UPPMAX Introduction

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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!!!

Uppsala Multidisciplinary Center for Advanced Computational Science

http://www.uppmax.uu.se

2 (3) **computer clusters**

- **Rackham**: ~ 500 nodes à 20 cores (128 & 512 GB RAM)
- **Bianca**: 200 nodes à 16 cores (128, 256 & 512 GB RAM) - virtual cluster
- **(Milou**: 208 nodes with 16 cores (128GB RAM) decommissioned, will be resurrected)

>12 PB fast parallel **storage**

Bioinformatics **software**
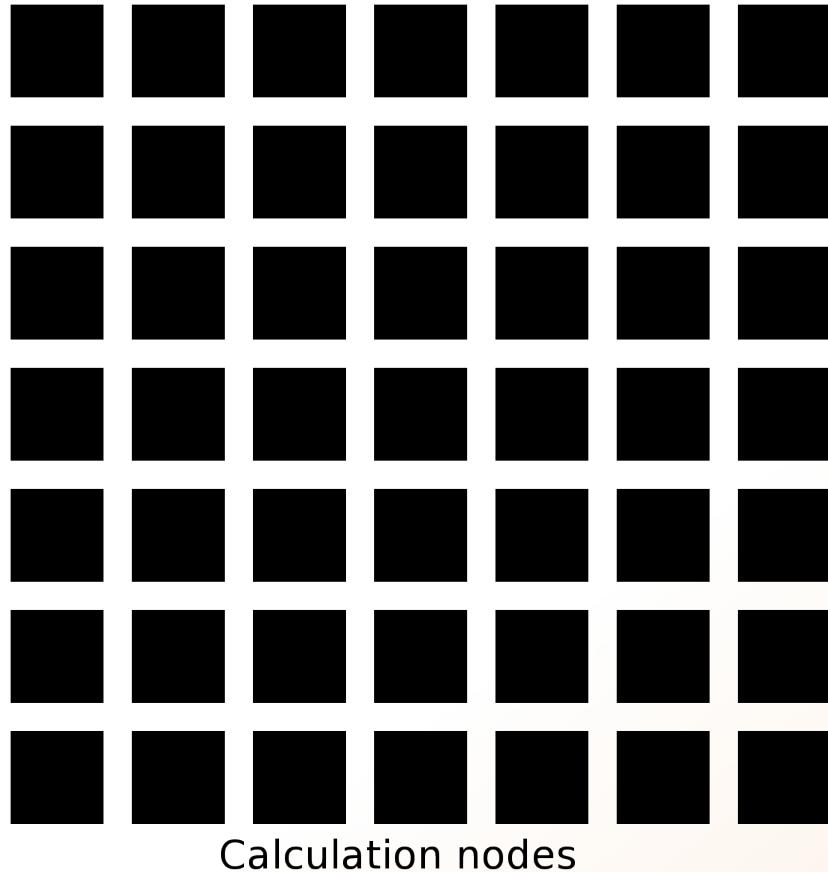
The basic structure of supercomputer

node = computer
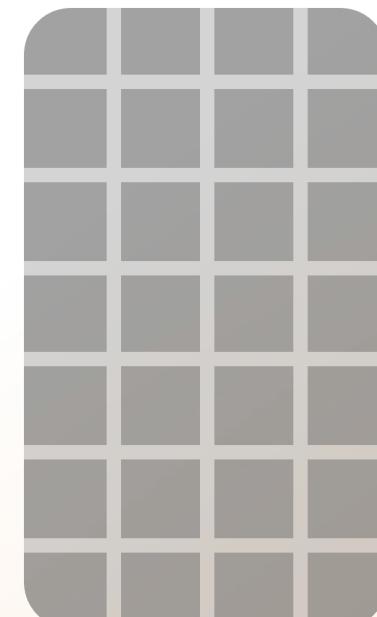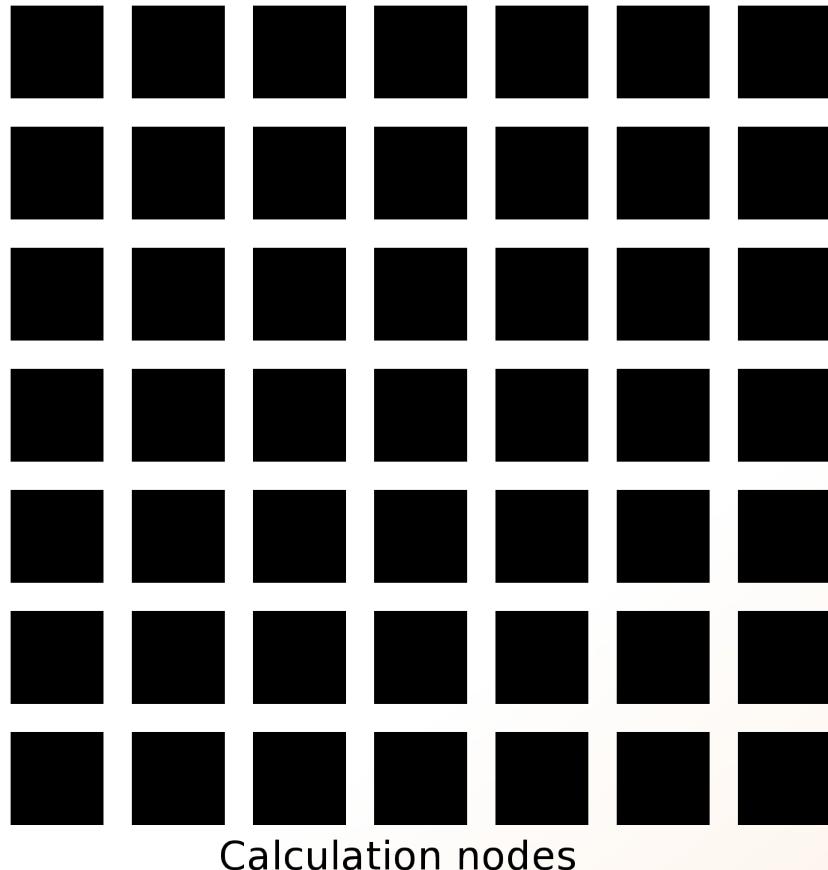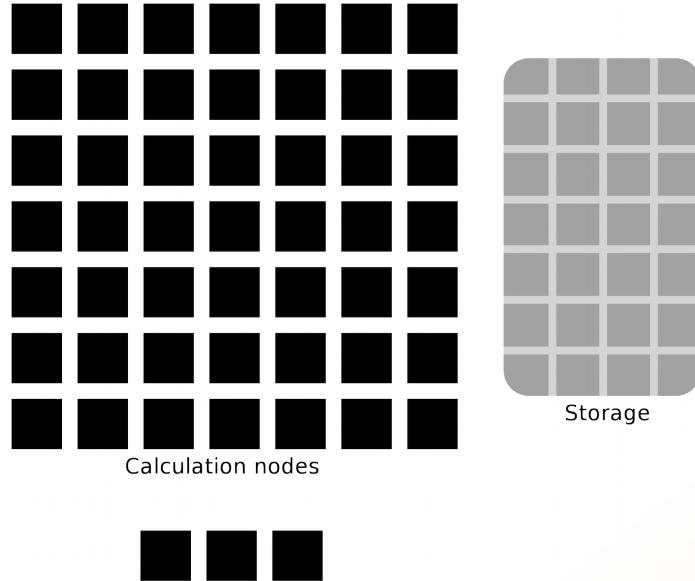
Login nodes

