SciLifeLab
UPPSALA

UPPMAX Introduction

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Enabler for Life Sciences

SciLifeLab
Uppsala Multidisciplinary Center for Advanced Computational Science
UPPMAX
UPPNEX
UPPSALA UNIVERSITET

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

3 clusters

- Milou, 208 computers à 16 cores (128GB RAM)
  - 17 with 256, 17 with 512 - until end of 2017
- Rackham, 334(600) computers à 20 cores (128GB RAM)
- Bianca, 200 nodes à 16 cores (128GB RAM)

~12 PB fast parallel storage

Bioinformatics software

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UPPMAX

The basic structure of supercomputer

node = computer

Login nodes

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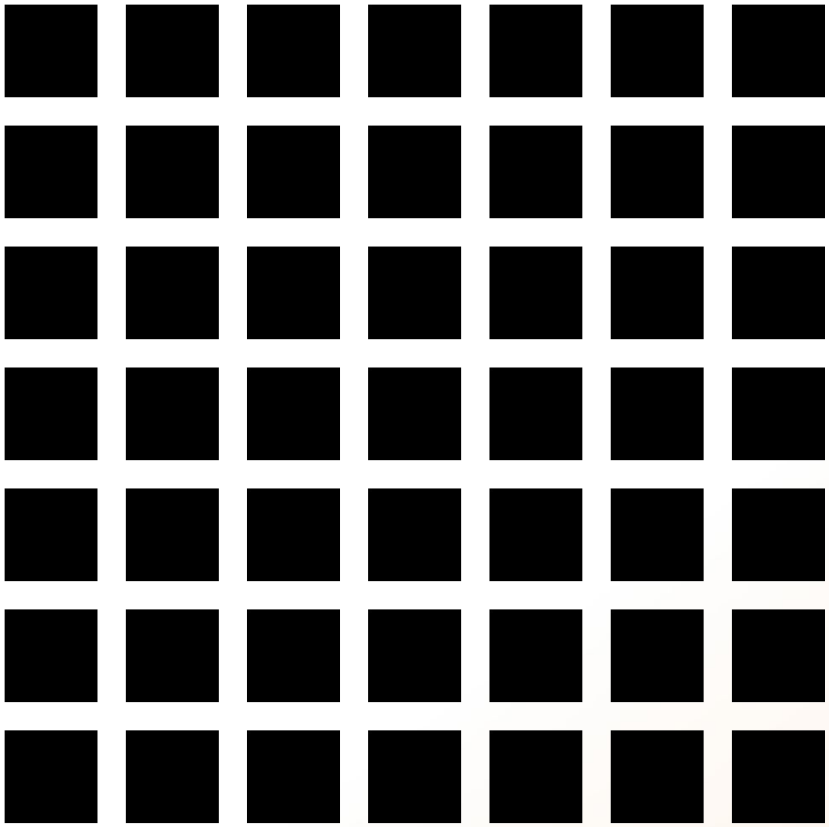
UPPMAX

The basic structure of supercomputer



Calculation nodes

Login nodes

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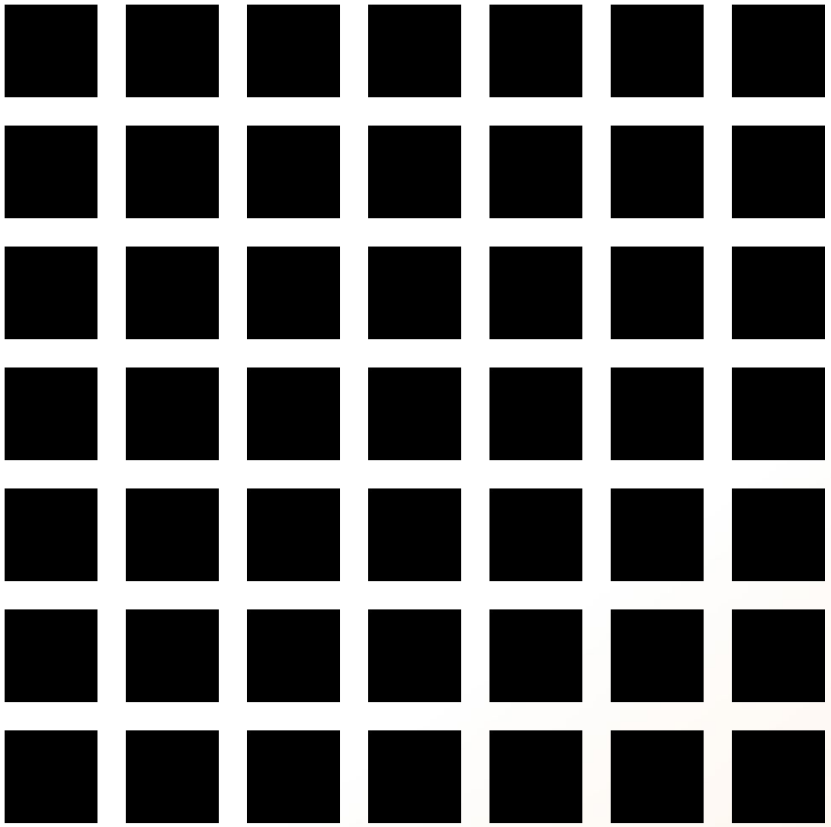
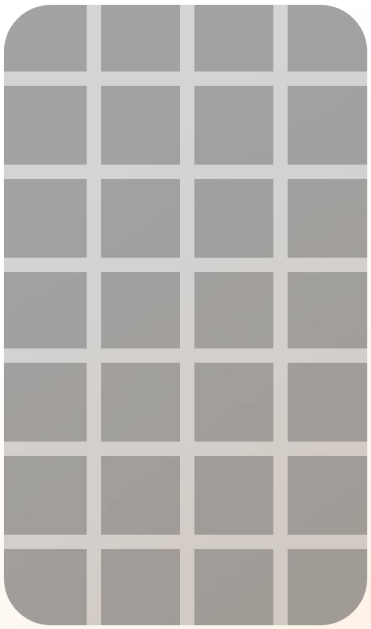
UPPMAX

The basic structure of supercomputer



Calculation nodes



Storage

Login nodes

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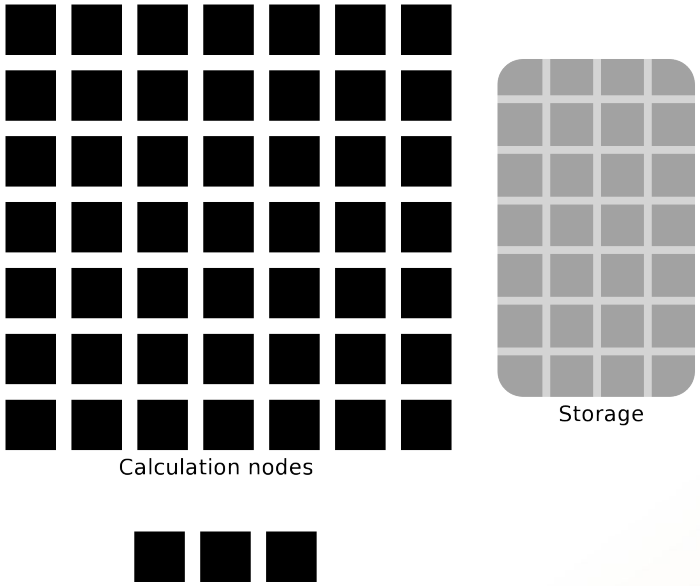
UPPMAX



