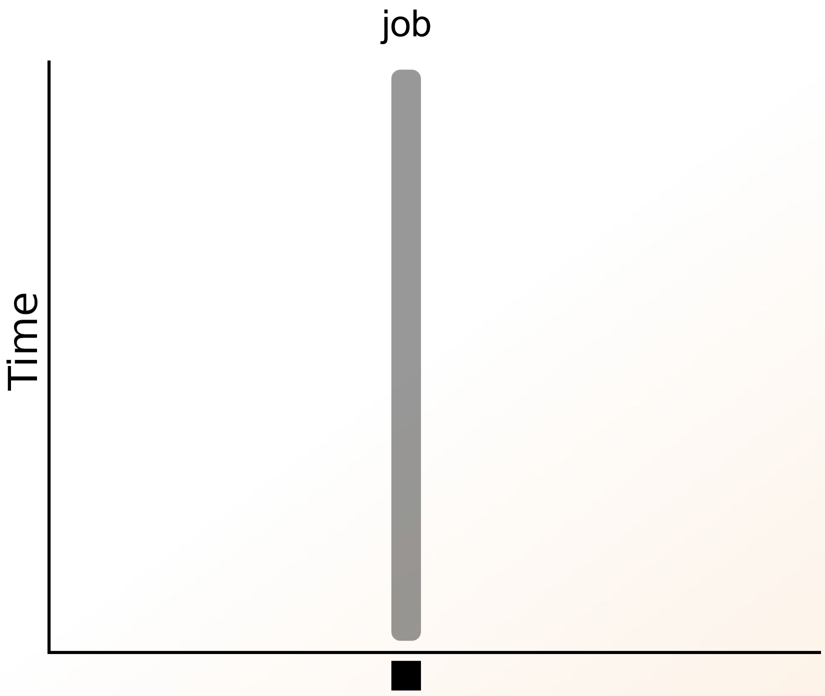
Read/open files

Do something with the data

Print/save output

Job

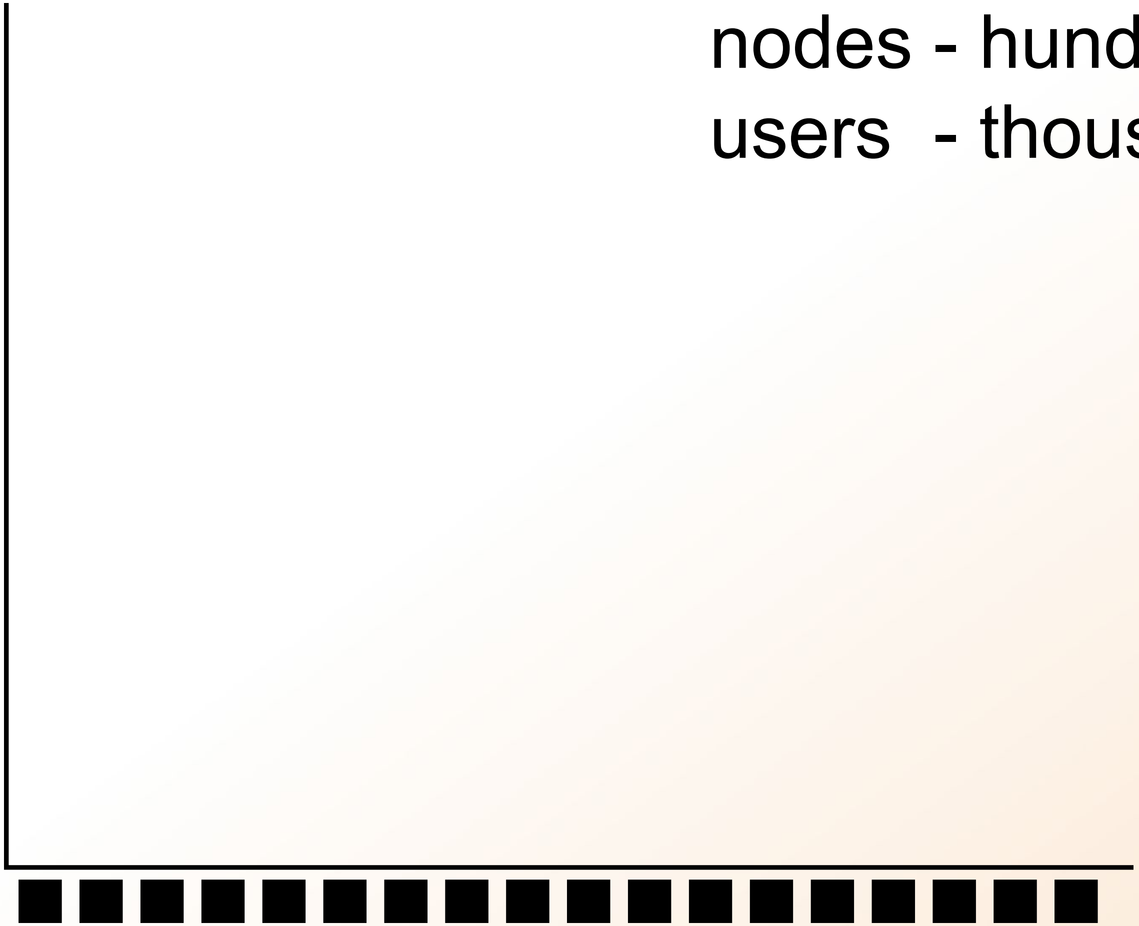
Standard way of running jobs



Parallel computing

Queue System

- More users than nodes
  - Need for a queue



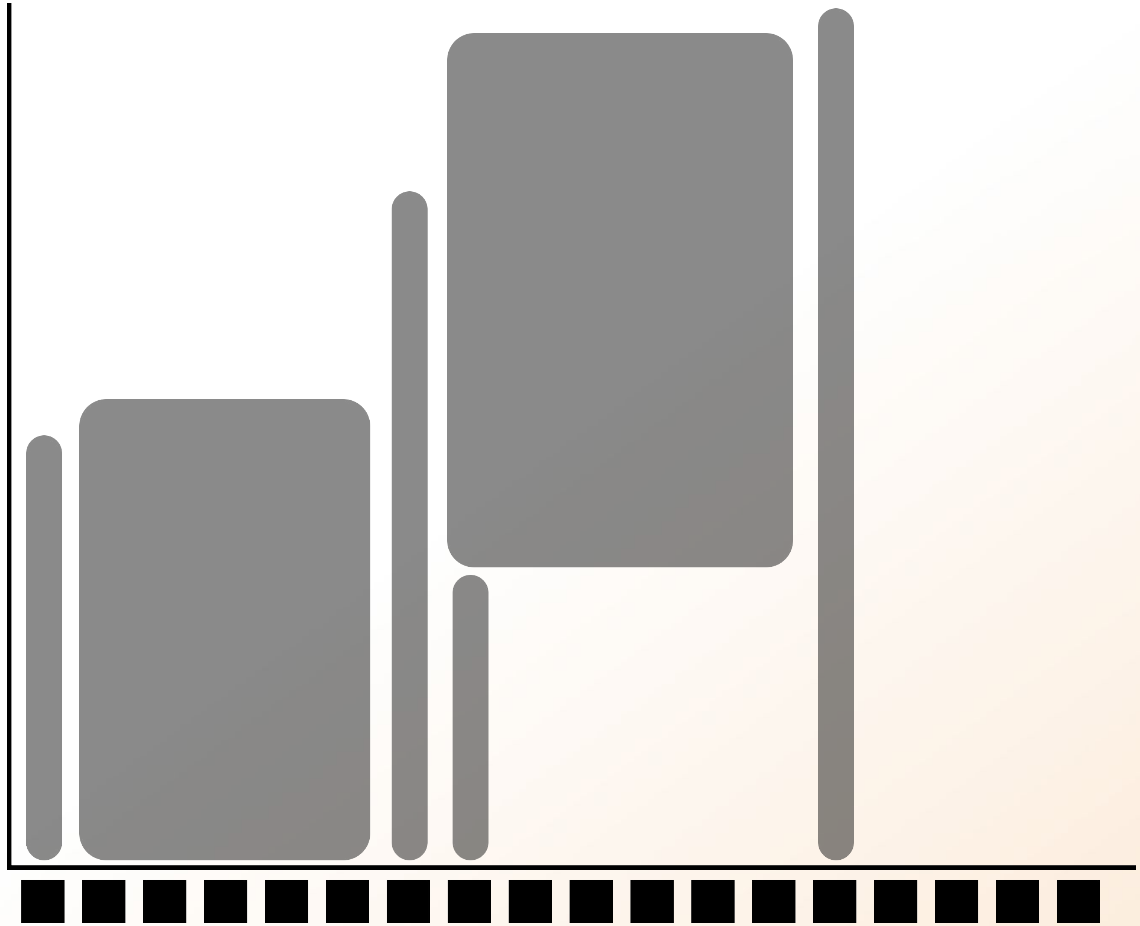
nodes - hundreds

users - thousands

Queue System

More users than nodes

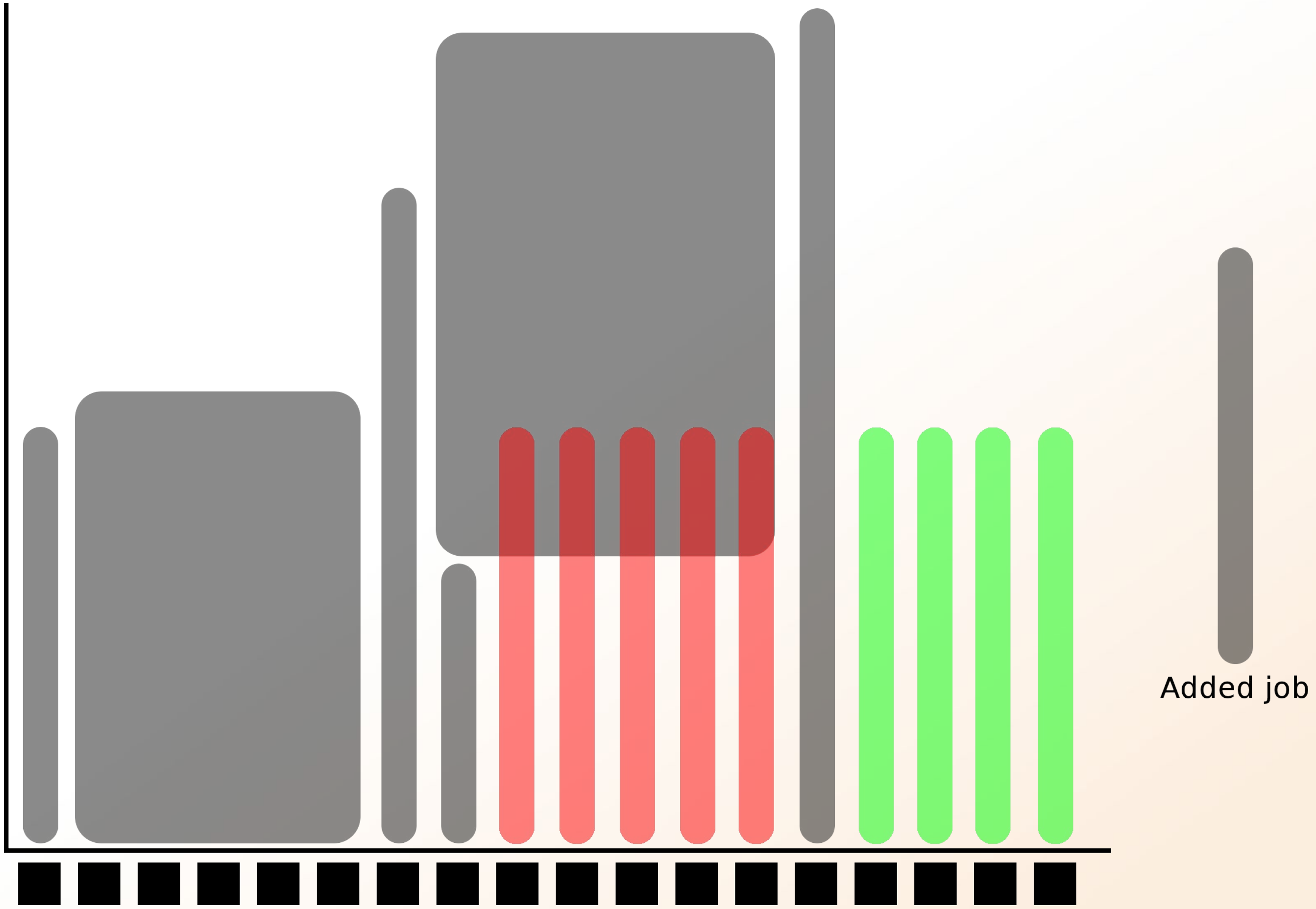
- Need for a queue



Queue System

More users than nodes

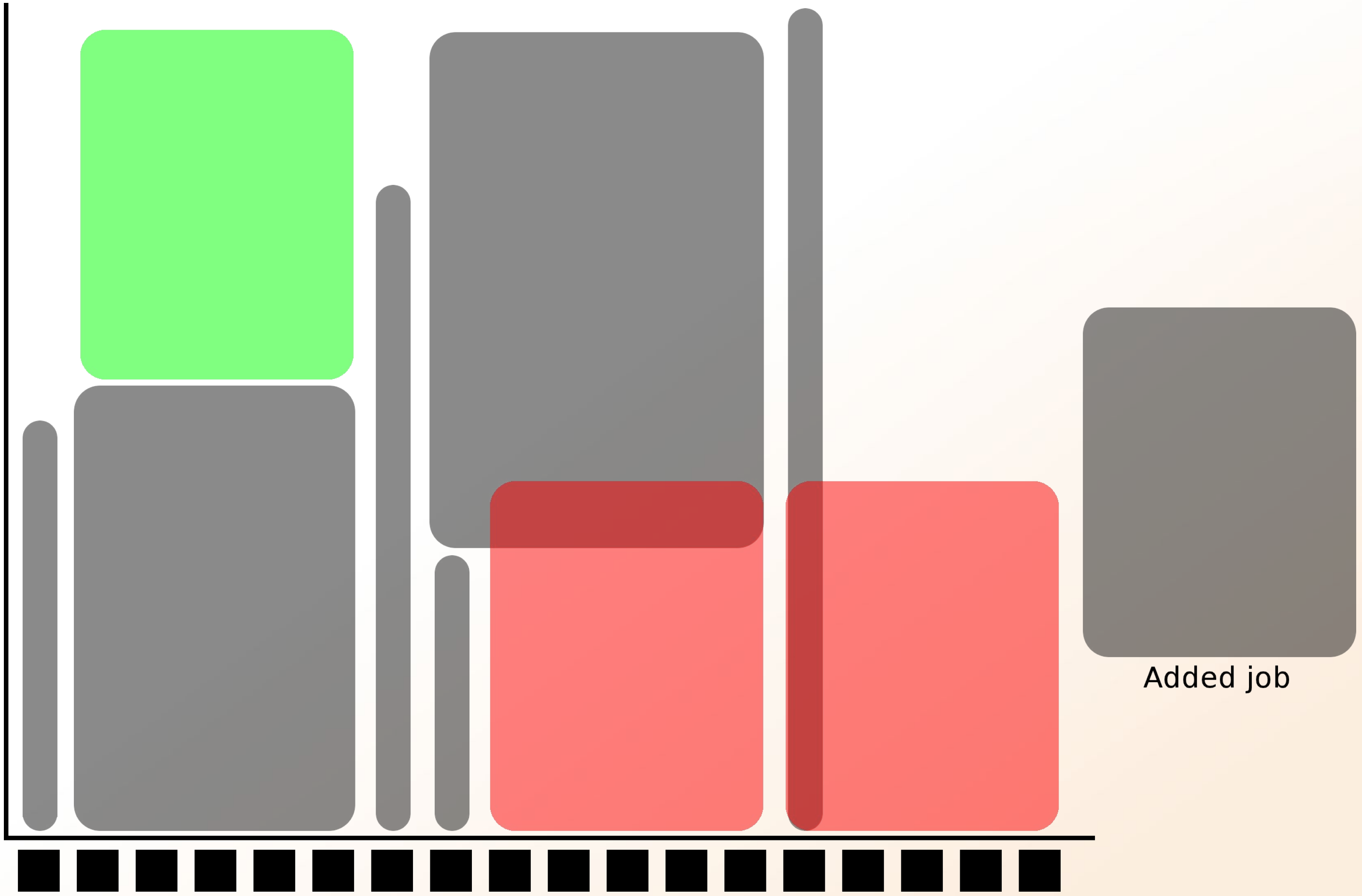
- Need for a queue



Queue System

More users than nodes

Need for a queue



SLURM

queue system
workload manager