The basic structure of supercomputer

Calculation nodes

Login nodes

The basic structure of supercomputer

Calculation nodes

Storage

Login nodes

SciLifeLab UPPSALA

UPPMAX

Calculation nodes

Storage

UPPMAX provides

Compute and **Storage**

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How to access UPPMAX
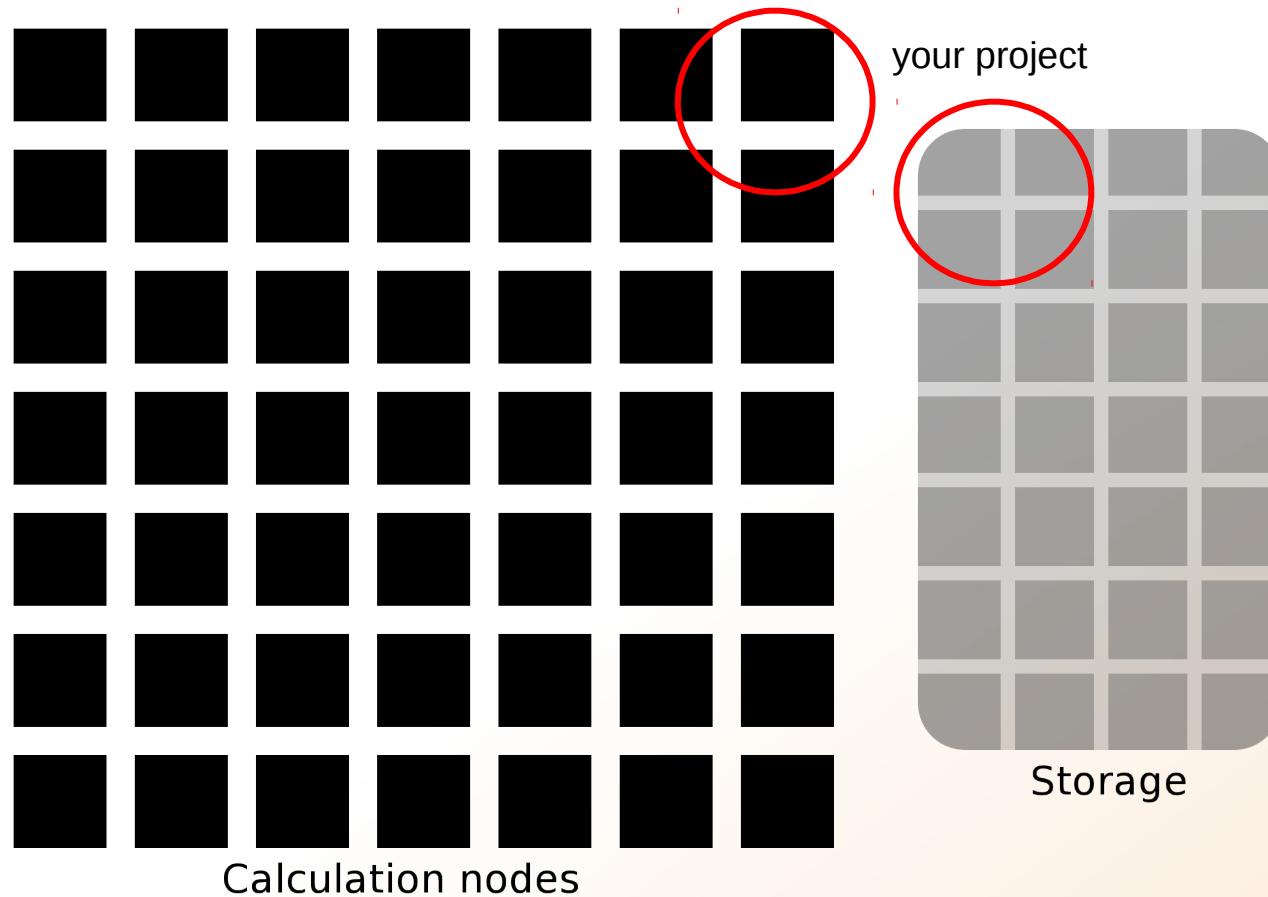
Jobs and queuing systems

How to use the resources of UPPMAX

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

UPPMAX provides its resources via

projects

Projects

your project

Storage

Calculation nodes

Resources:

compute
(core-hours/month)

storage
(GB)

Two separate projects:

SNIC project:
    cluster **Rackham**
        2000 - 100 000+ core-hours/month
        128 GB

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

SciLifeLab UPPSALA

SNIC SUPR

| Admin | User |

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

Uppsala universitet [SE] | https://supr.snic.se/round/2018smalluppmax/

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.

| Create New Proposal for SNAC Small UPPMAX, 2018 | View Committee Overview |

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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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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        FAQ: http://www.uppmax.uu.se/support/faq