UPPMAX provides

Compute and **Storage**

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Objectives

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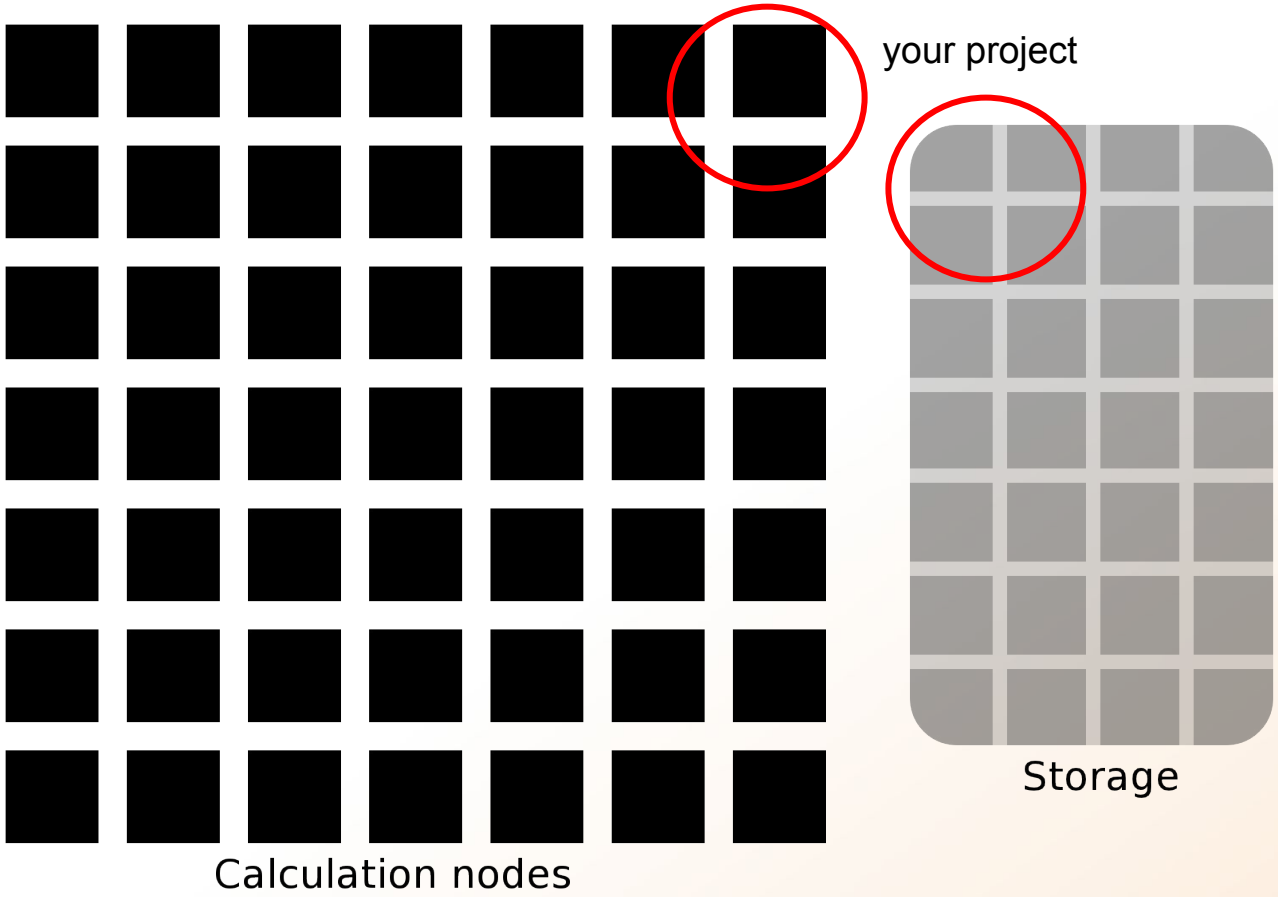
Efficiency!!!

Projects

UPPMAX provides its resources via

projects

Projects



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Projects

Resources:

compute
(core-hours/month)

storage
(GB)

Projects

before - UPPNEX projects:

cluster **Milou**

2000 core-hours/month

1 TB

This course's project ID: g2017024

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Projects

now - two separate projects:

SNIC project:

cluster **Rackham**

2000 core-hours/month

128 GB

Scilifelab Storage project:

storage system **CREX**

1 - 100 TB

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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 Milou

```
VG-MBP:~ valentingeorgiev$ ssh -Y valent@milou.uppmax.uu.se
Last login: Sun Oct 22 10:02:44 2017 from host-95-195-196-83.mobileonline.telia.com
 _    _ ____  ____  __  __     _     __  __
| |  | |  _ \|  _ \|  \/  |   / \    \ \/ /    | System:    milou2
| |  | | |_) | |_) | |\/| |  / _ \    \  /     | 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@milou2 ~]$
```

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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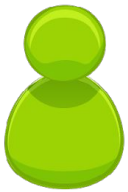
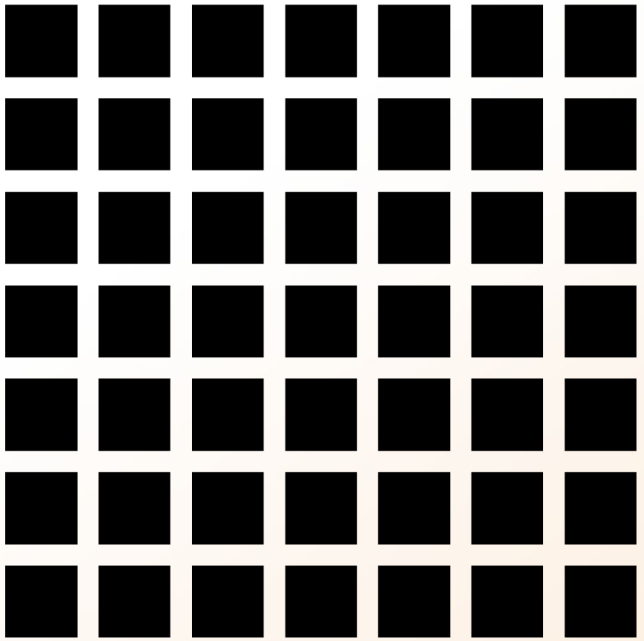
SSH