job queue
batch queue
job scheduler

SLURM (Simple Linux Utility for Resource Management)

free and open source

SciLifeLab UPPSALA

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Efficiency!!!

SLURM

1) Ask for resource and run jobs manually

mainly for testing and small jobs

2)Write a script and submit it to SLURM

do the real job

SLURM

1) Ask for resource and run jobs manually

submit a request for resources

↓

ssh to a calculation node

↓

run programs

SLURM

1) Ask for resource and run jobs manually

<u>submit a request for resources</u>

```
salloc -A b2015245 -p core -n 1 -t 00:05:00
```

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

SLURM

-A	project ID you have to be a member
-p	1 node = 16 cores 1 hour walltime = 16 core-hours
-n	number of cores (default value = 1)
-N	number of nodes
-t	format - hh:mm:ss default value= 7-00:00:00

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

SLURM

Information about your jobs

squeue -u <user>

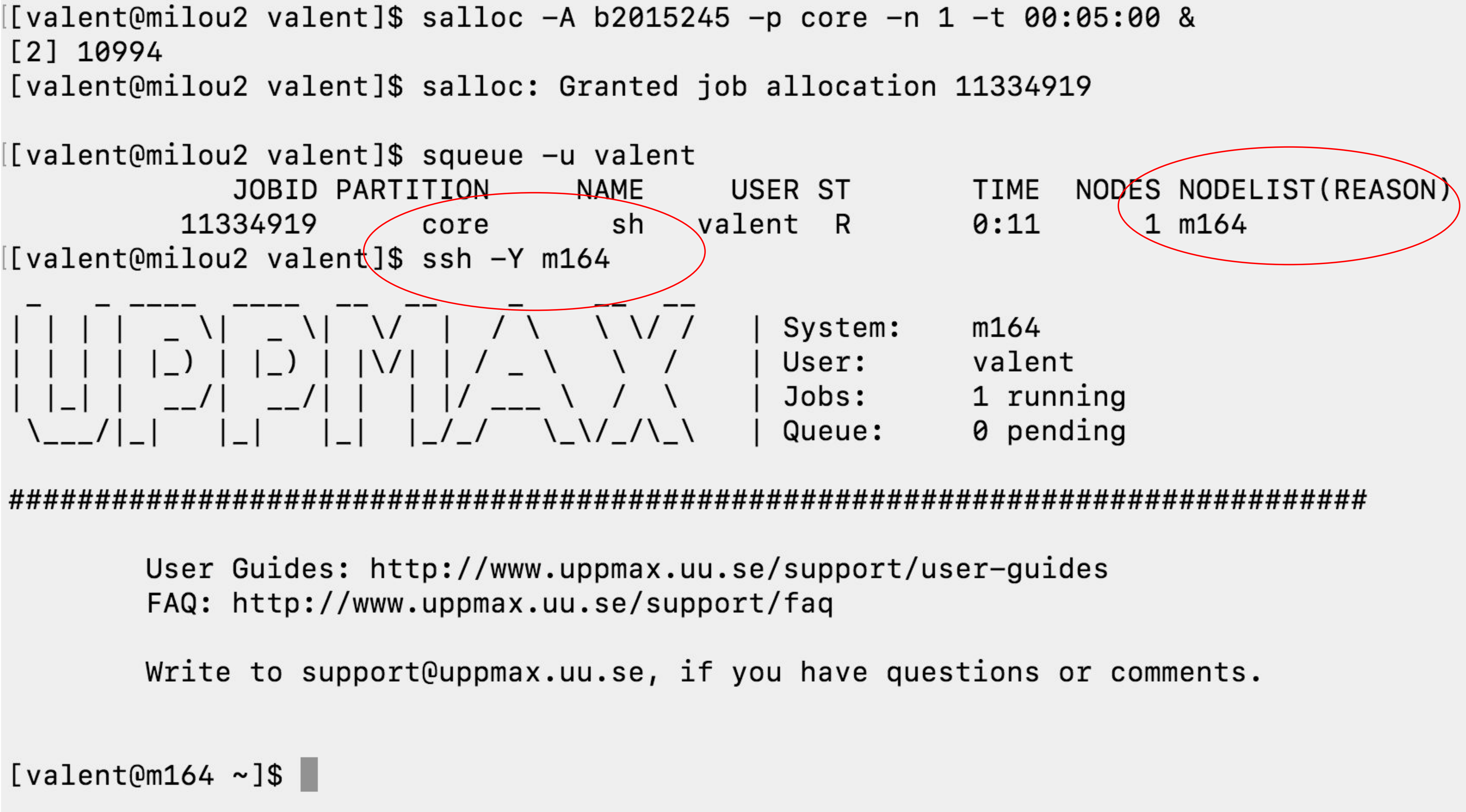
```
[valent@milou2 valent]$ squeue -u valent
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          11334919      core       sh   valent  R       0:11      1 m164
```

SLURM

SSH to a calculation node (from a login node)

