

UPPMAX Introduction

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Enabler for Life Sciences

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, 256 & 1024 GB RAM)
+ **Snowy (old Milou):** ~ 200 nodes à 16 cores (128, 256 & 512 GB RAM)
- **Bianca:** 200 nodes à 16 cores (128, 256 & 512 GB RAM) -
virtual cluster

>12 PB fast parallel **storage**

Bioinformatics **software**

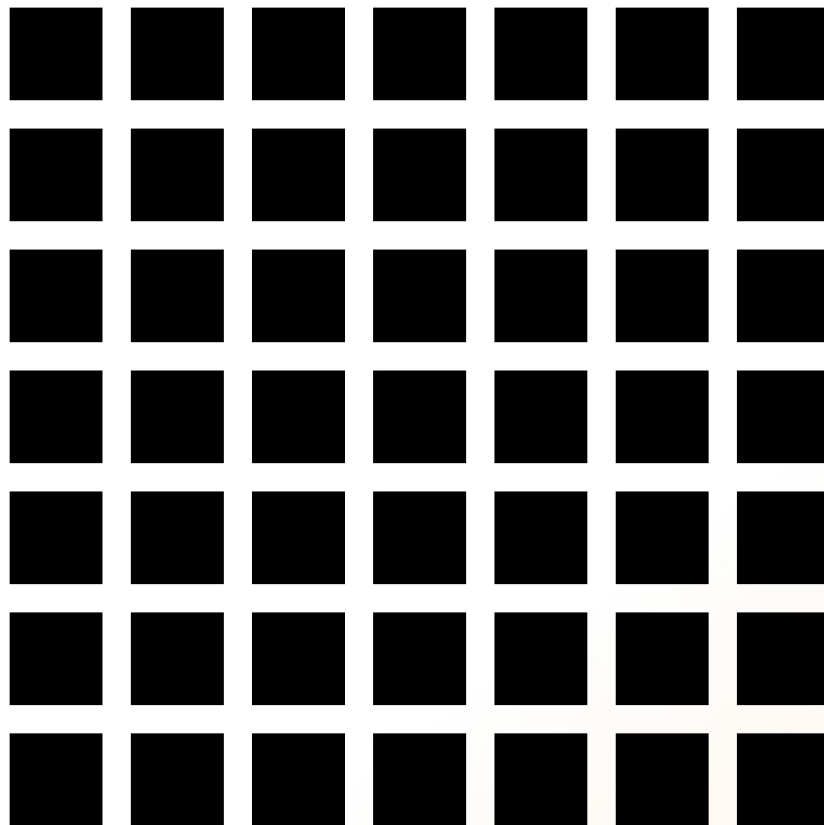
The basic structure of supercomputer

node = computer



Login nodes

The basic structure of supercomputer

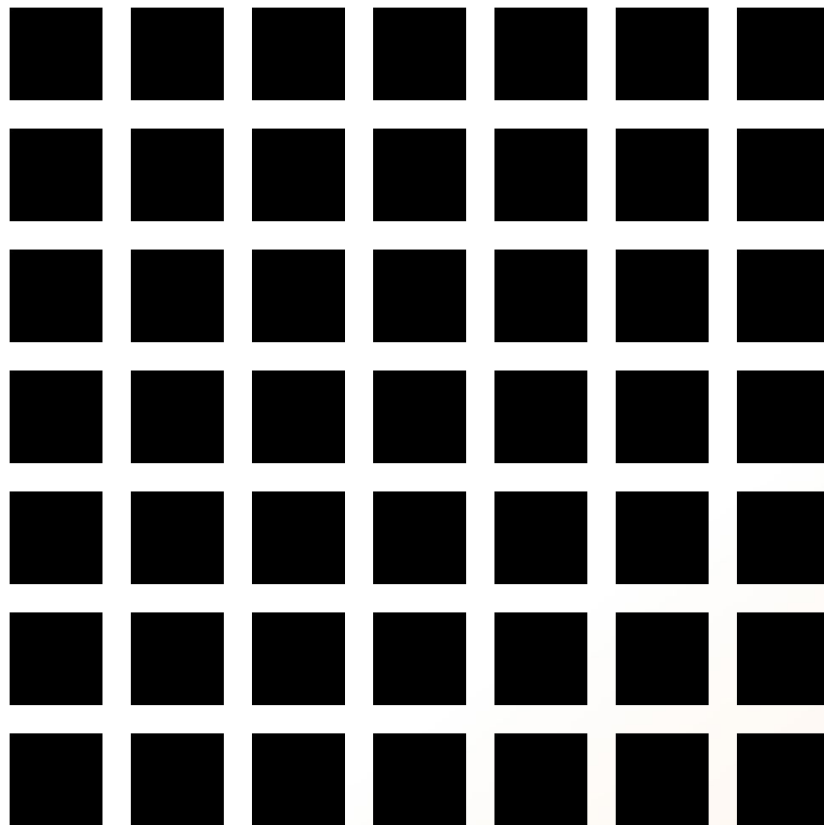


Calculation nodes

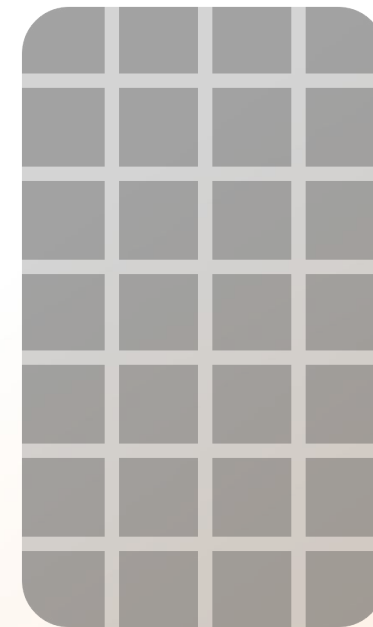


Login nodes

The basic structure of supercomputer