Local computer

Login nodes



Computation nodes

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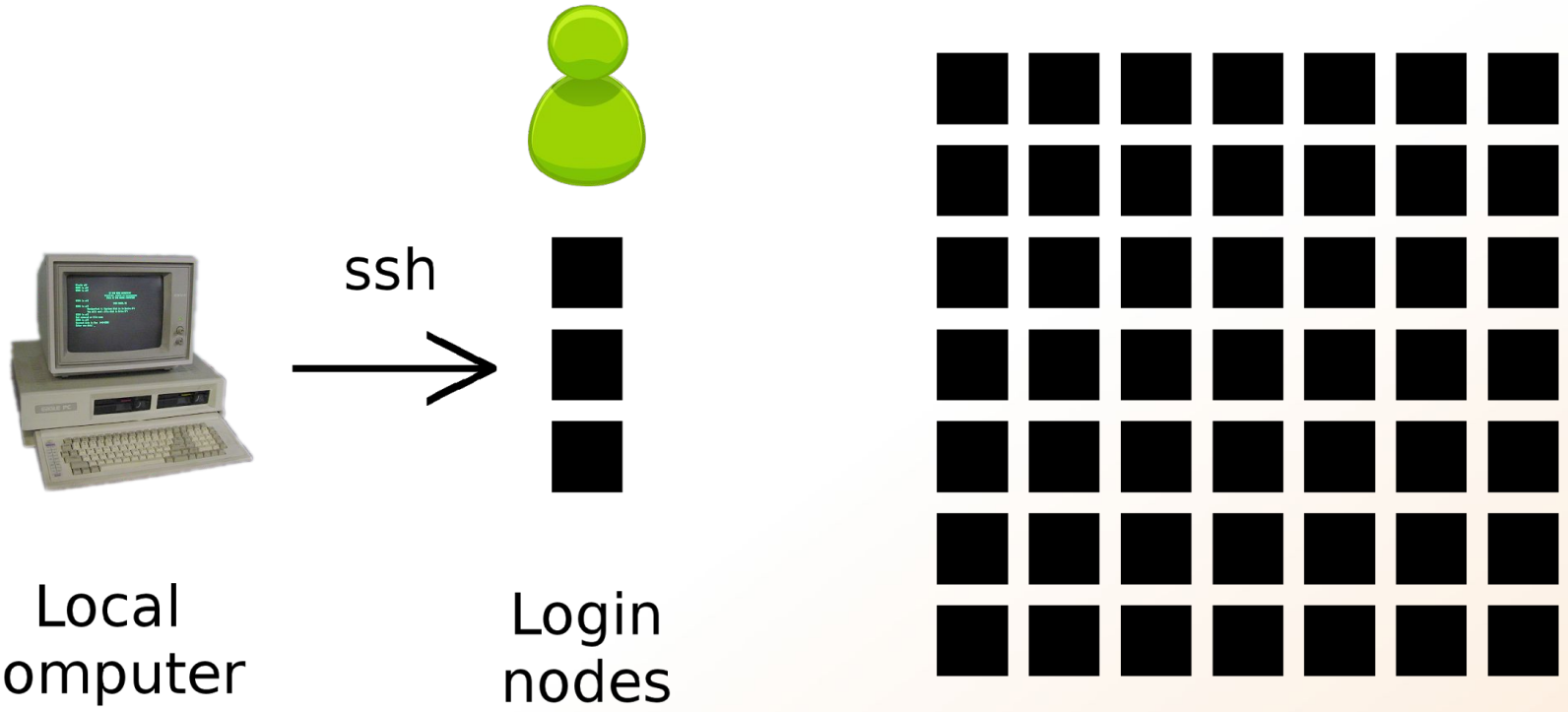
SSH



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How to use UPPMAX

Login nodes

use them to access UPPMAX
never use them to run **jobs**
don't even use them to do "quick stuff"

Calculation nodes

do your work here - testing and running

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How to use UPPMAX

Calculation nodes

not accessible directly

SLURM (queueing system) gives you access

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Efficiency!!!

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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Job

Read/open files

Do something with the data

Print/save output

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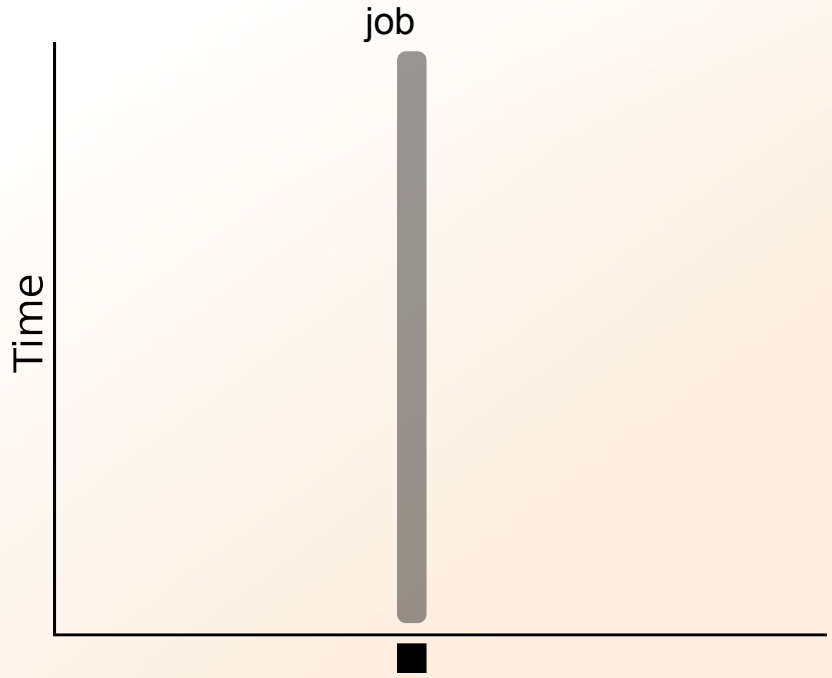
Job