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

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 ~]$ 
```
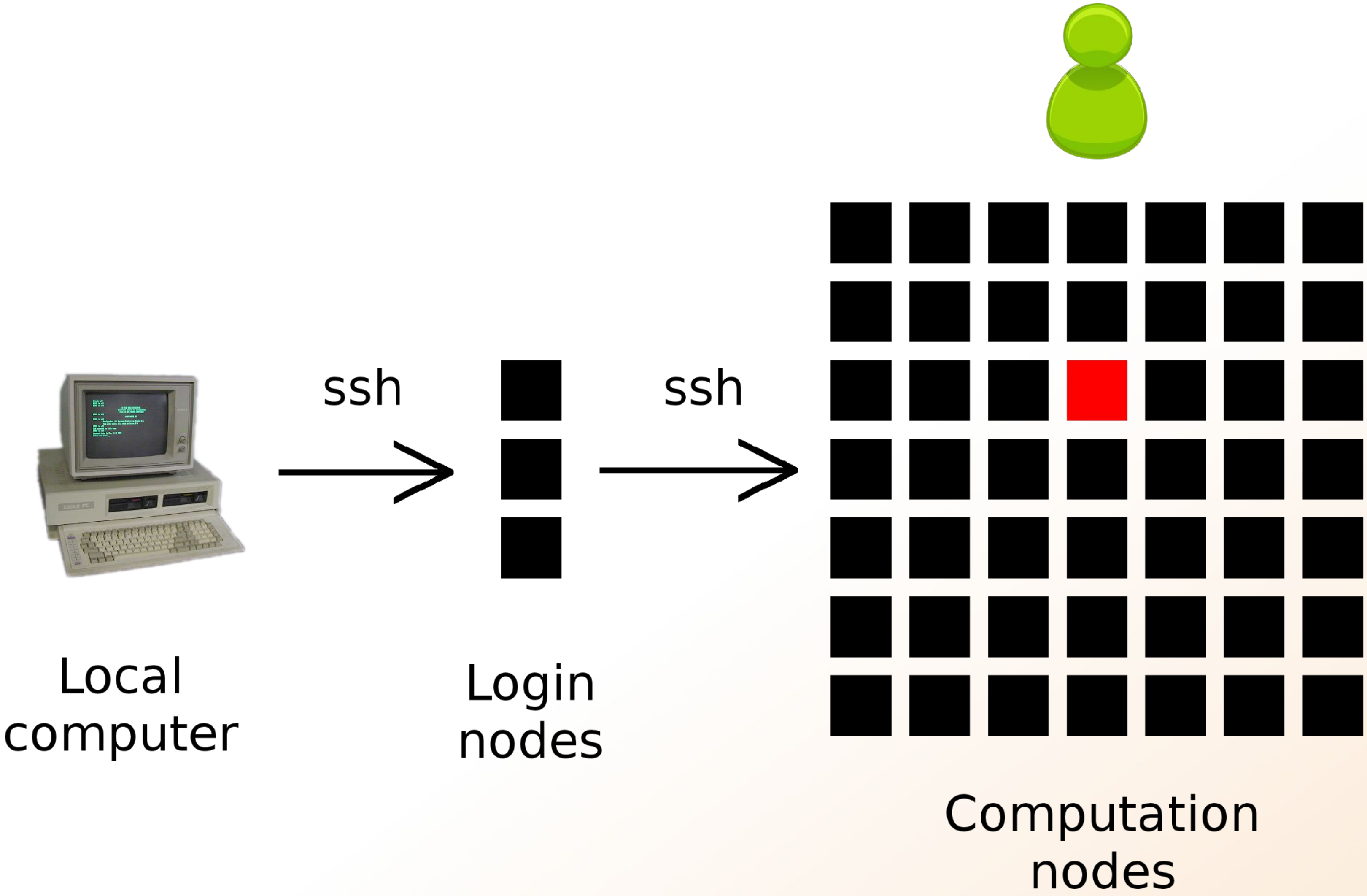

SLURM



You can run programs now!

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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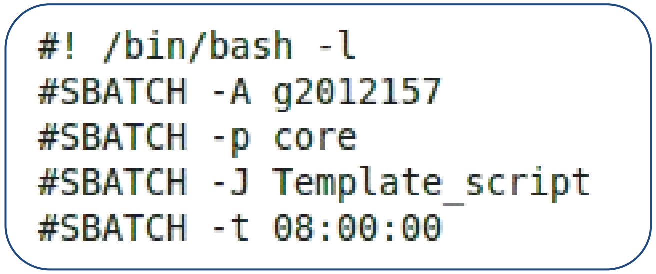
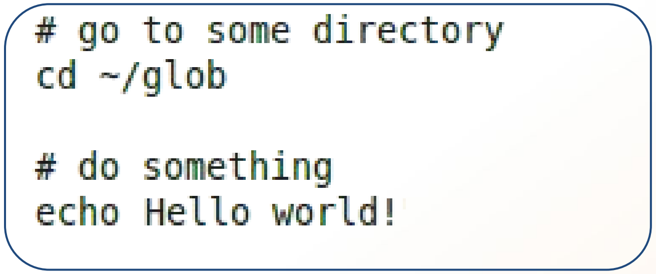
put all commands in a text file - script



```
#! /bin/bash -l
#SBATCH -A g2012157
#SBATCH -p core
#SBATCH -J Template_script
#SBATCH -t 08:00:00
```

job parameters

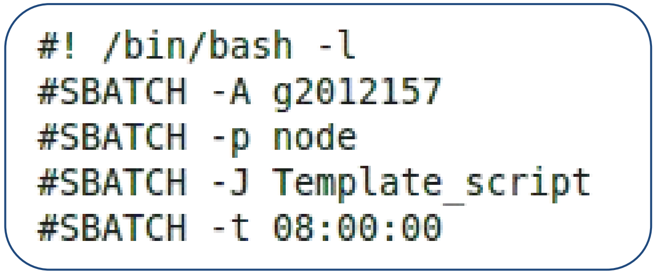


```
# go to some directory
cd ~/glob

# do something
echo Hello world!
```

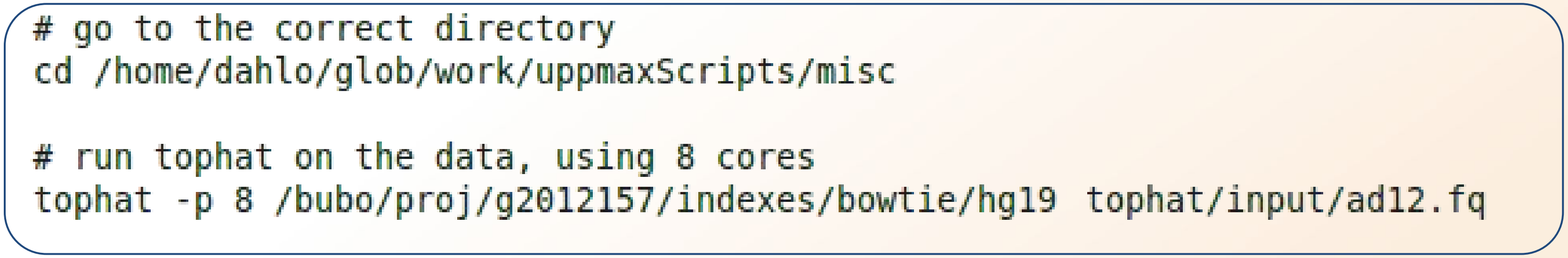
tasks to be done

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
```