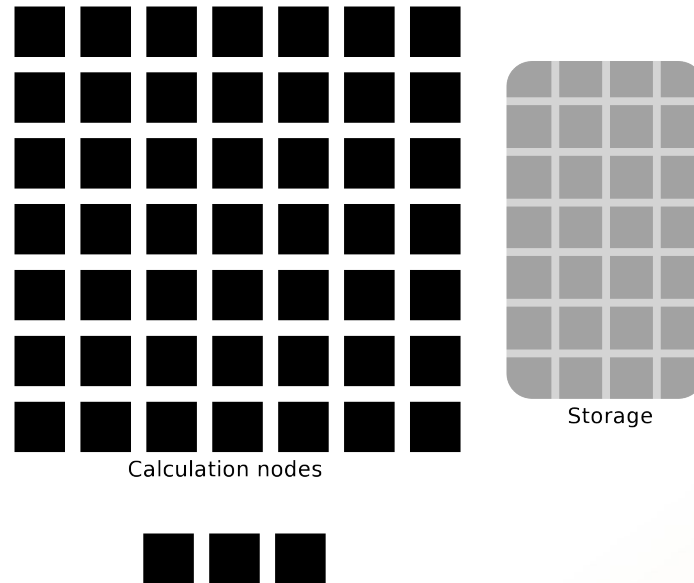
Calculation nodes



Storage



Login nodes



UPPMAX provides

Compute and Storage

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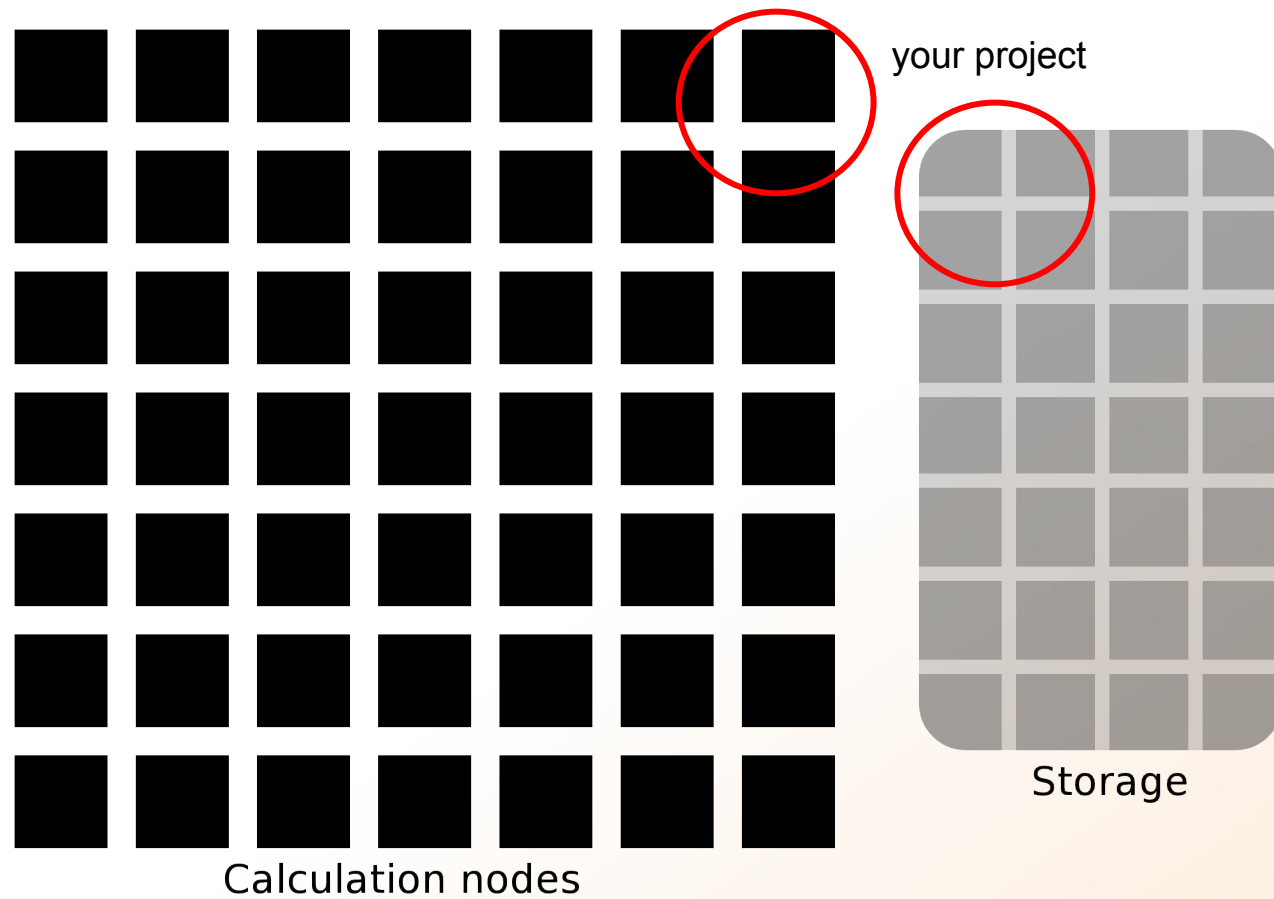
Jobs and queuing systems

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



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

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



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**

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	—



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

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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.