The basic structure of a supercomputer

Parallel computing is key

- Not one super fast



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Job

The basic structure of a supercomputer

Parallel computing is key

- Not one super fast

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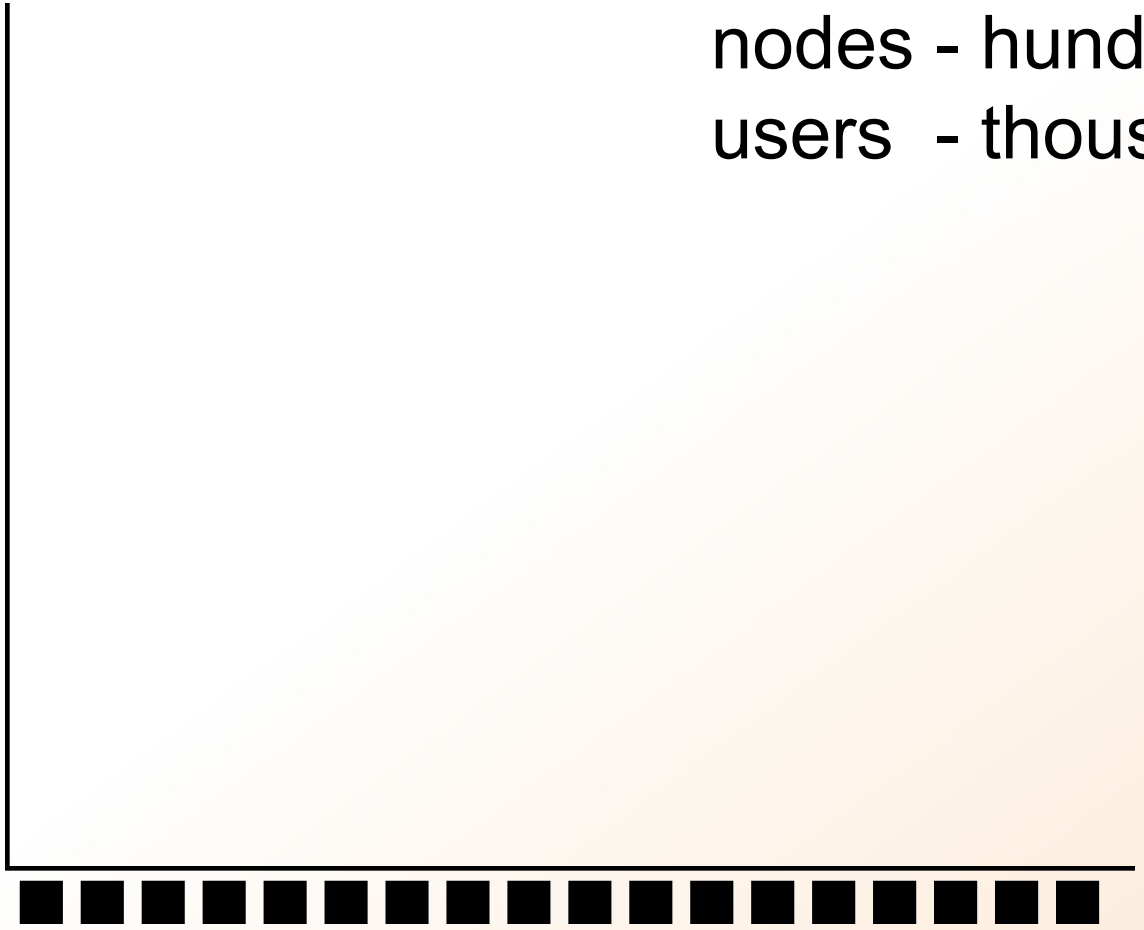
Queue System