SLURM

2)Write a script and submit it to SLURM

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

sbatch test.sbatch

SLURM

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

SLURM

2)Write a script and submit it to SLURM

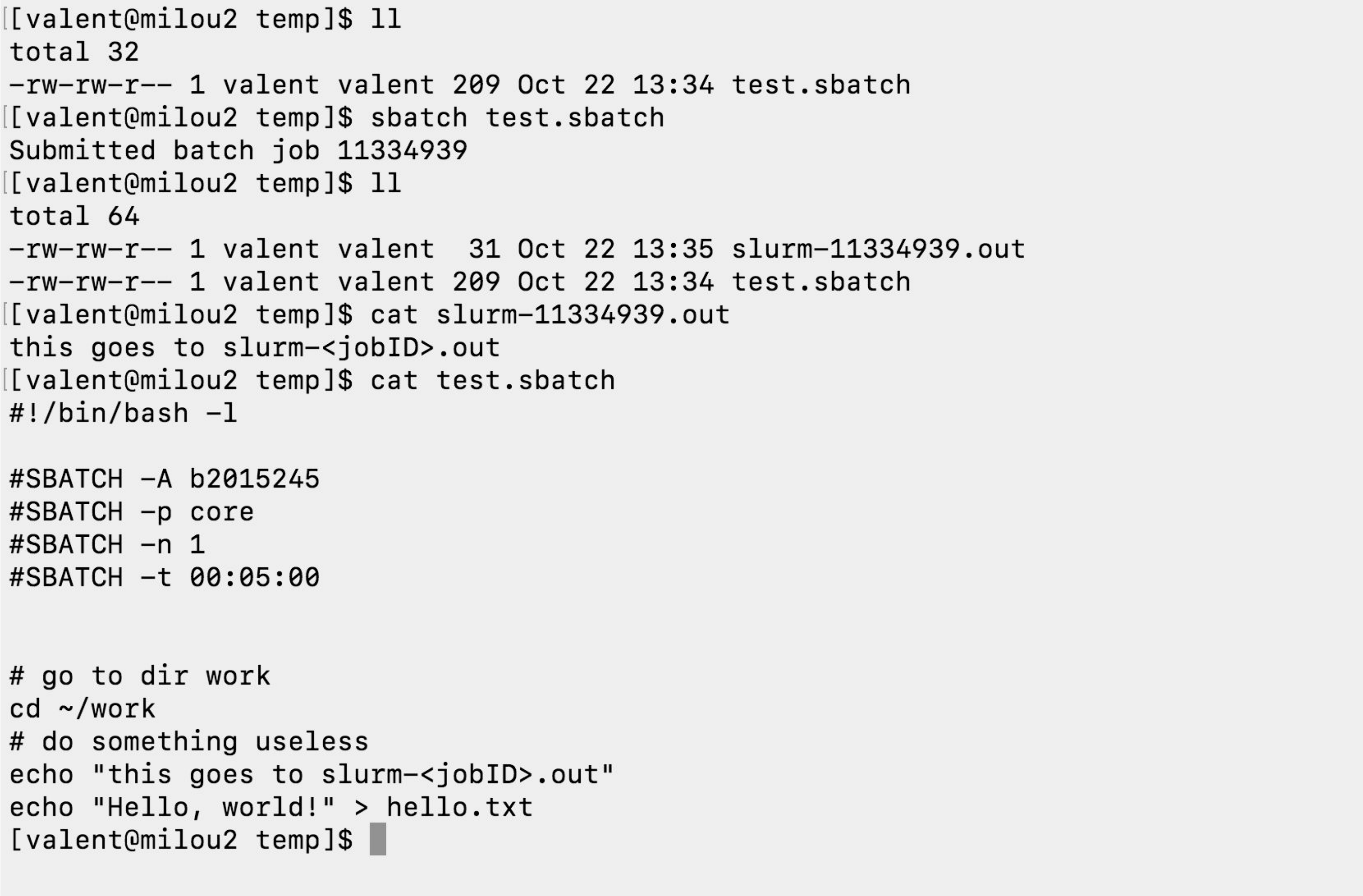
tell SLURM to run the script
(use the same job parameters)

```
sbatch -A b2015245 -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>

Queue System

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

or just google “uppmax slurm user guide”

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

UPPMAX Software

100+ programs installed

Managed by a 'module system'

Installed, but hidden

Manually loaded before use

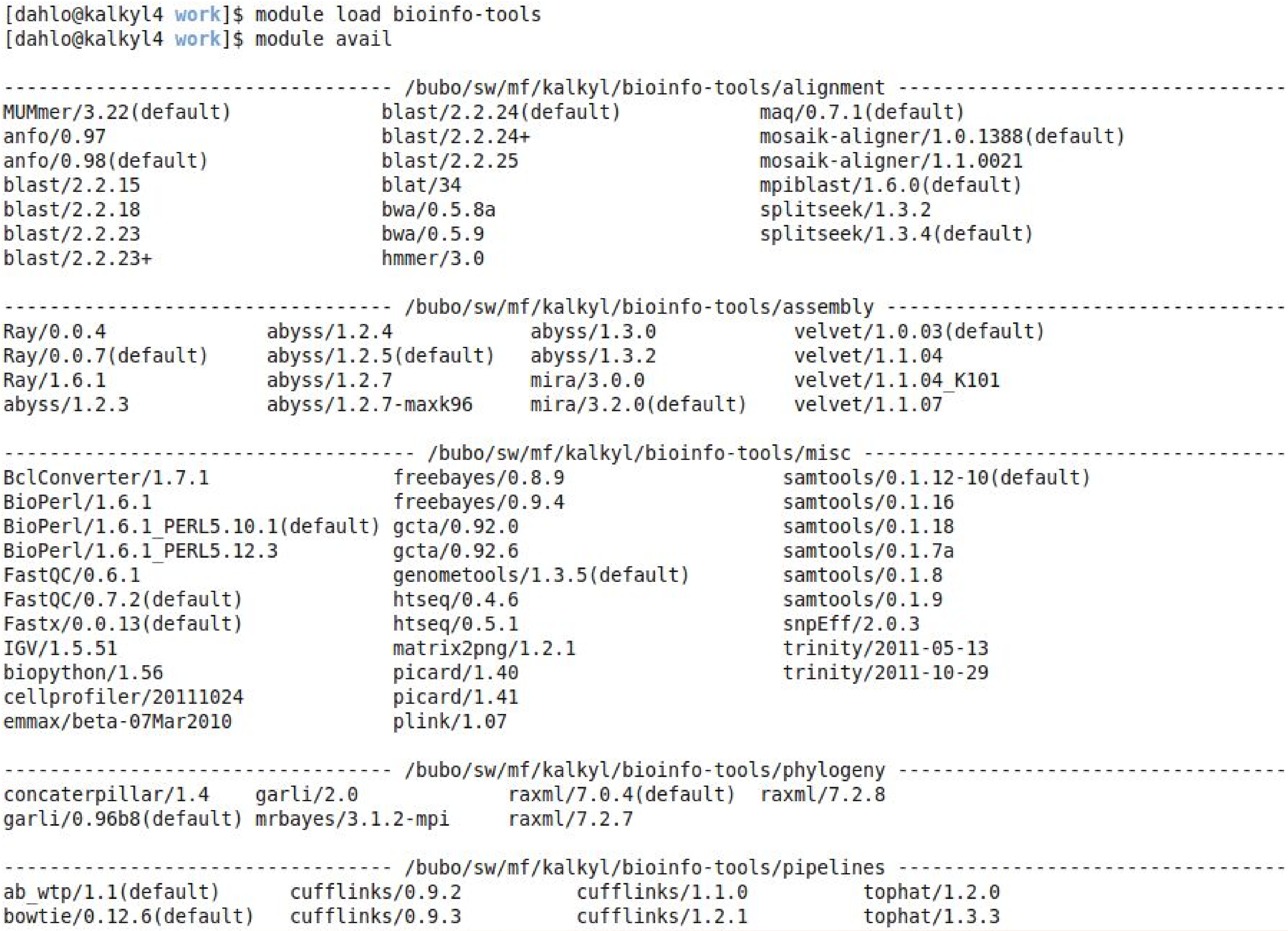
module avail - Lists all available modules

module load <module name> - Loads the module

module unload <module name> - Unloads the module

module list - Lists loaded modules

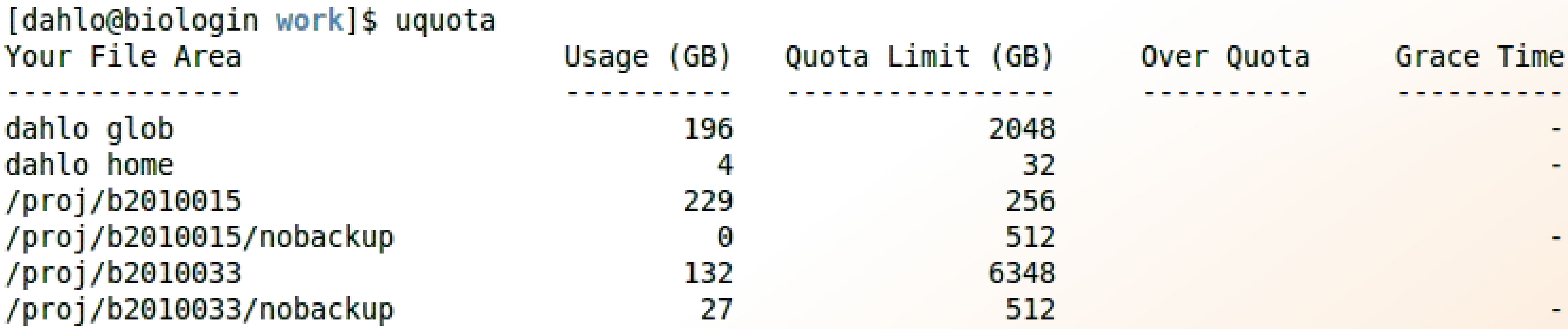
module spider <word> - Searches all modules after 'word'