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[valent@rackham1 ~]$
```

SSH

Local
computer

Login
nodes

Computation
nodes

ssh
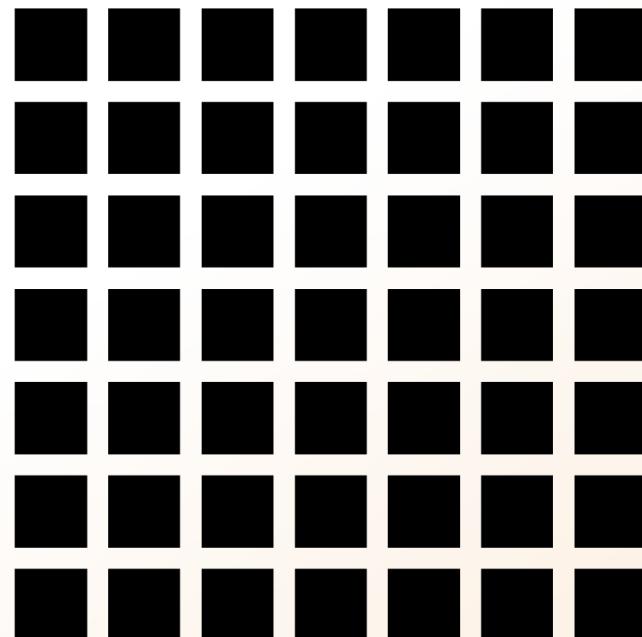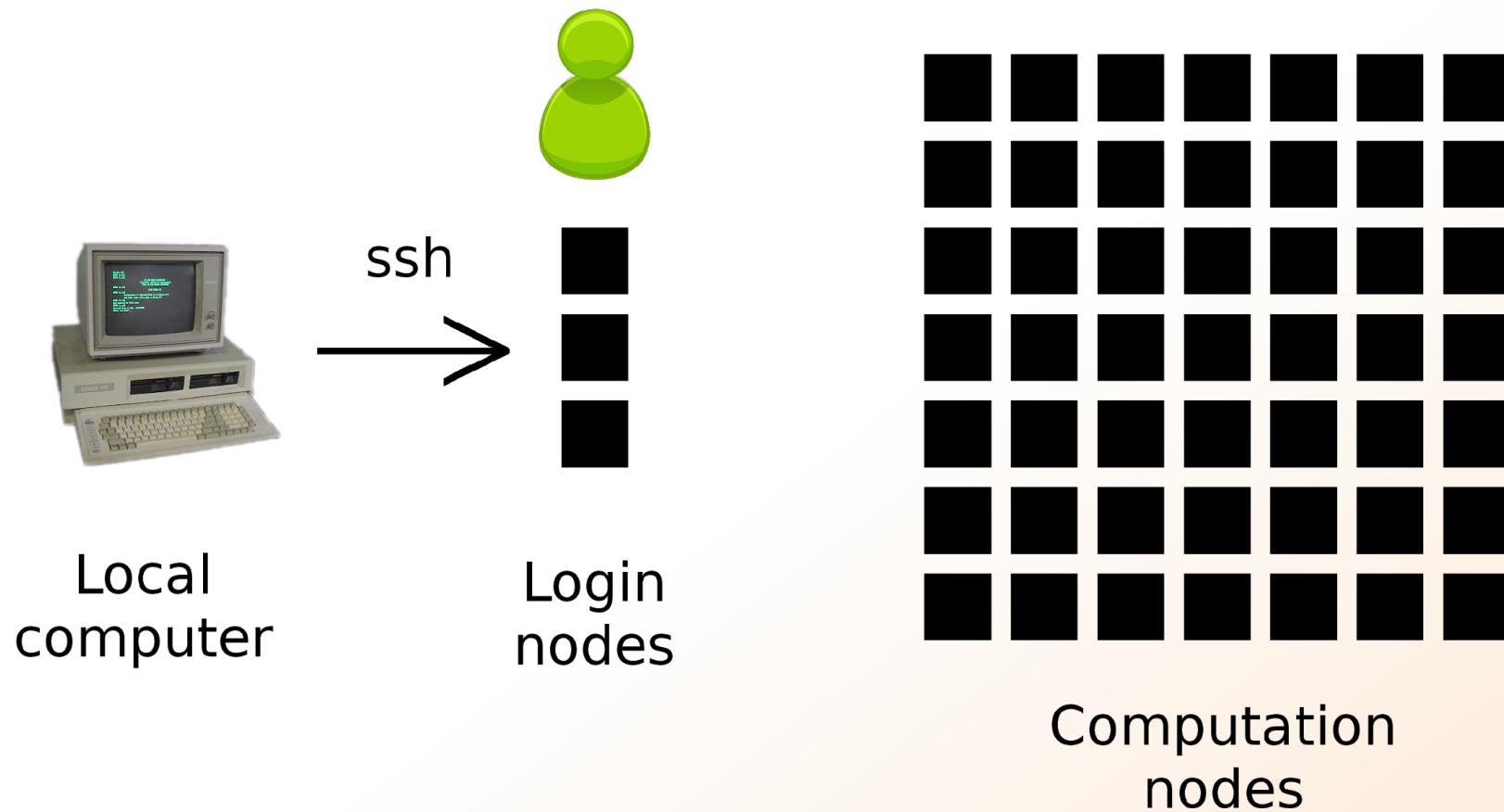
Local
computer

Login
nodes

Computation
nodes

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

Calculation nodes

not accessible directly

SLURM (queueing system) gives you access

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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.

Read/open files

Do something with the data

Print/save output

Read/open files
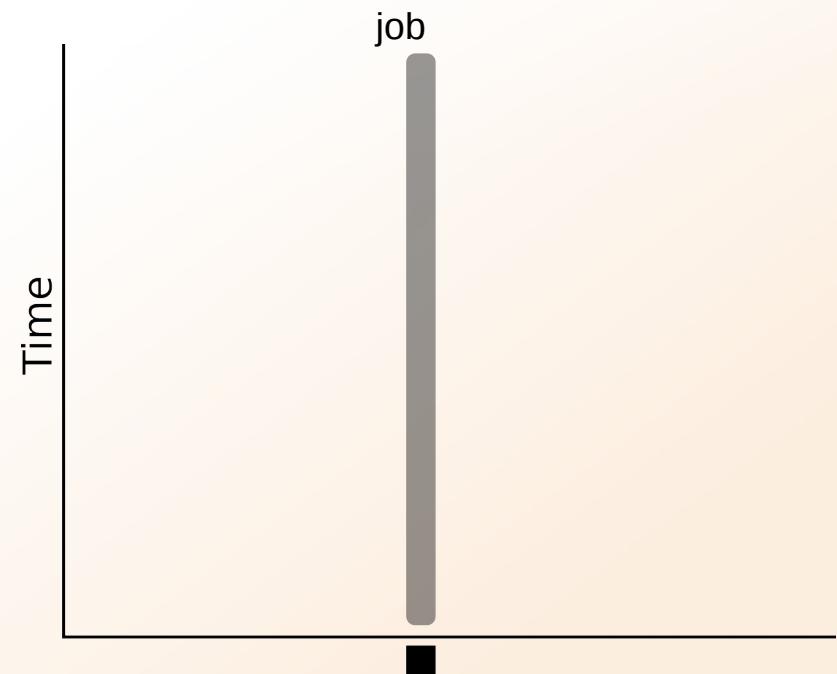
Do something with the data