[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
```

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.

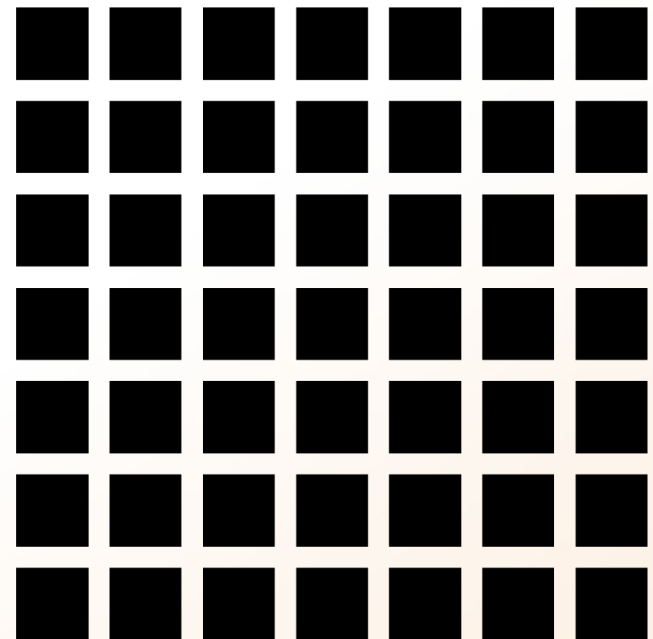
[valent@rackham1 ~]$
```