```
[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

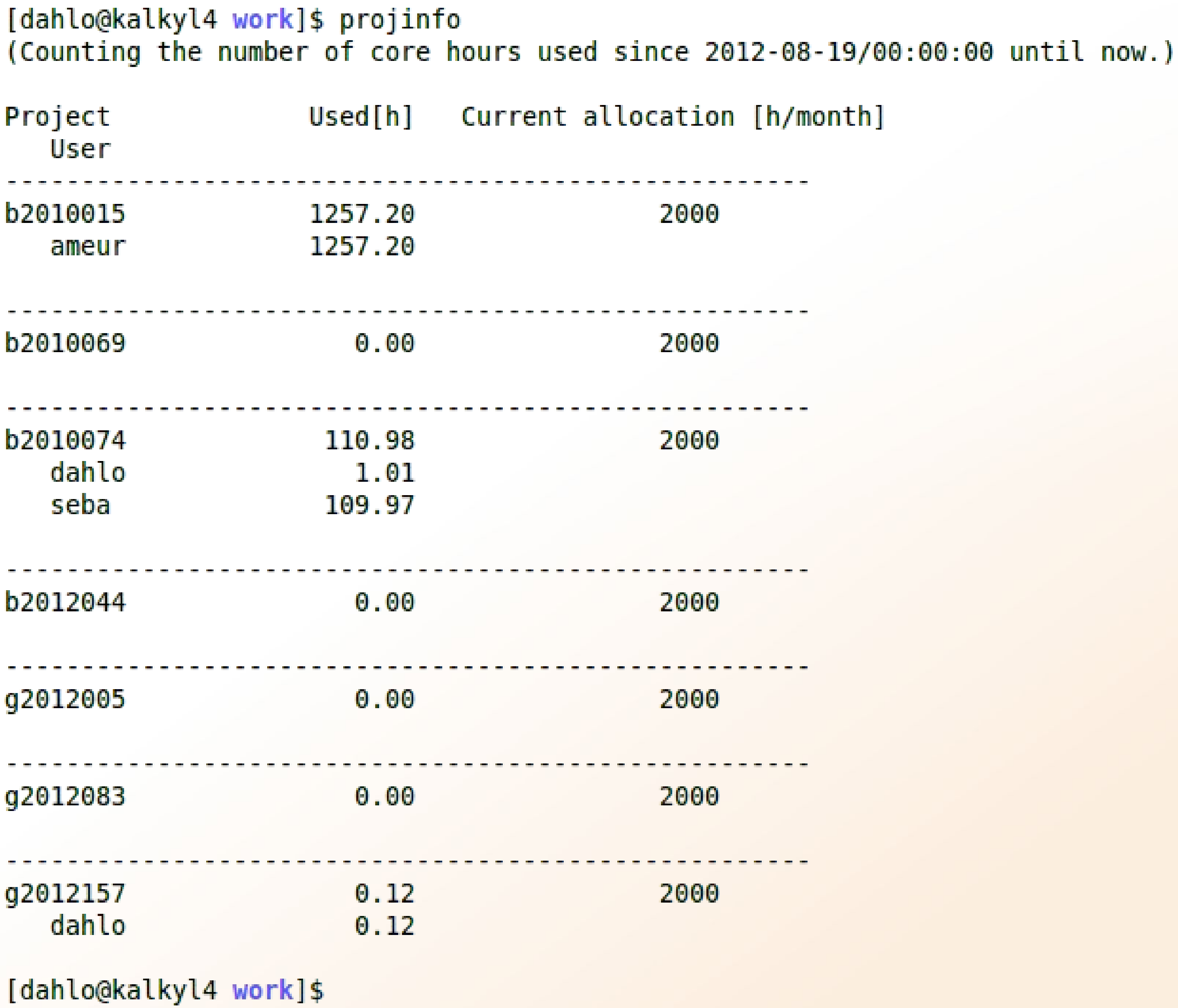
uquota



```
[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                             -
```

UPPMAX Commands

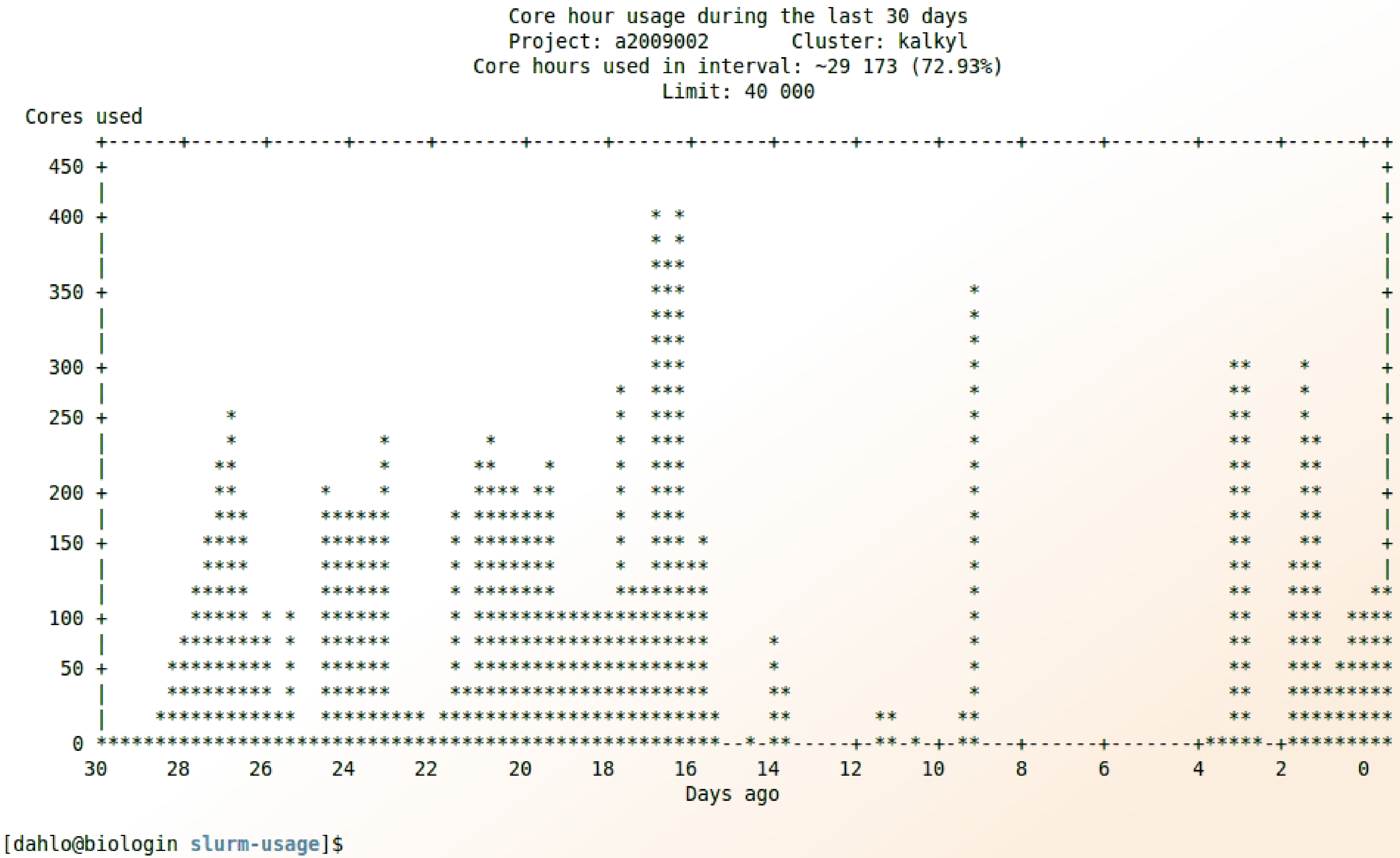
projinfo



```
[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)