Print/save output

The basic structure of a supercomputer
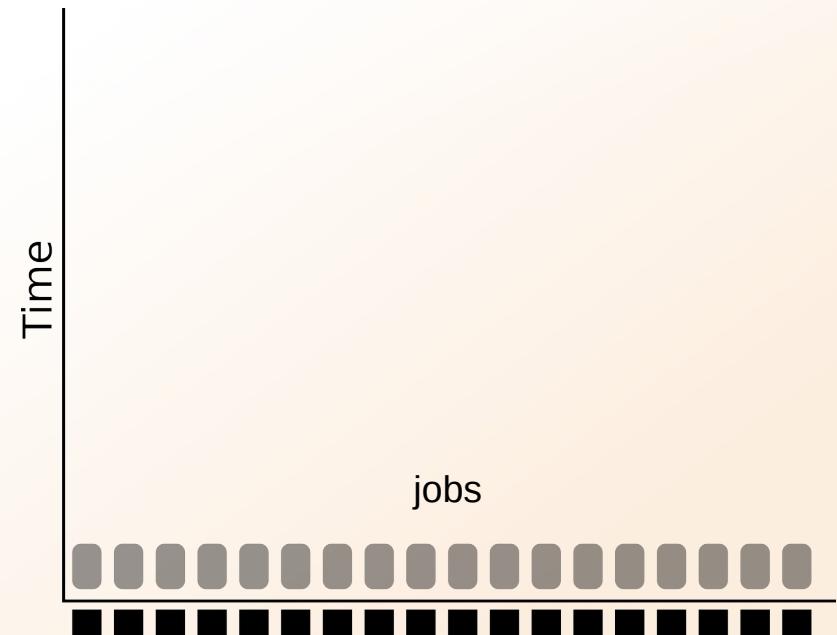
Parallel computing!!!
Not one super fast

The basic structure of a supercomputer

Parallel computing!!!
    Not one super fast
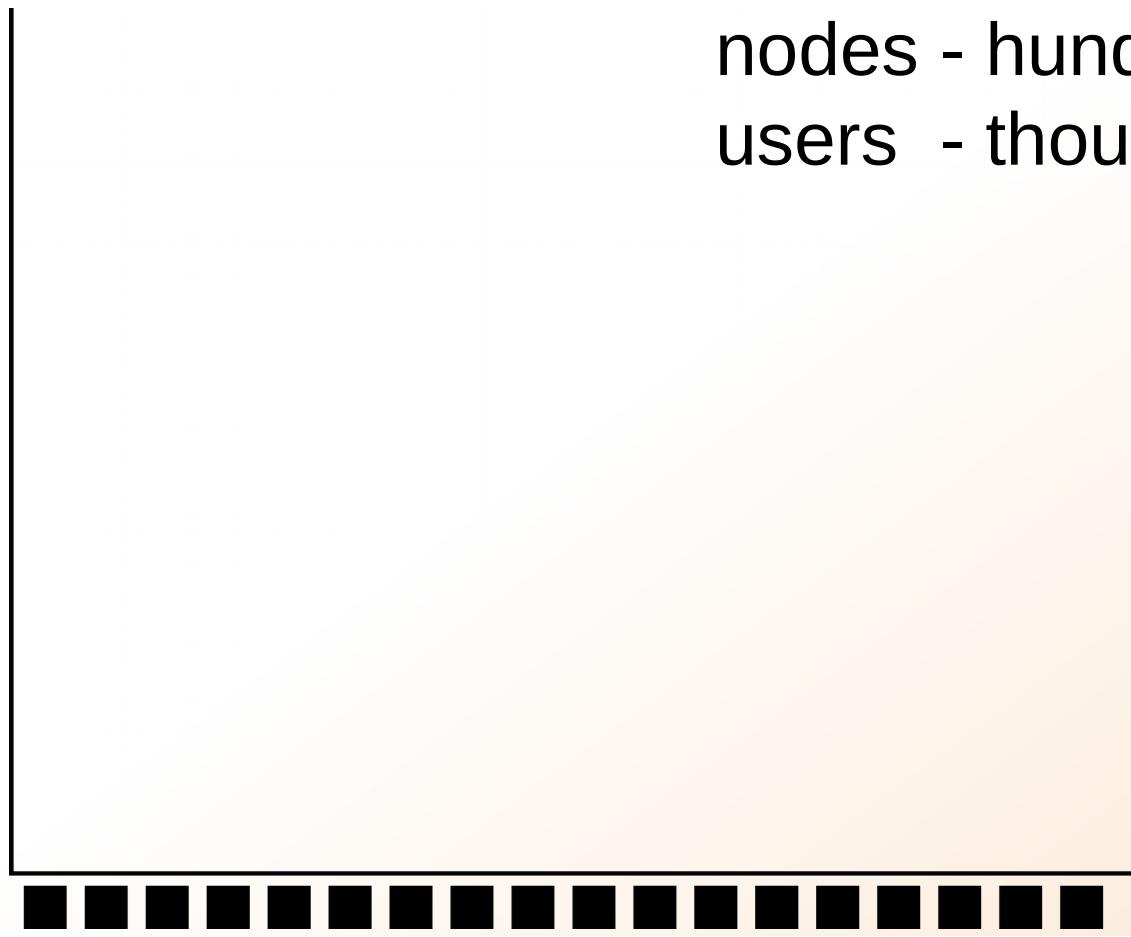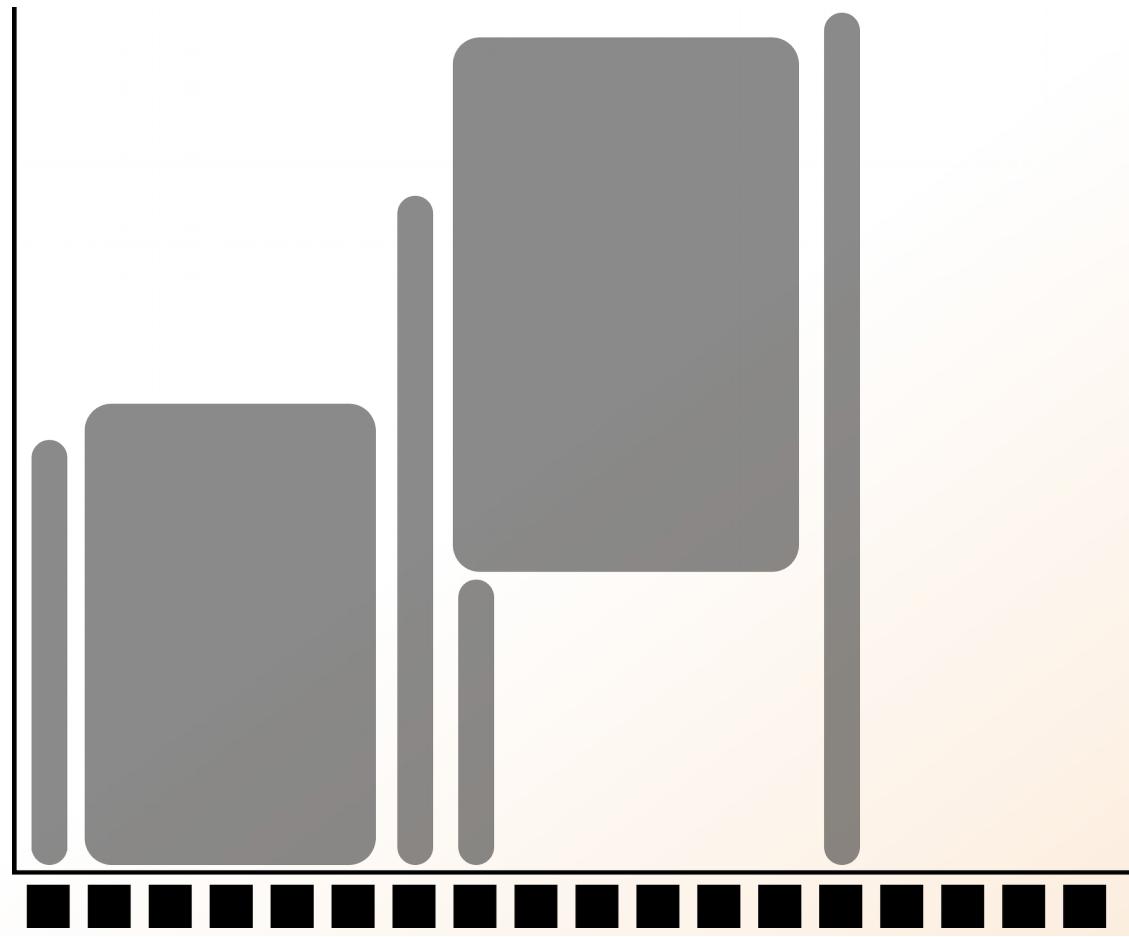
More users than nodes
Need for a queue

nodes - hundreds
users - thousands
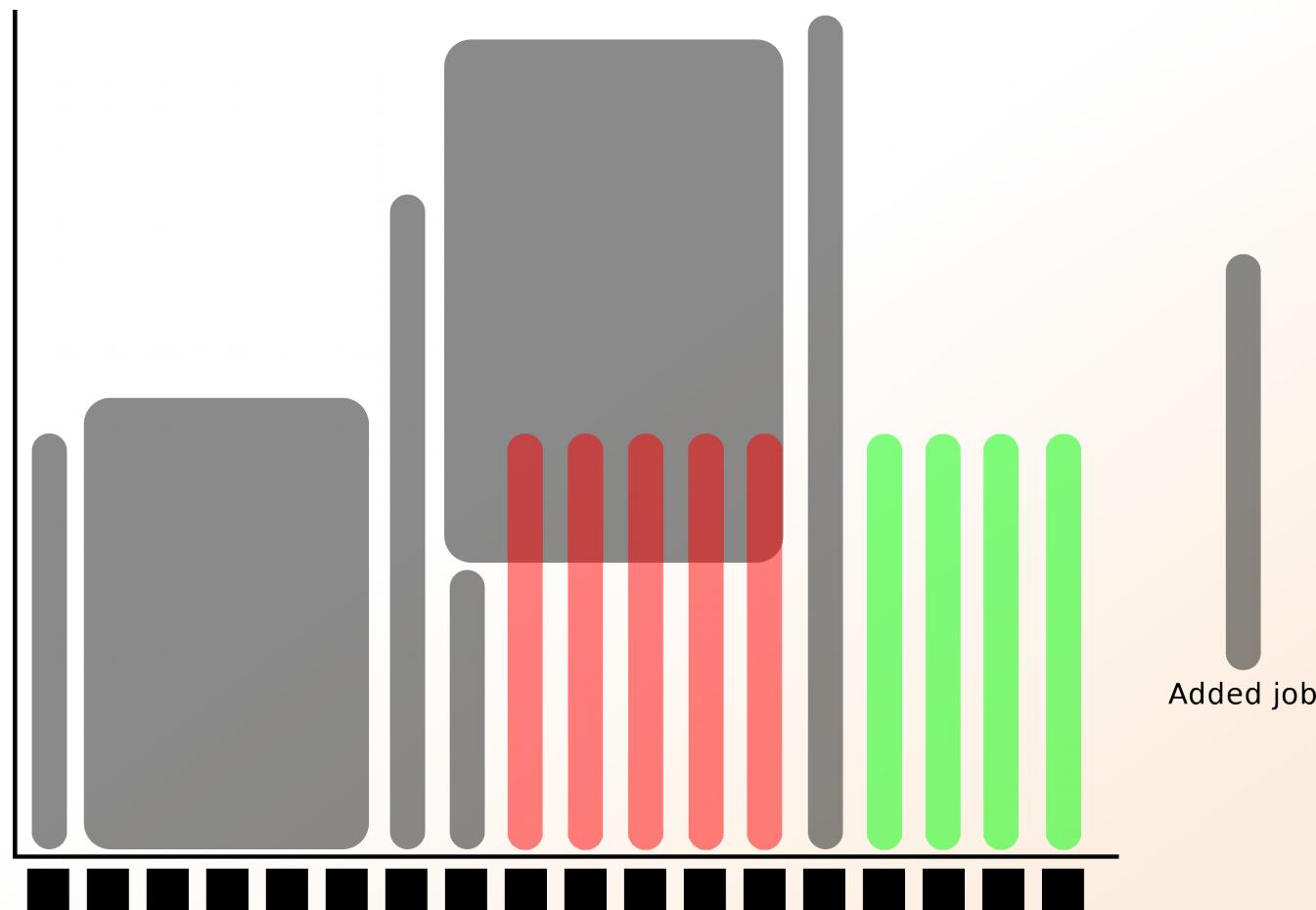
More users than nodes
Need for a queue
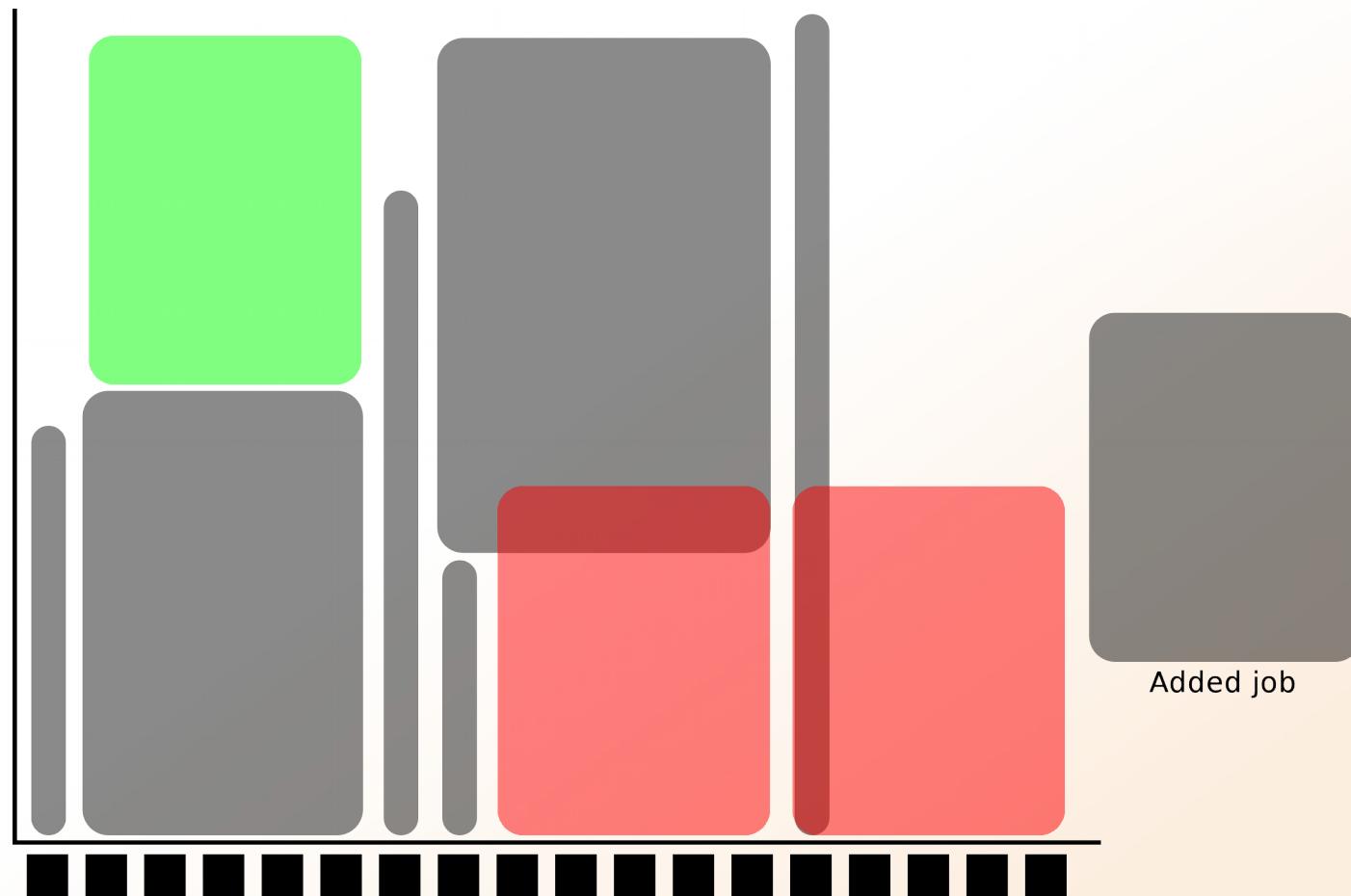
More users than nodes
Need for a queue

Added job

More users than nodes

Need for a queue

Added job

**workload manager
job queue
batch queue
job scheduler**

SLURM (Simple Linux Utility for Resource Management)
free and open source

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How to use the resources of UPPMAX

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

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

1) Ask for resource and run jobs manually

submit a request for resources

ssh to a calculation node

run programs

1) Ask for resource and run jobs manually

salloc -A snic2018-0-001 -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

-A   this course project g2018018

            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%

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>*