More users than nodes

Need for a queue



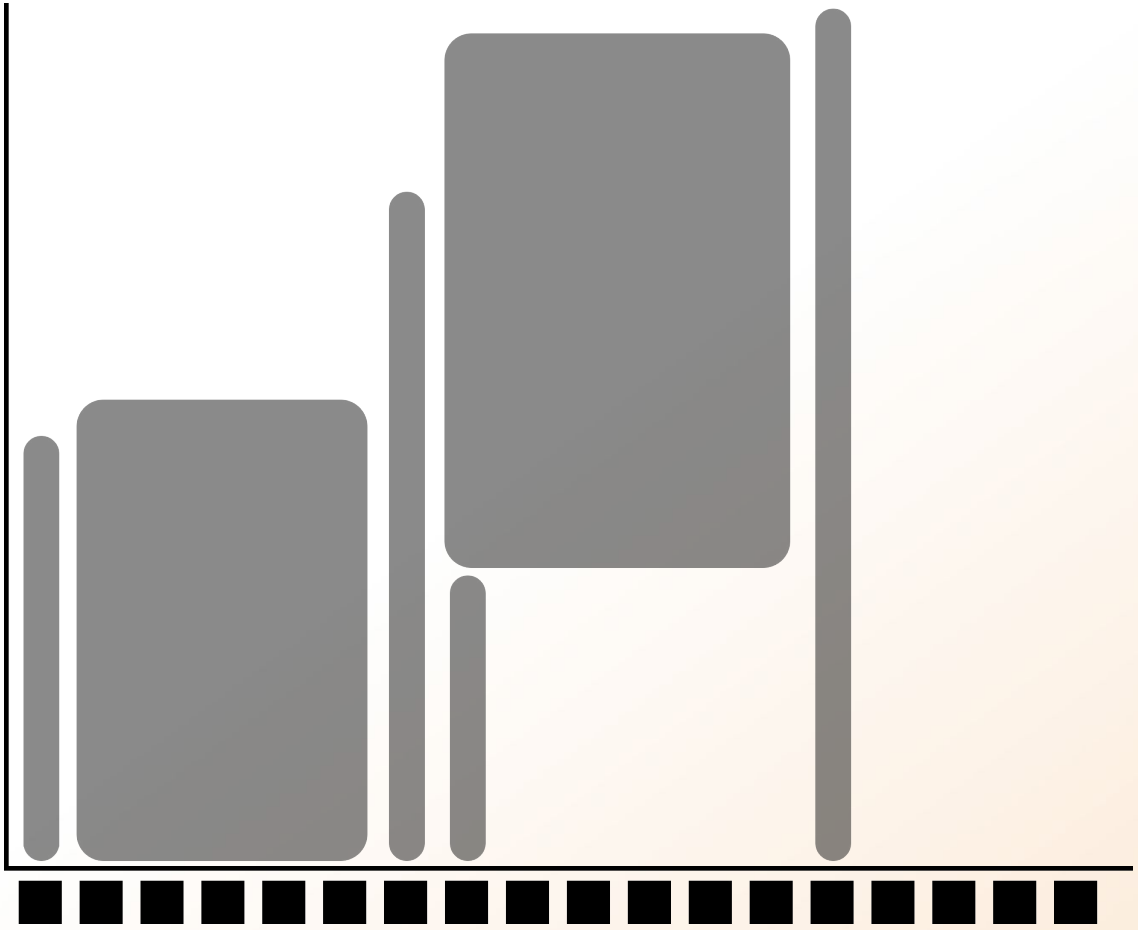
nodes - hundreds

users - thousands

Queue System

More users than nodes

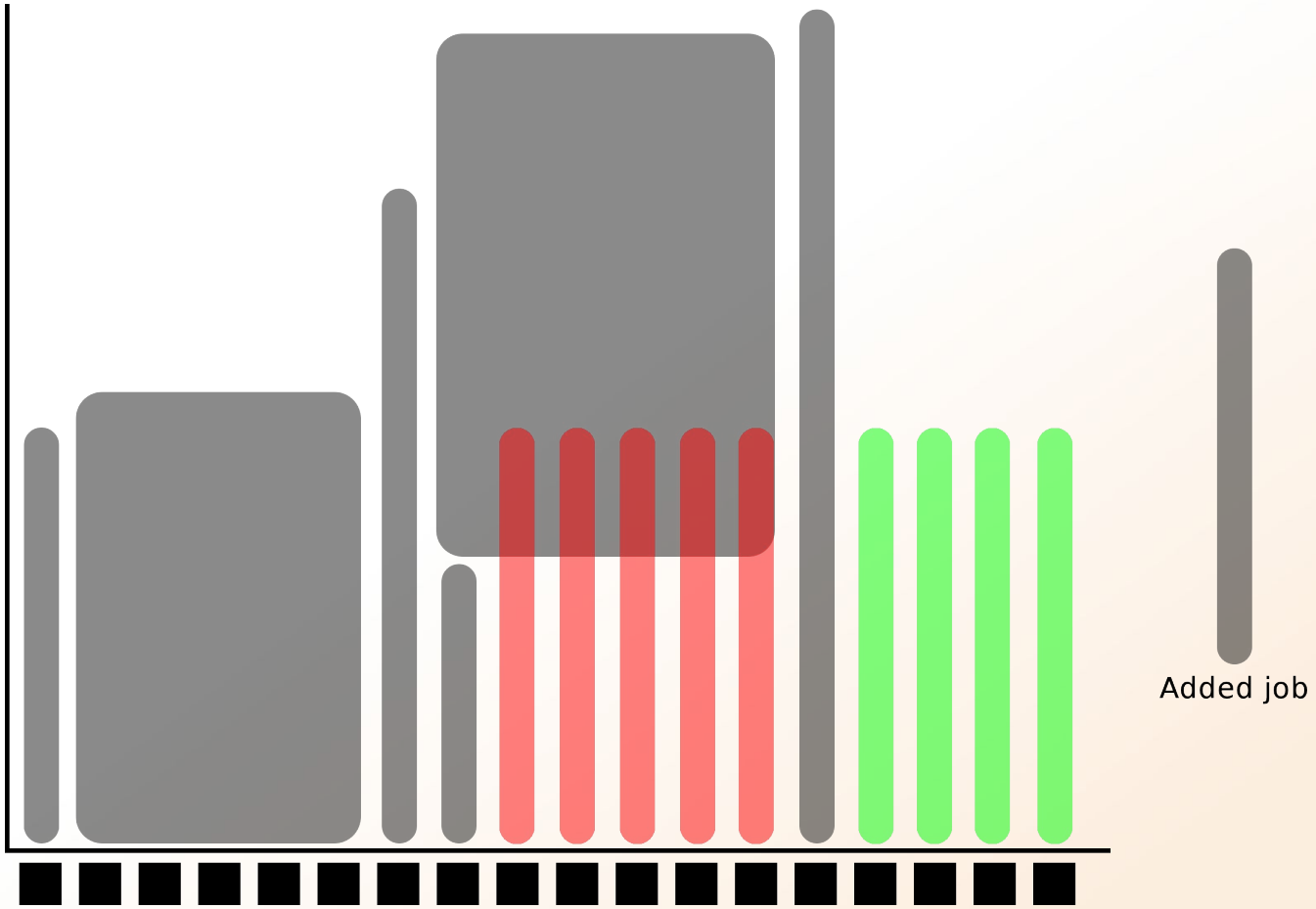
Need for a queue



Queue System

More users than nodes

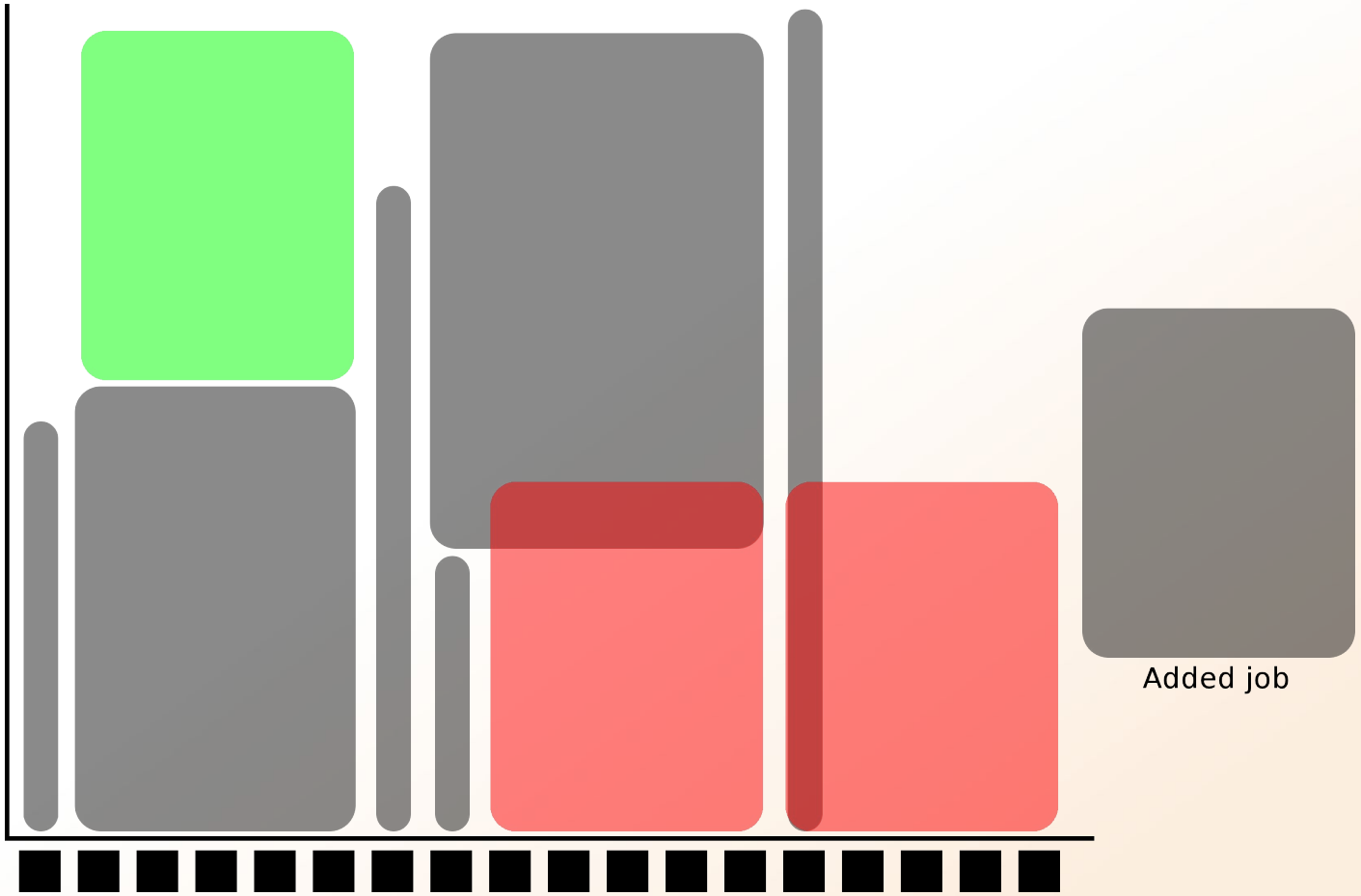
Need for a queue



Queue System

More users than nodes

Need for a queue



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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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Efficiency!!!