```
                                           Core hour usage during the last 30 days
                                           Project: a2009002       Cluster: kalkyl
                                        Core hours used in interval: ~29 173 (72.93%)
                                                        Limit: 40 000
  Cores used
        +------+------+------+------+-------+------+------+------+------+------+------+------+-------+------+------+-+
    450 +                                                                                                            +
        |                                                                                                            |
    400 +                                              * *                                                           +
        |                                              * *                                                           |
        |                                              ***                                                           |
    350 +                                              ***                        *                                  +
        |                                              ***                        *                                  |
        |                                              ***                        *                                  |
    300 +                                              ***                        *                     **    *      +
        |                                          *  ***                        *                     **    *      |
    250 +          *                                *  ***                        *                     **    *      +
        |          *            *        *          *  ***                        *                     **    **     |
        |         **            *       **    *     *  ***                        *                     **    **     |
    200 +         **       *    *       **** **     *  ***                        *                     **    **     +
        |         ***      ******     * *******     *  ***                        *                     **    **     |
    150 +        ****      ******     * *******     *  *** *                      *                     **    **     +
        |        ****      ******     * *******     *  *****                      *                     **   ***     |
        |       *****      ******     * *******     ********                      *                     **   ***    **
    100 +       ***** * *  ******     * ********************                      *                     **   ***  ****
        |      ******** *  ******     * ********************     *                *                     **   ***  ****
     50 +     ********* *  ******     * ********************     *                *                     **   *** *****
        |     ********* *  ******     **********************     **               *                     **   *********
        |    ************  ********* ************************    **       **     **                     **   *********
      0 *****************************************************--*-**-----+-**-*-+-**---+------+-------+*****-+*********
       30     28     26     24     22      20     18     16     14     12     10      8      6       4      2      0
                                                          Days ago