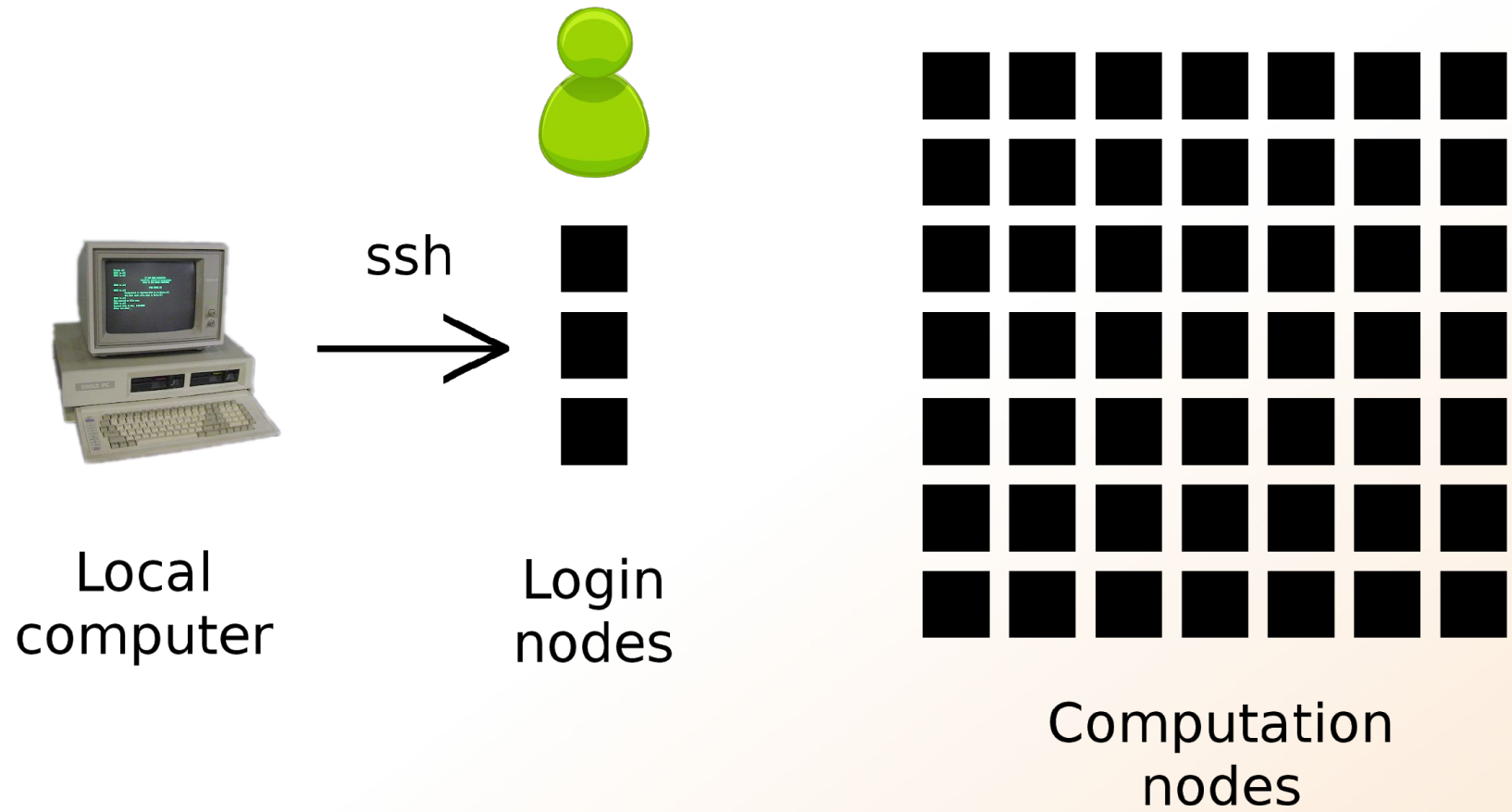
Local
computer



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

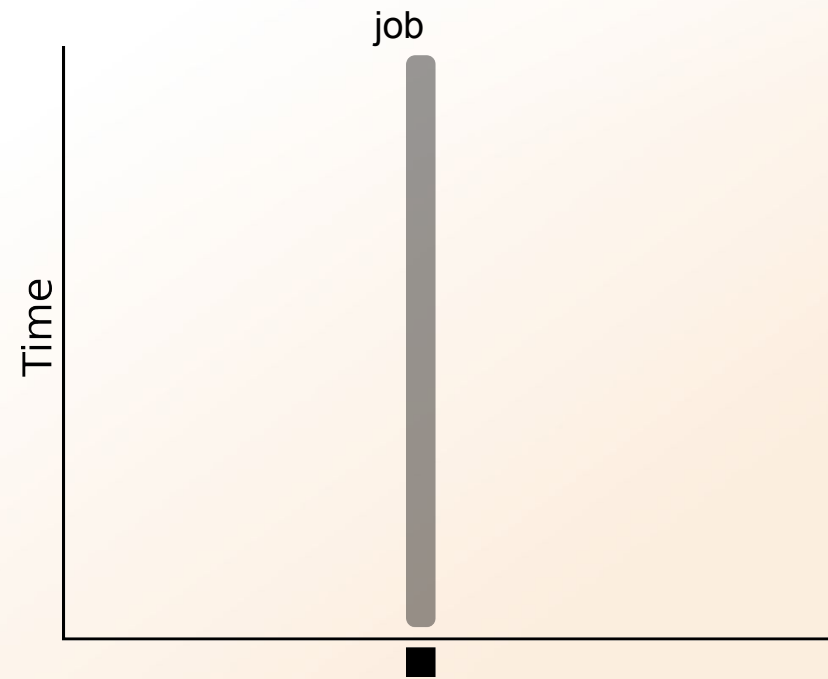
Read/open files

Do something with the data

Print/save output

The basic structure of a supercomputer

Parallel computing!!!
Not one super fast



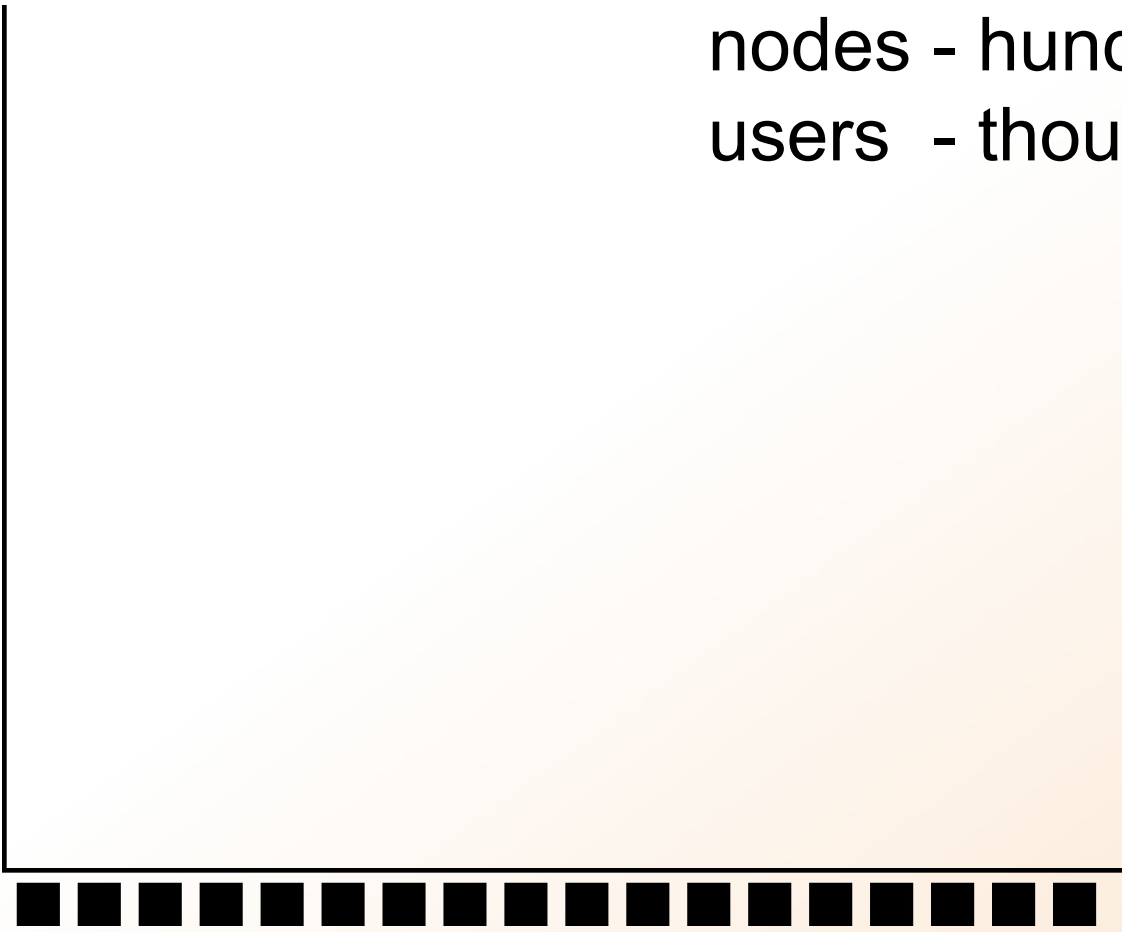
The basic structure of a supercomputer