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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

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SLURM

1) Ask for resource and run jobs manually

submit a request for resources

ssh to a calculation node

run programs

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SLURM

1) Ask for resource and run jobs manually

salloc -A b2015245 -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

-A this course project g2017024
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%

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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
```

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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

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

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

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[valent@m164 ~]$
```

SSH to a calculation node (from a login node)

ssh -Y *<node_name>*

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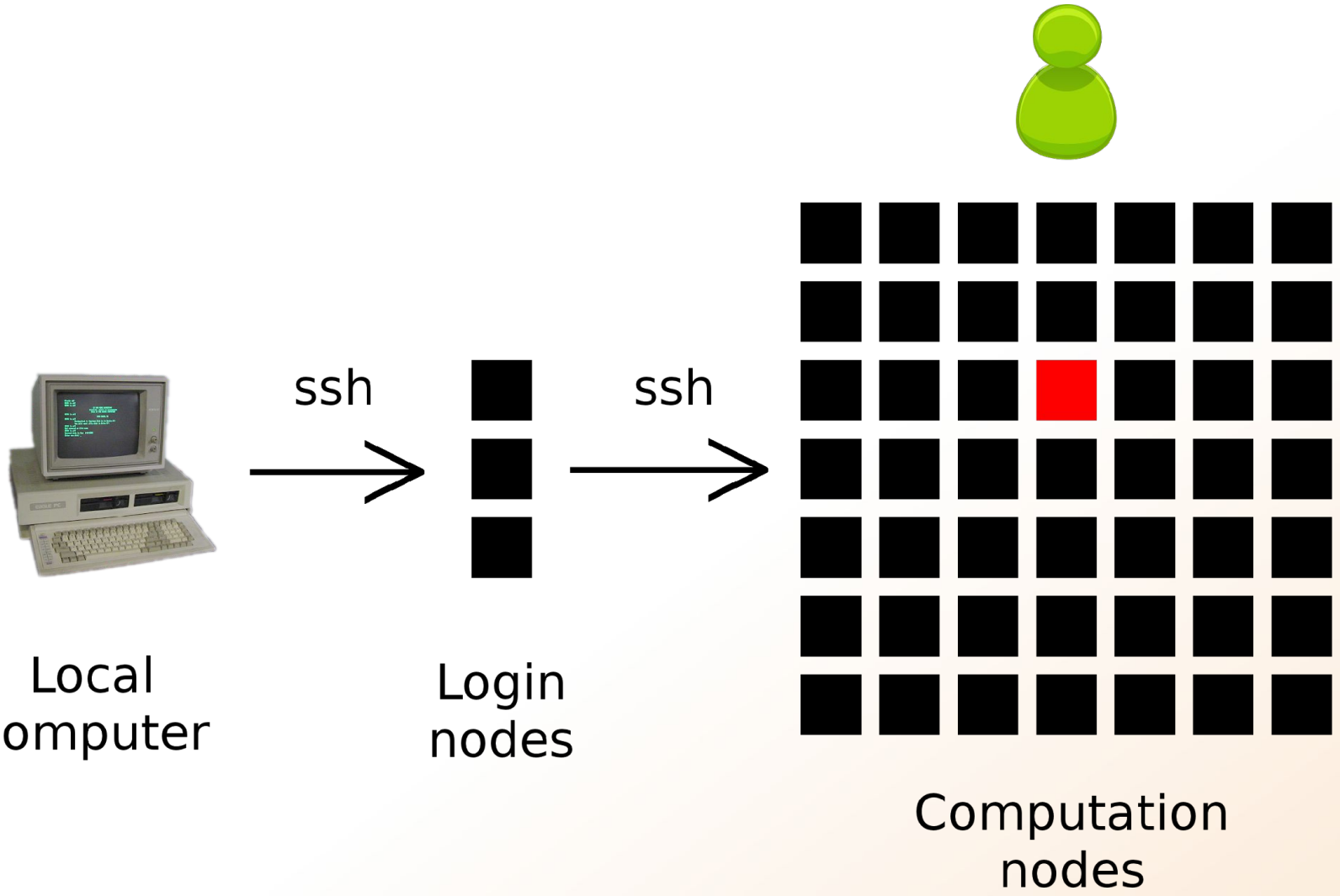
SLURM



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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 b2015245 -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)

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 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'