```
[[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 ~]$ █
```
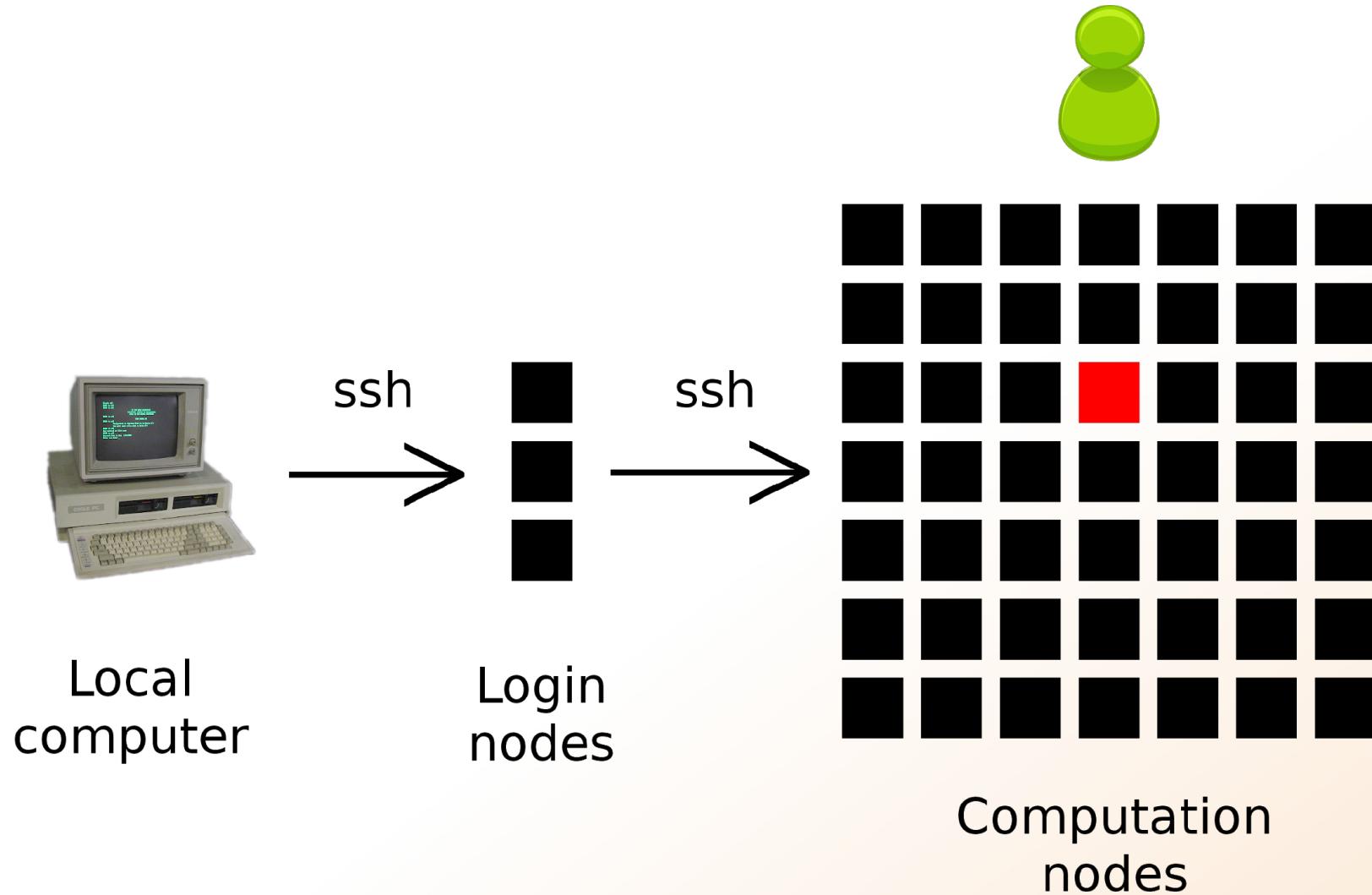
SLURM

Local computer

ssh

Login nodes

ssh

Computation nodes

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

Interactive - books a node and connects you to it

interactive -A b2018-0-001 -p core -n 1 -t 00:05:00

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

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

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

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 g2018000 -p core -n 1 -t 00:05:00 test.sbatch

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]$ 
```