Parallel computing!!!
Not one super fast



More users than nodes
Need for a queue

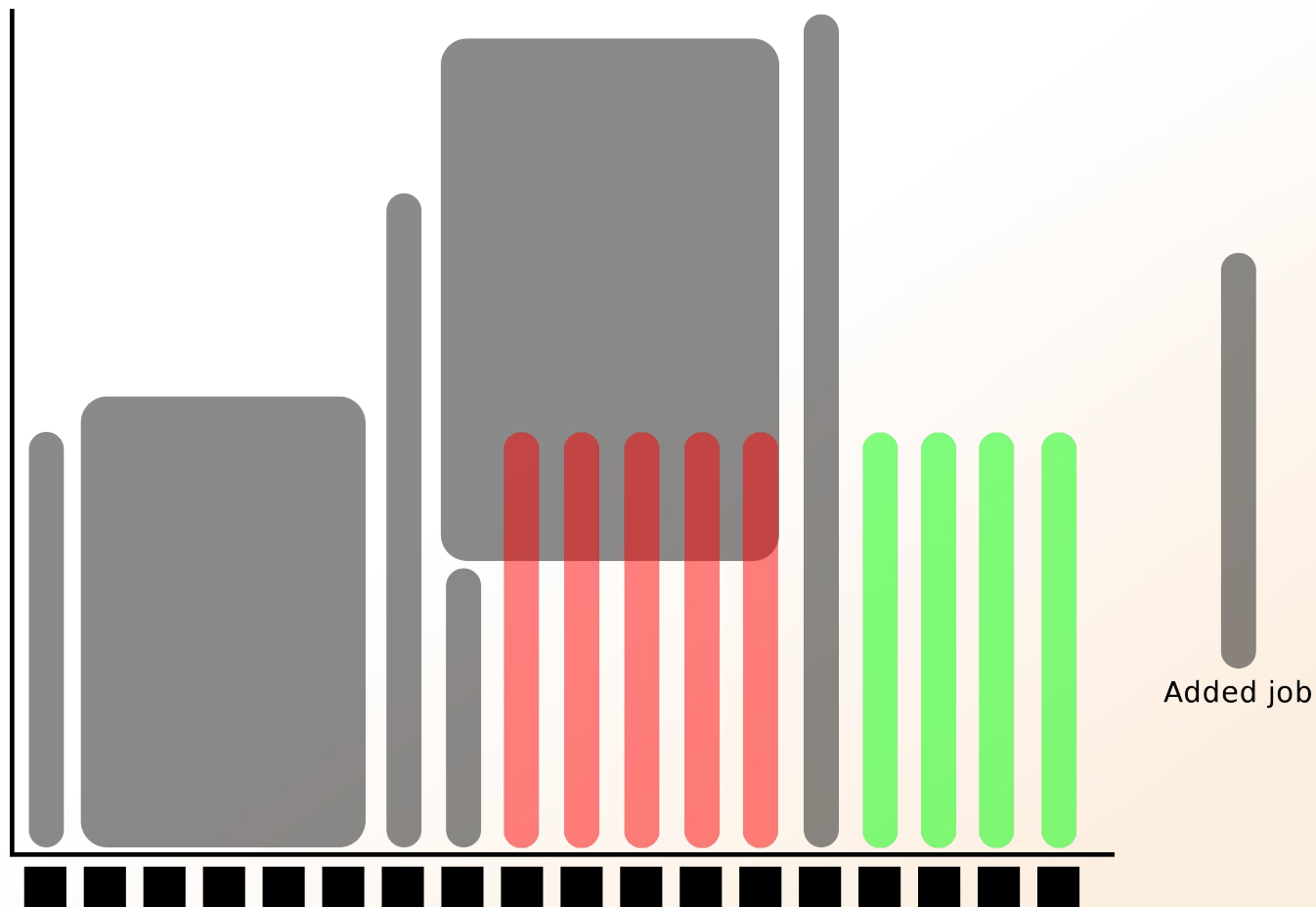
nodes - hundreds
users - thousands



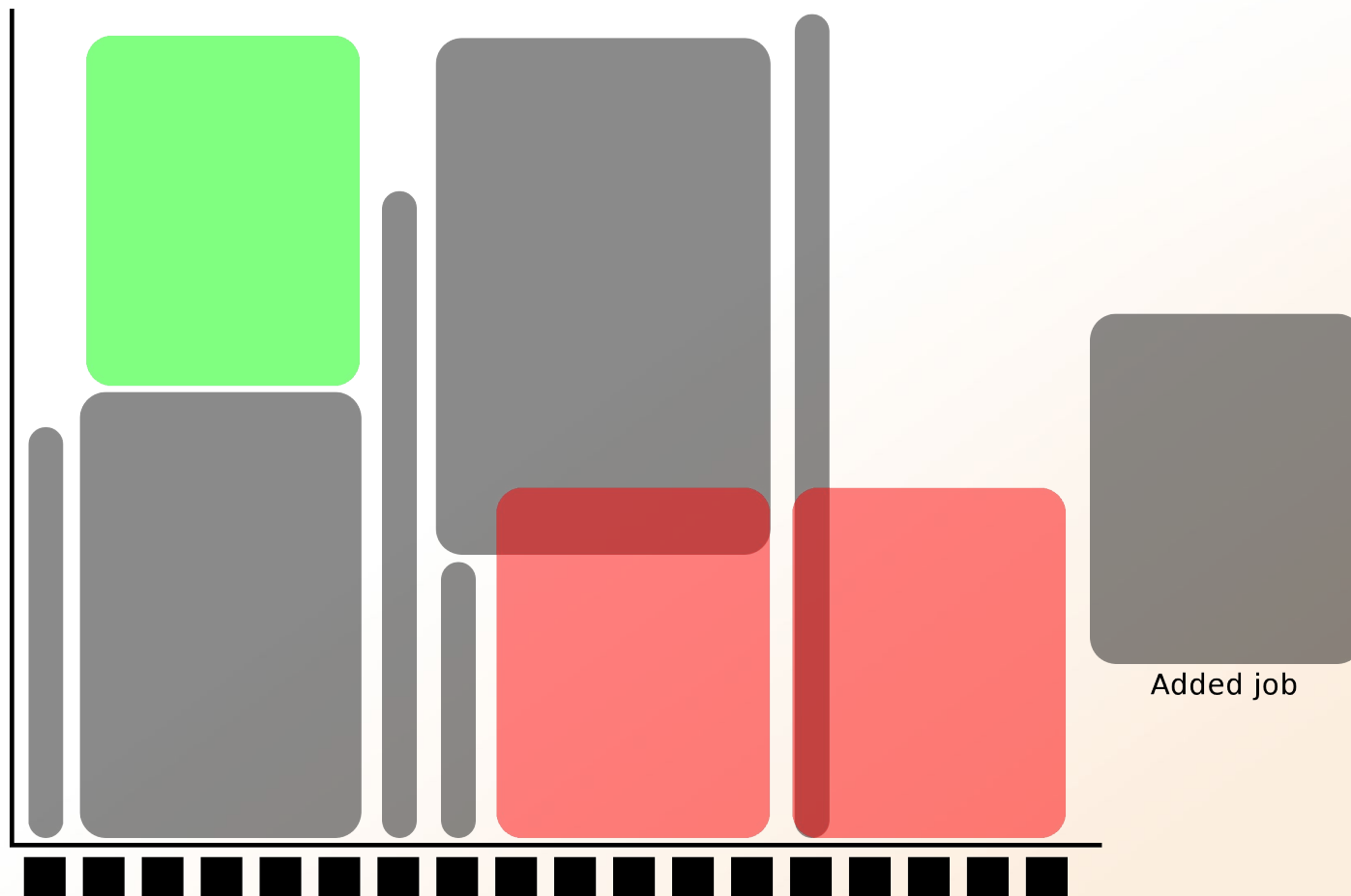
More users than nodes
Need for a queue



More users than nodes
Need for a queue



More users than nodes
Need for a queue



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