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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                             -
```

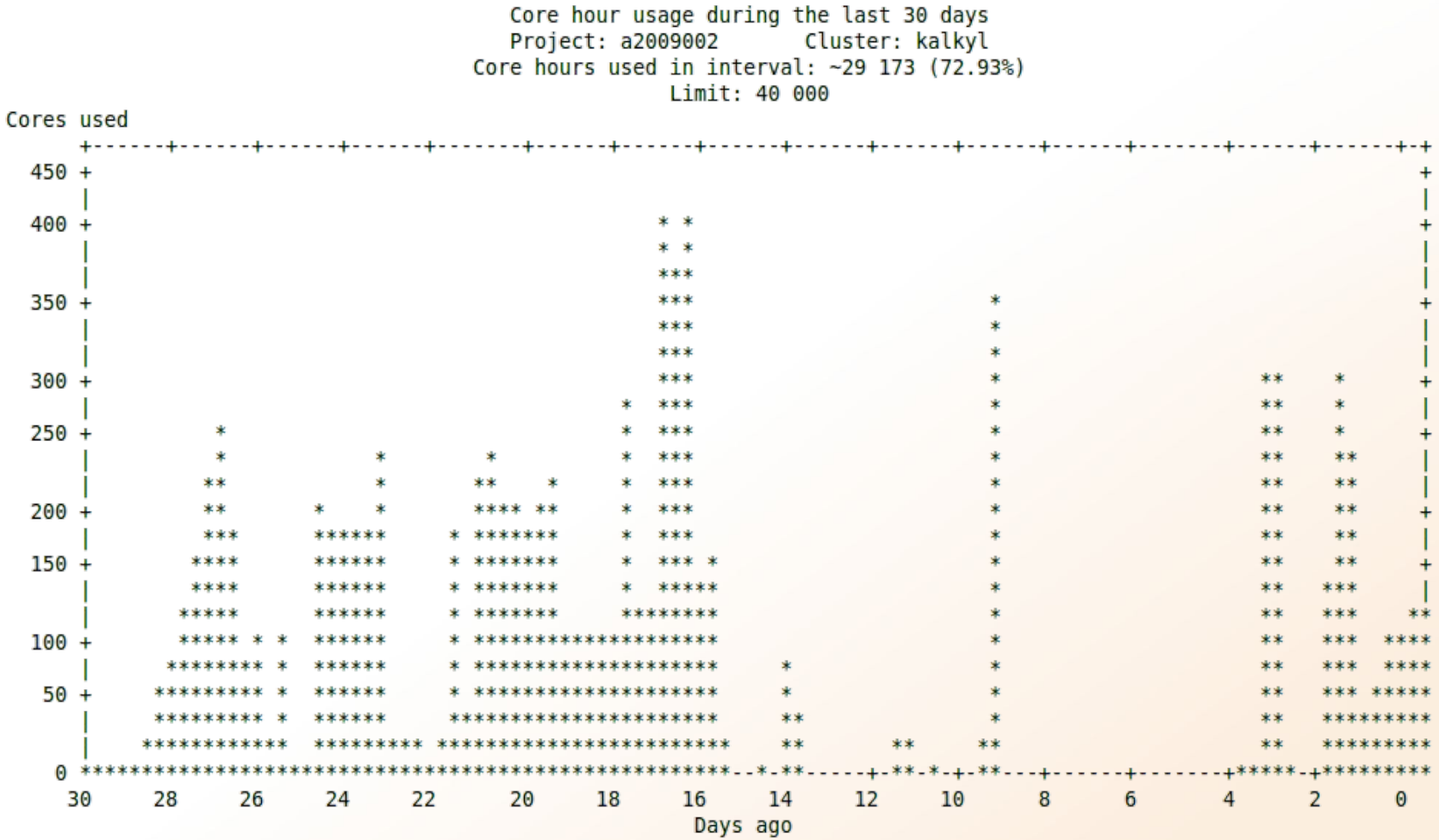
UPPMAX Commands

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)




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

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!!!

UPPMAX Commands

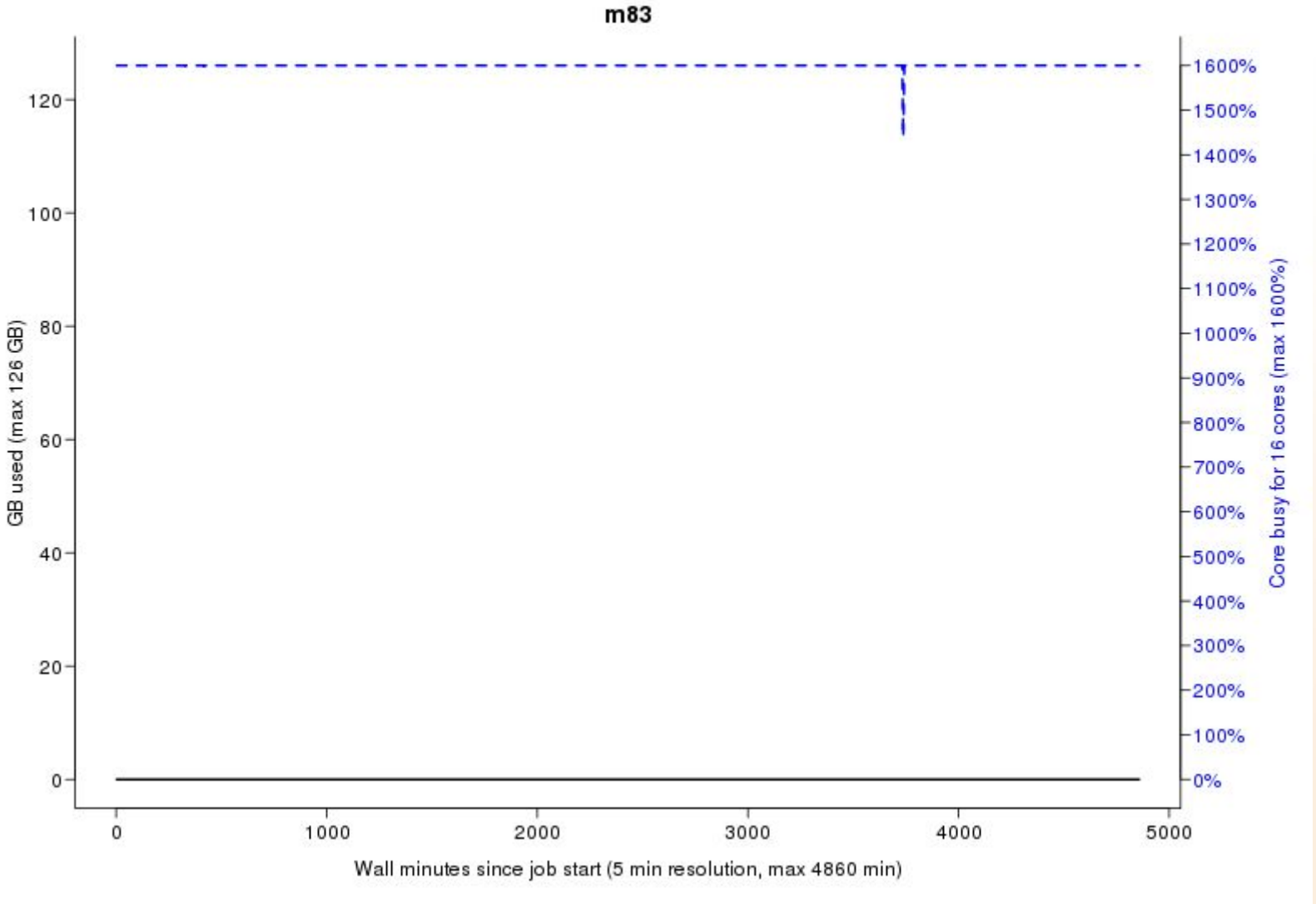
Plot efficiency

jobstats -p -A <projid>

SciI