[dahlo@biologin slurm-usage]$
```

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!!!

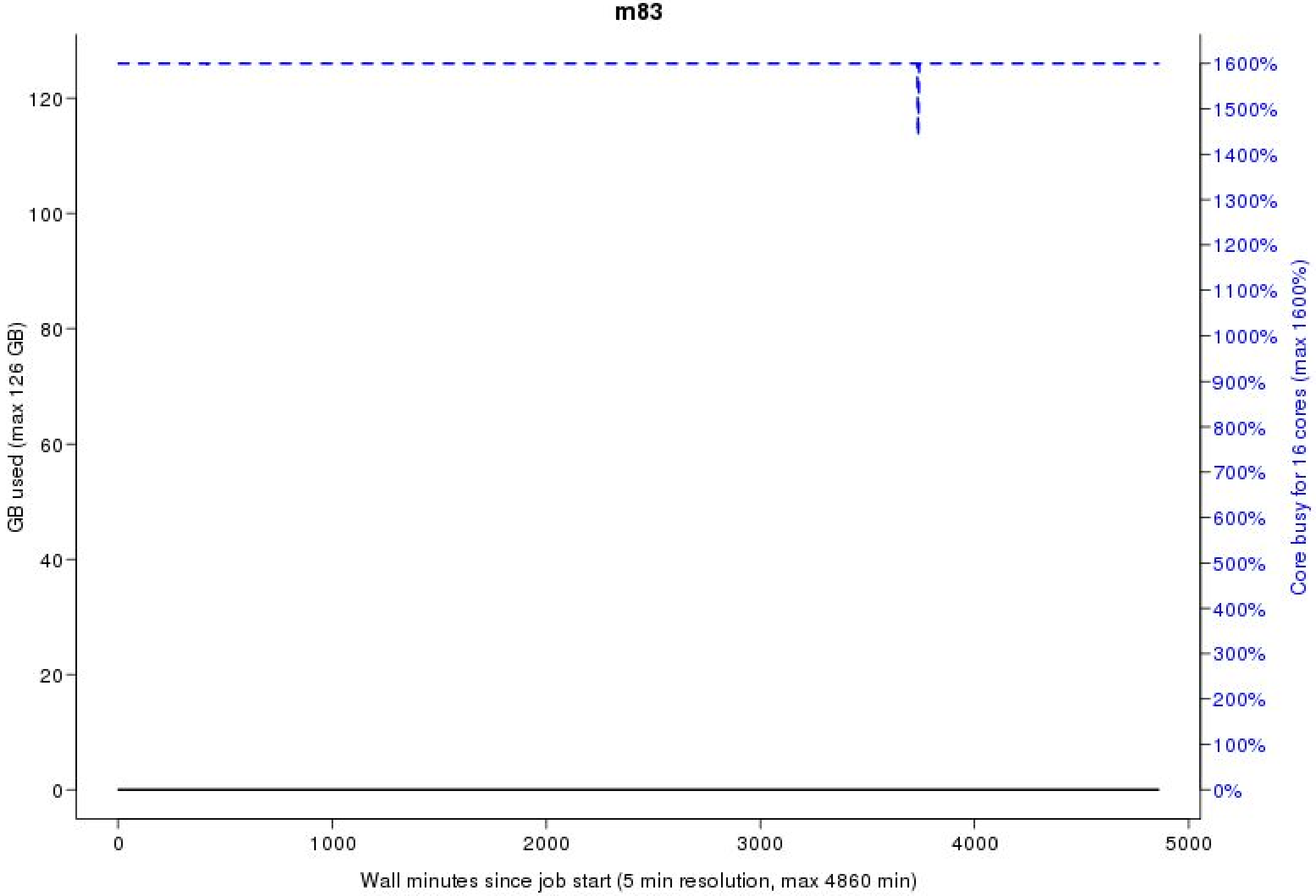
UPPMAX Commands

Plot efficiency

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

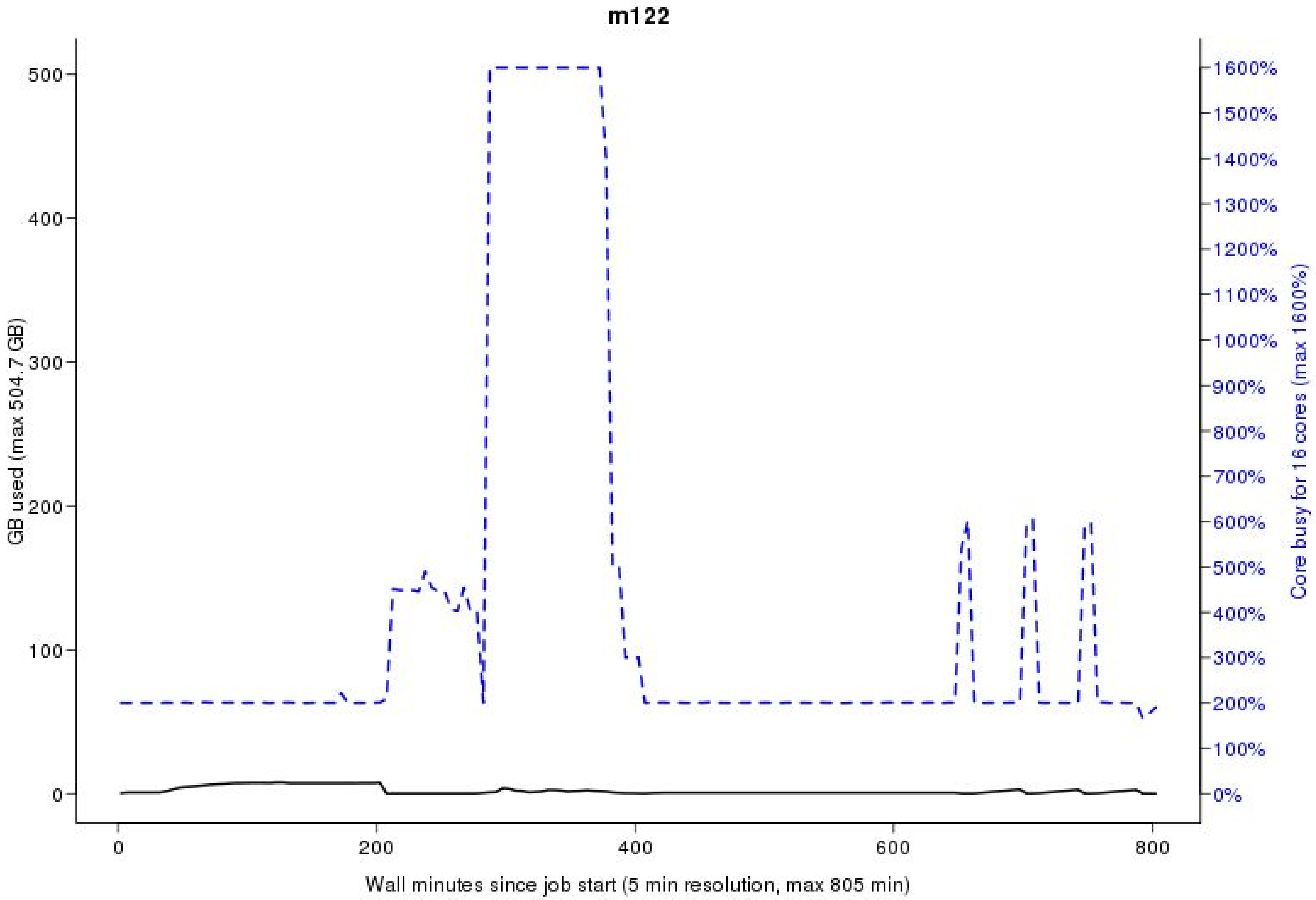
2719328 on 'milou' end: 2014-09-09T08:26:34 runtime: 03-08:59:53

Flags: mem_underused:126:0



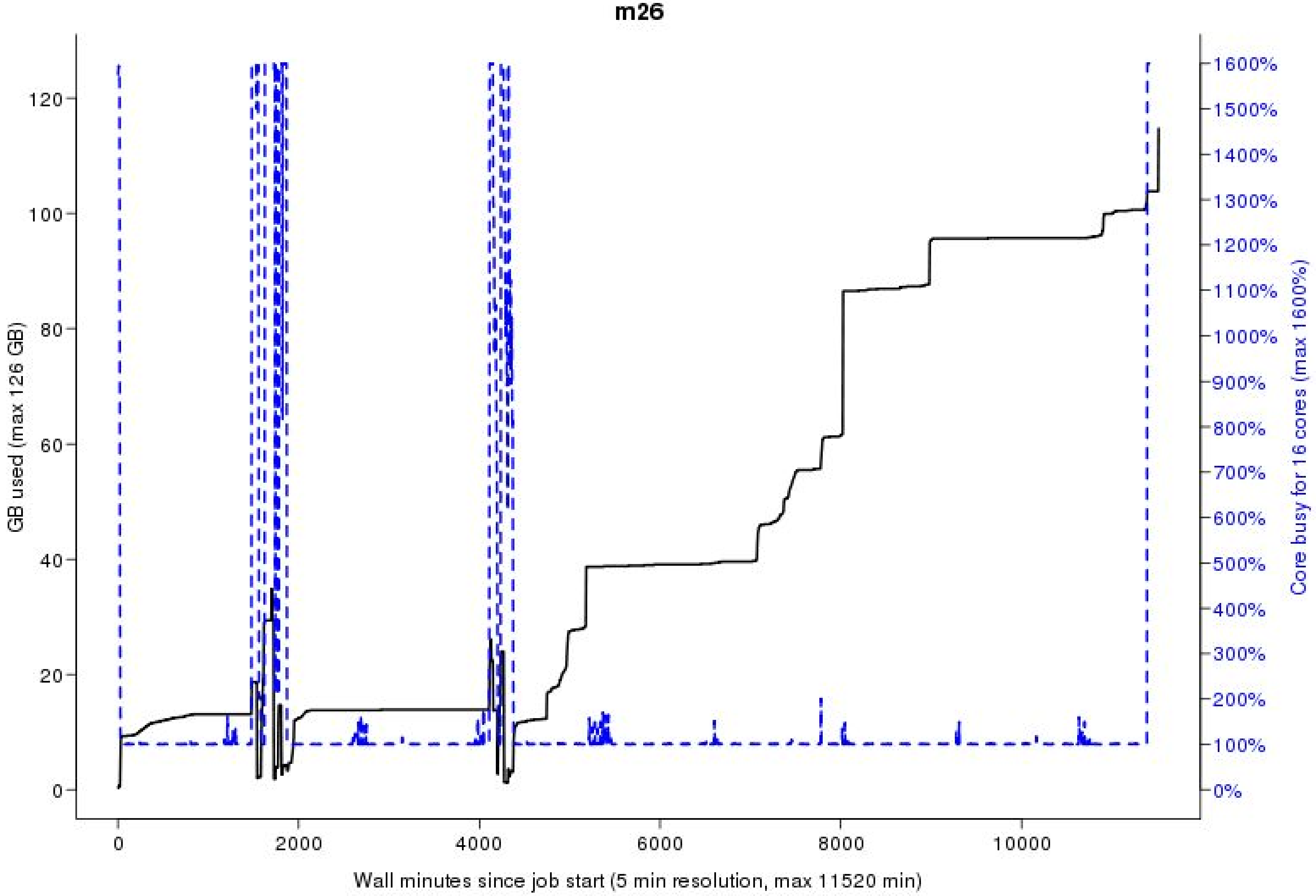
2934193 on 'milou' end: 2014-09-26T01:40:23 runtime: 13:30:23

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



UPPMAX

Summary

- All jobs are run on nodes through queue system
- 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

More info on UPPMAX homepage

- http://www.uppmax.uu.se/milou-user-guide