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

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 g2018028
you have to be a member

- p** 1 node = 20 cores
1 hour walltime = 20 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

```

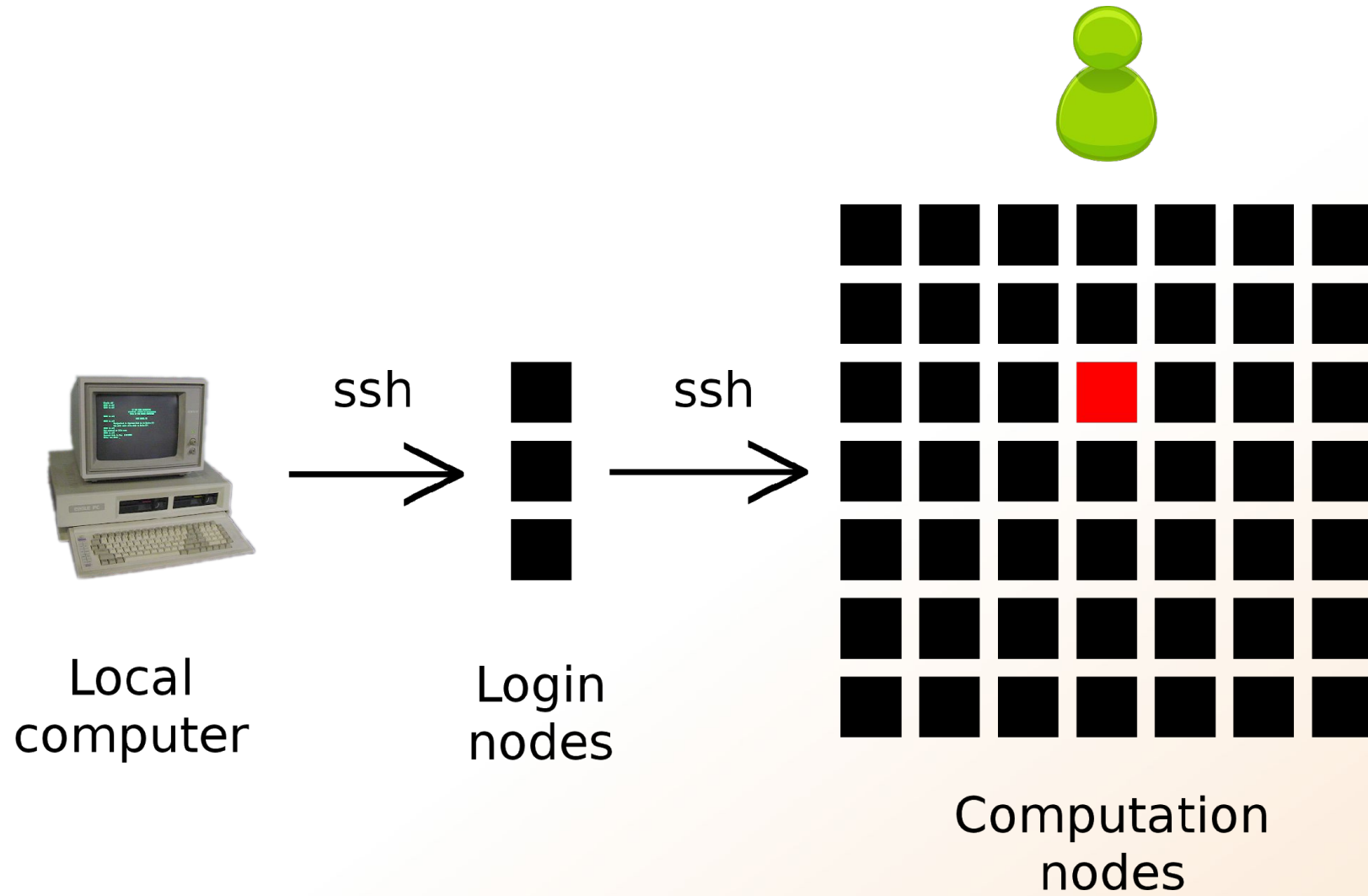
```
#####
```

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```
[valent@m164 ~]$ █
```