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>

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

or just google "uppmax slurm user guide"

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

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'

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                          -
```

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]$
```

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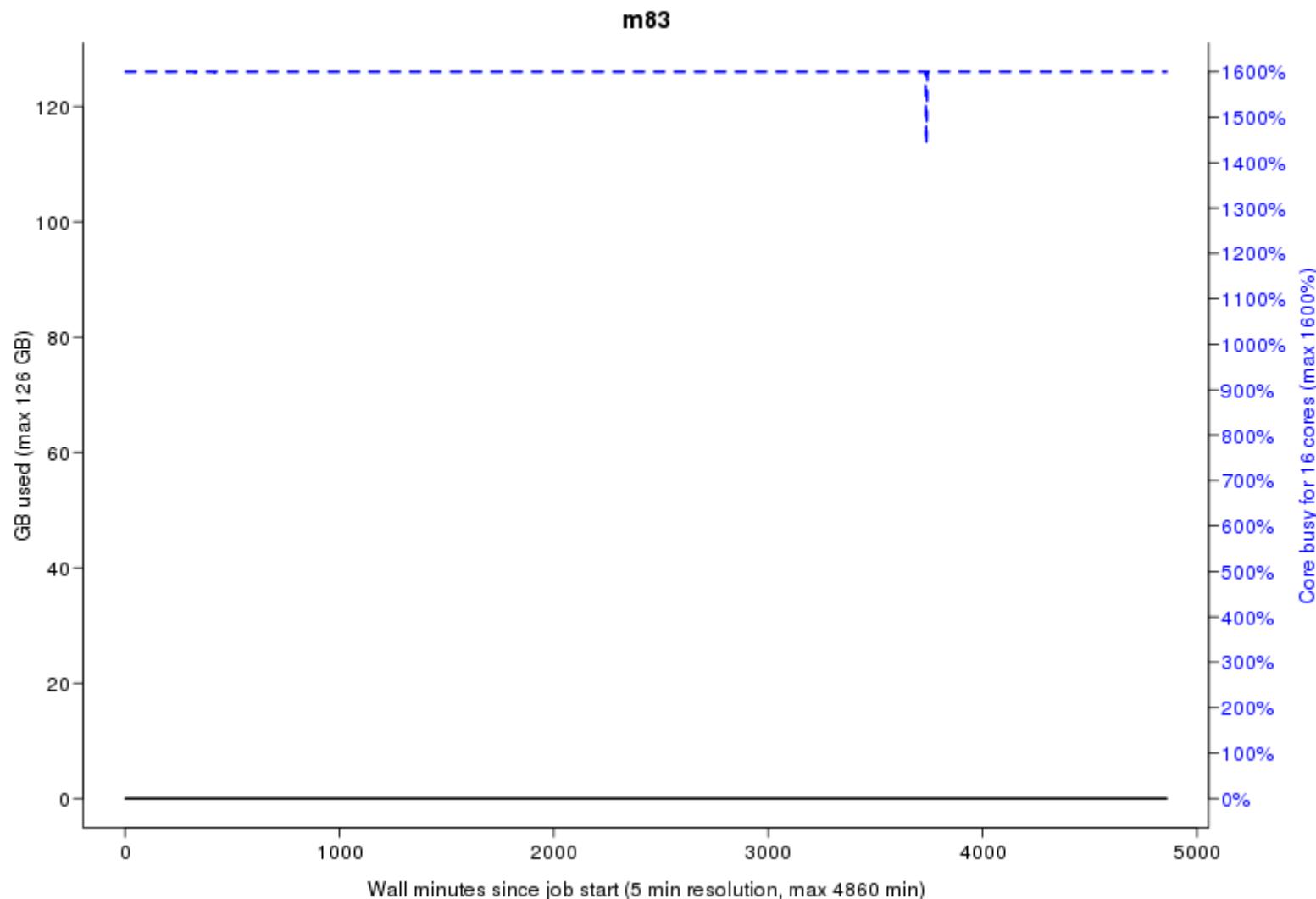
**How to use the resources of UPPMAX in a good way!**
                                                    Efficiency!!!