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

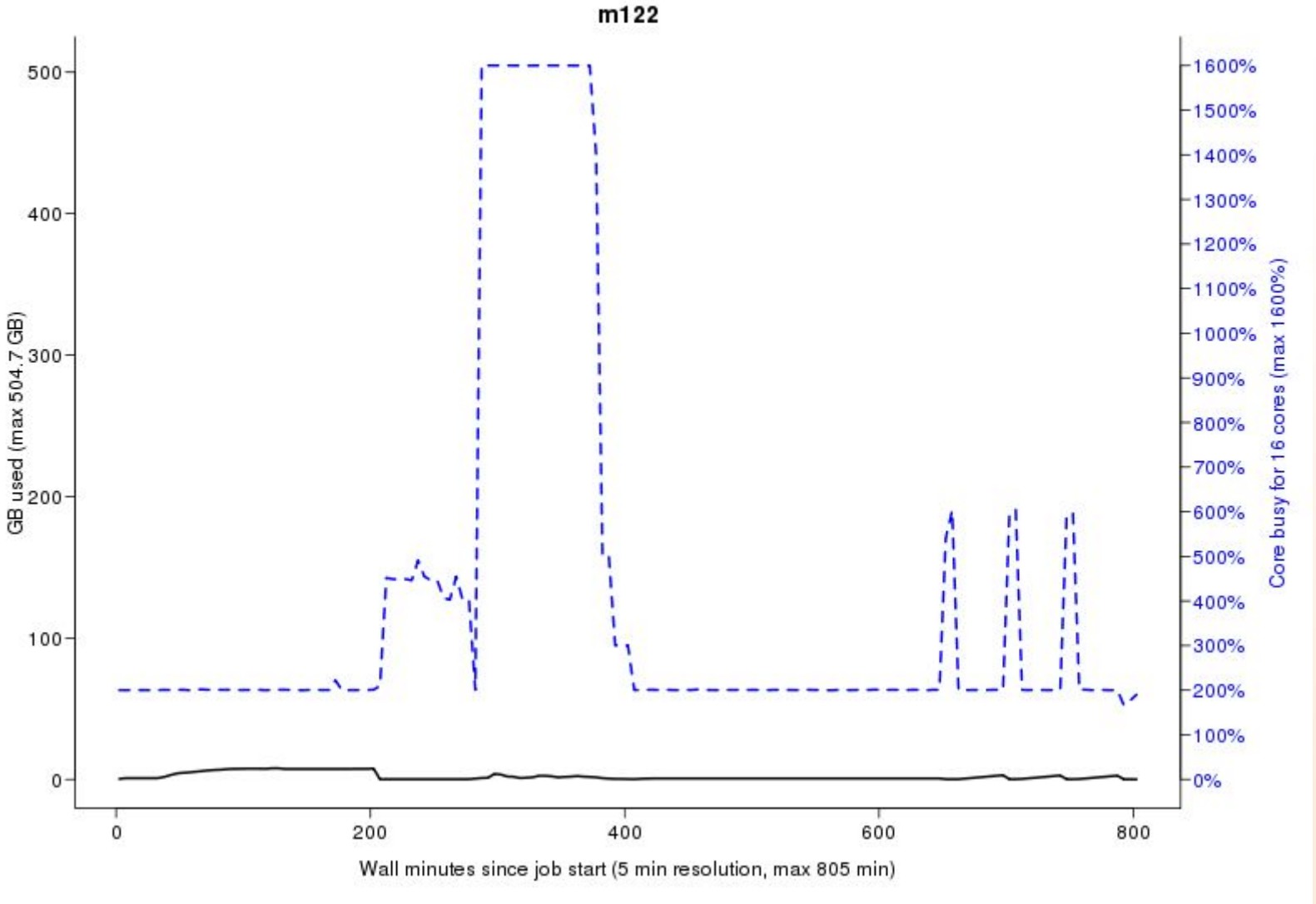
Flags: mem_underused:126:0



SciI

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

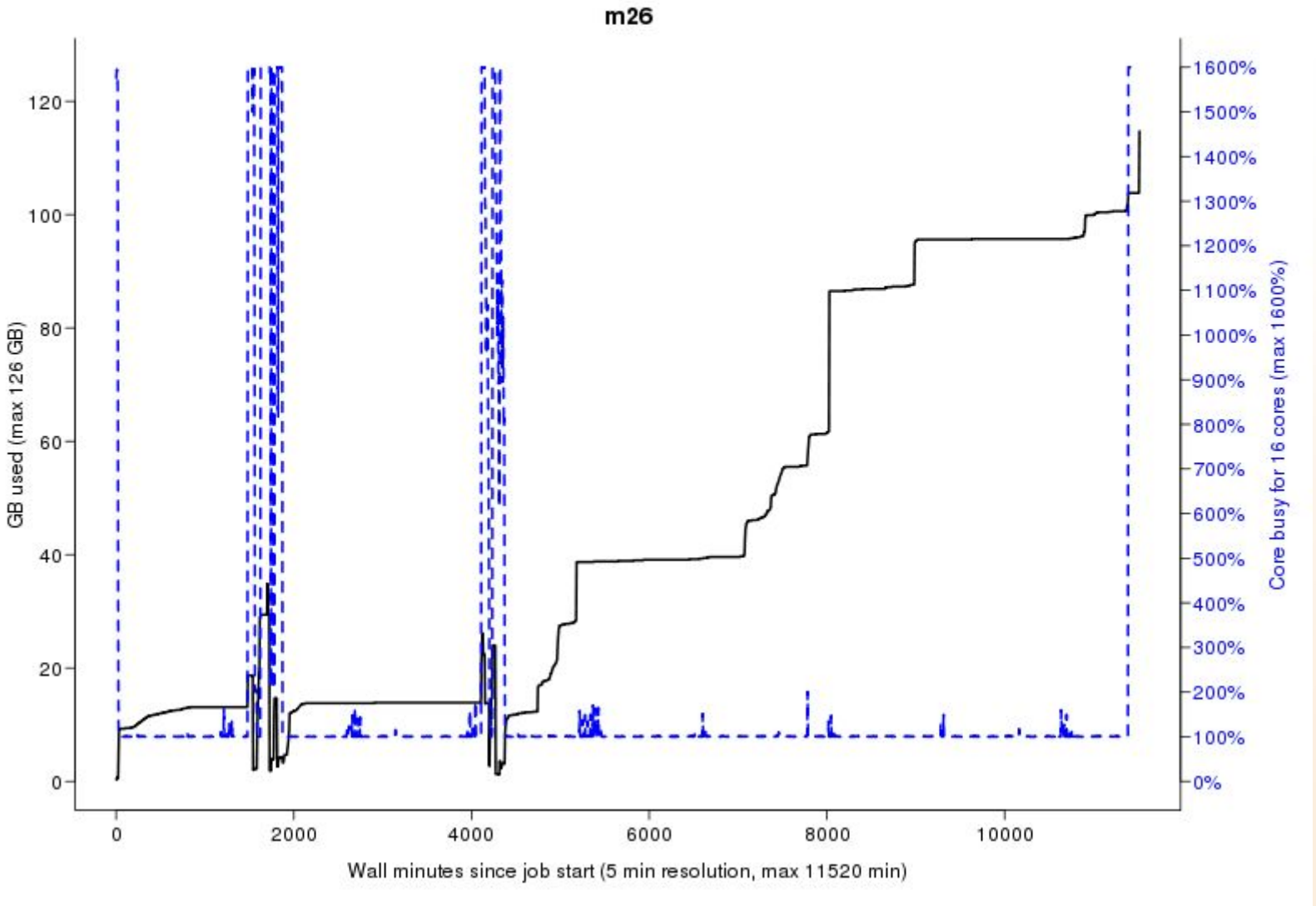
Flags: mem_underused:504.7:7.9 node_type_misbooked:mem512GB:mem128GB



SciI

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

Flags: none



SciLifeLab UPPSALA

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

SciLifeLab
UPPSALA

Laboratory time! (again)