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

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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             genomertools/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 -----
concatpillar/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.)
```

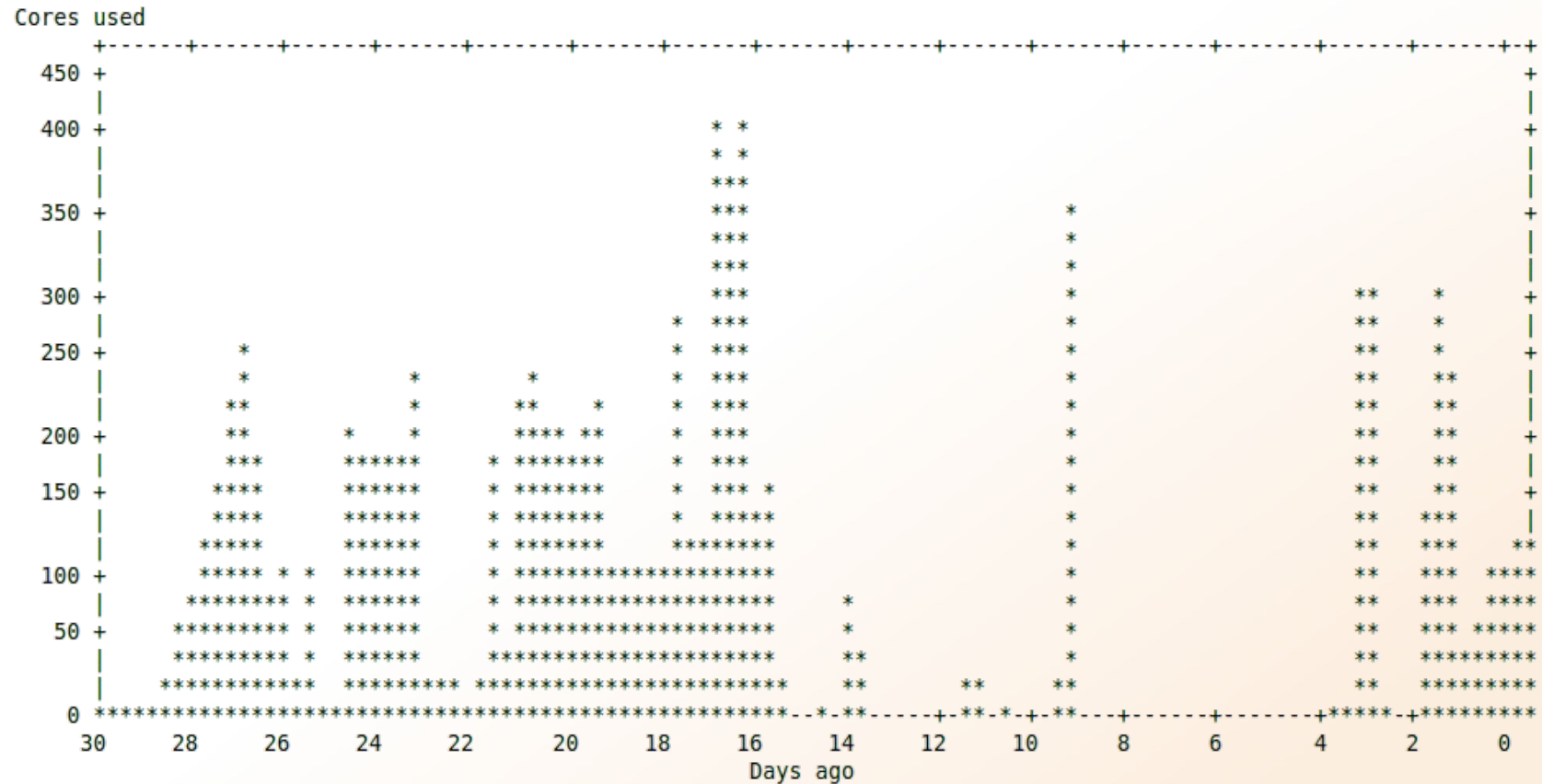
Project User	Used[h]	Current allocation [h/month]
b2010015	1257.20	2000
ameur	1257.20	
b2010069	0.00	2000
b2010074	110.98	2000
dahlo	1.01	
seba	109.97	
b2012044	0.00	2000
g2012005	0.00	2000
g2012083	0.00	2000
g2012157	0.12	2000
dahlo	0.12	

```
[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



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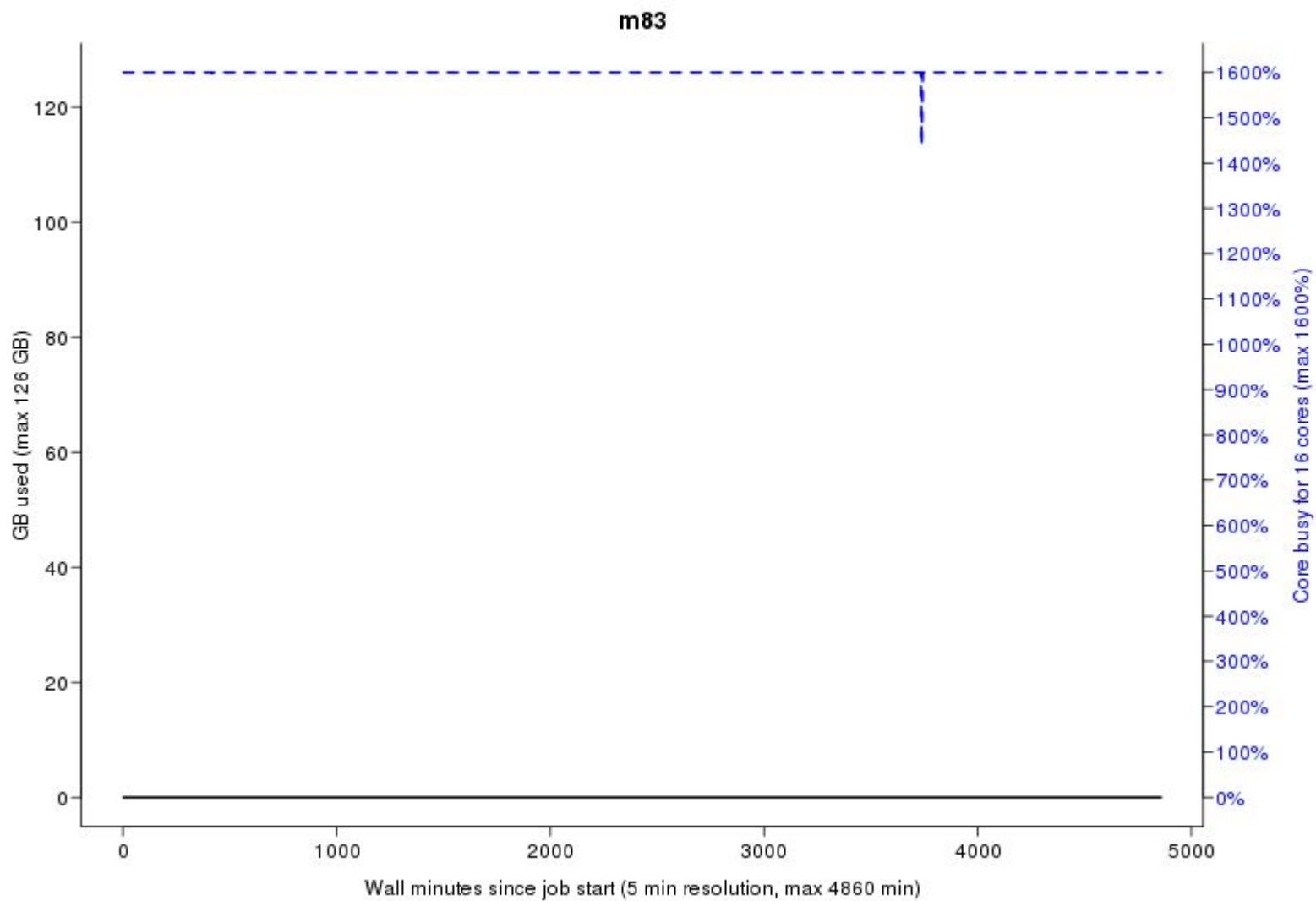
**How to use the resources of UPPMAX in a good way!
Efficiency!!!**