Plot efficiency
    jobstats -p -A <projid>
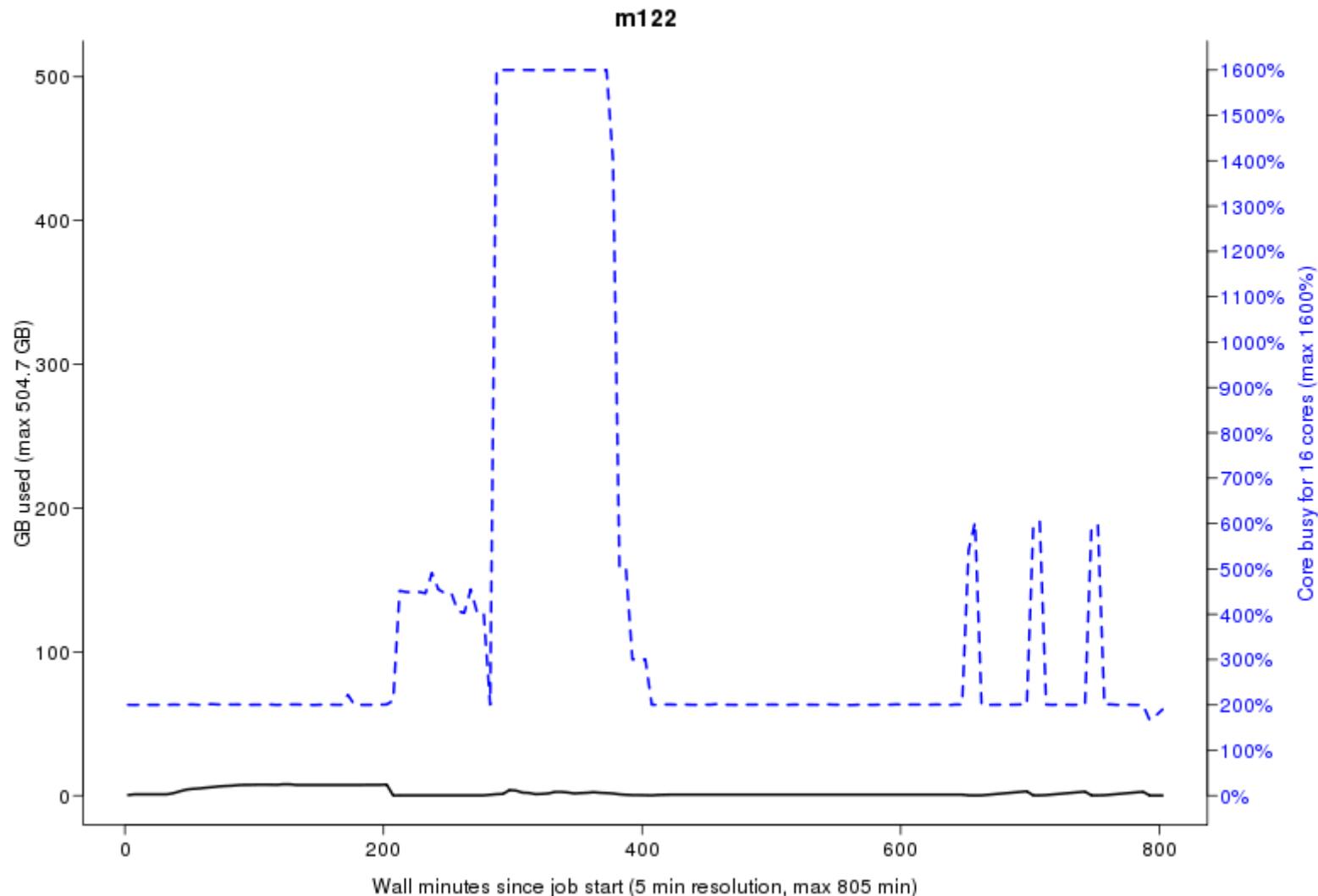
2719328 on 'milou' end: 2014-09-09T08:26:34 runtime: 03-08:59:53

Flags: mem_underused:126:0

m83

# 2934193 on 'milou' end: 2014-09-26T01:40:23 runtime: 13:30:23
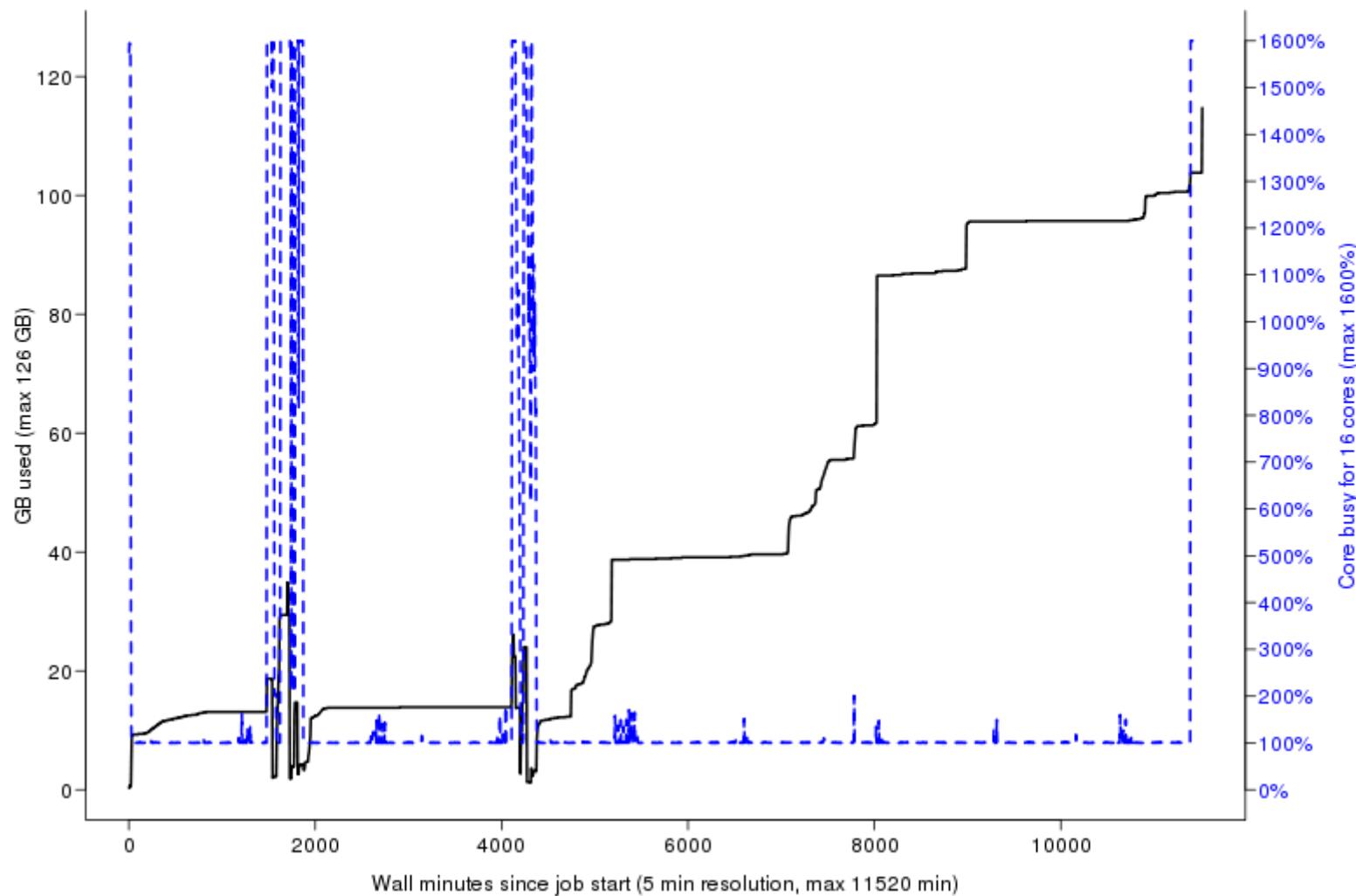
Flags: mem_underused:504.7:7.9   node_type_misbooked:mem512GB:mem128GB

m122

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

Flags: none

m26

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
- 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)