Plot efficiency

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

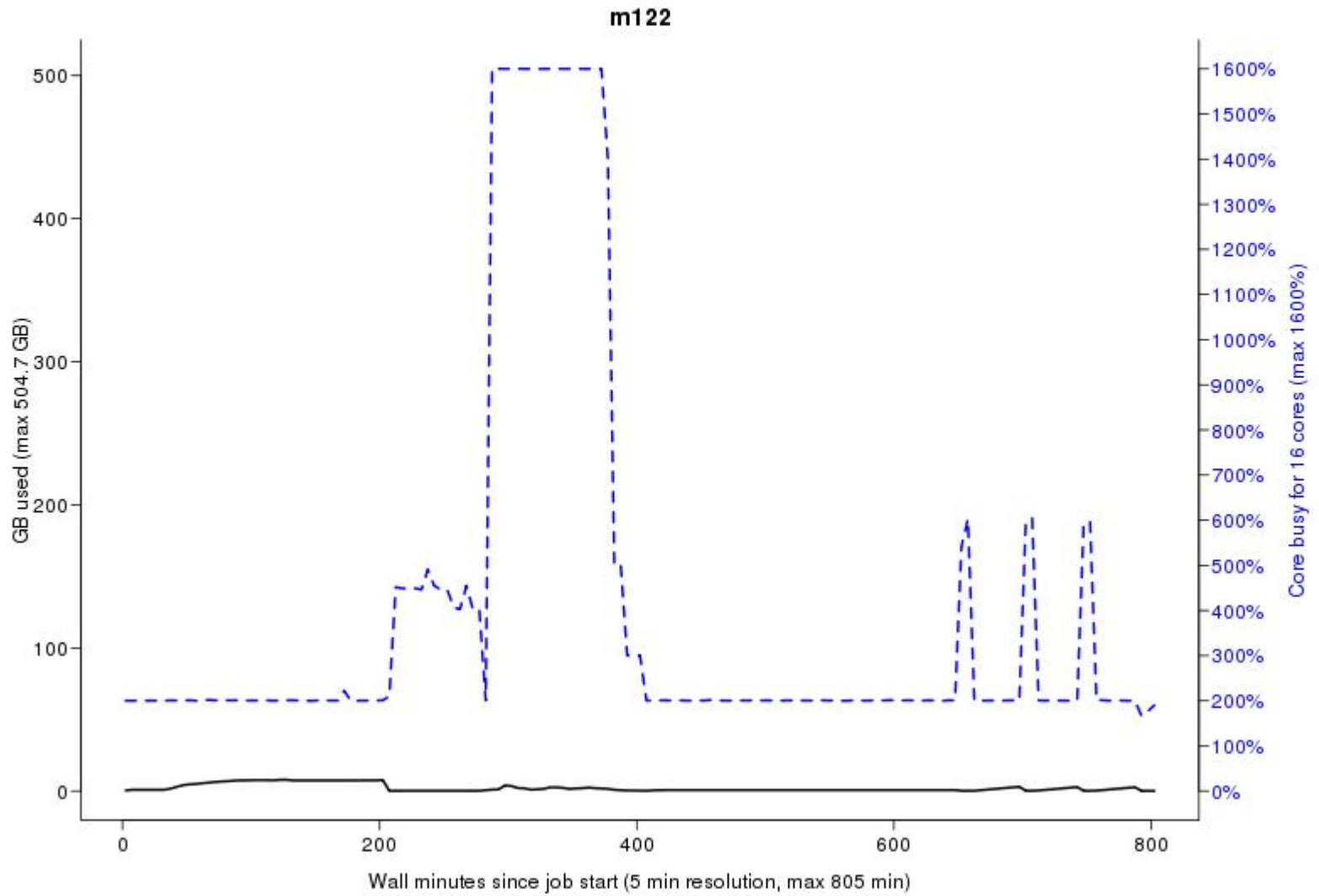
2719328 on 'milou' end: 2014-09-09T08:26:34 runtime: 03-08:59:53

Flags: mem_underused:126:0



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

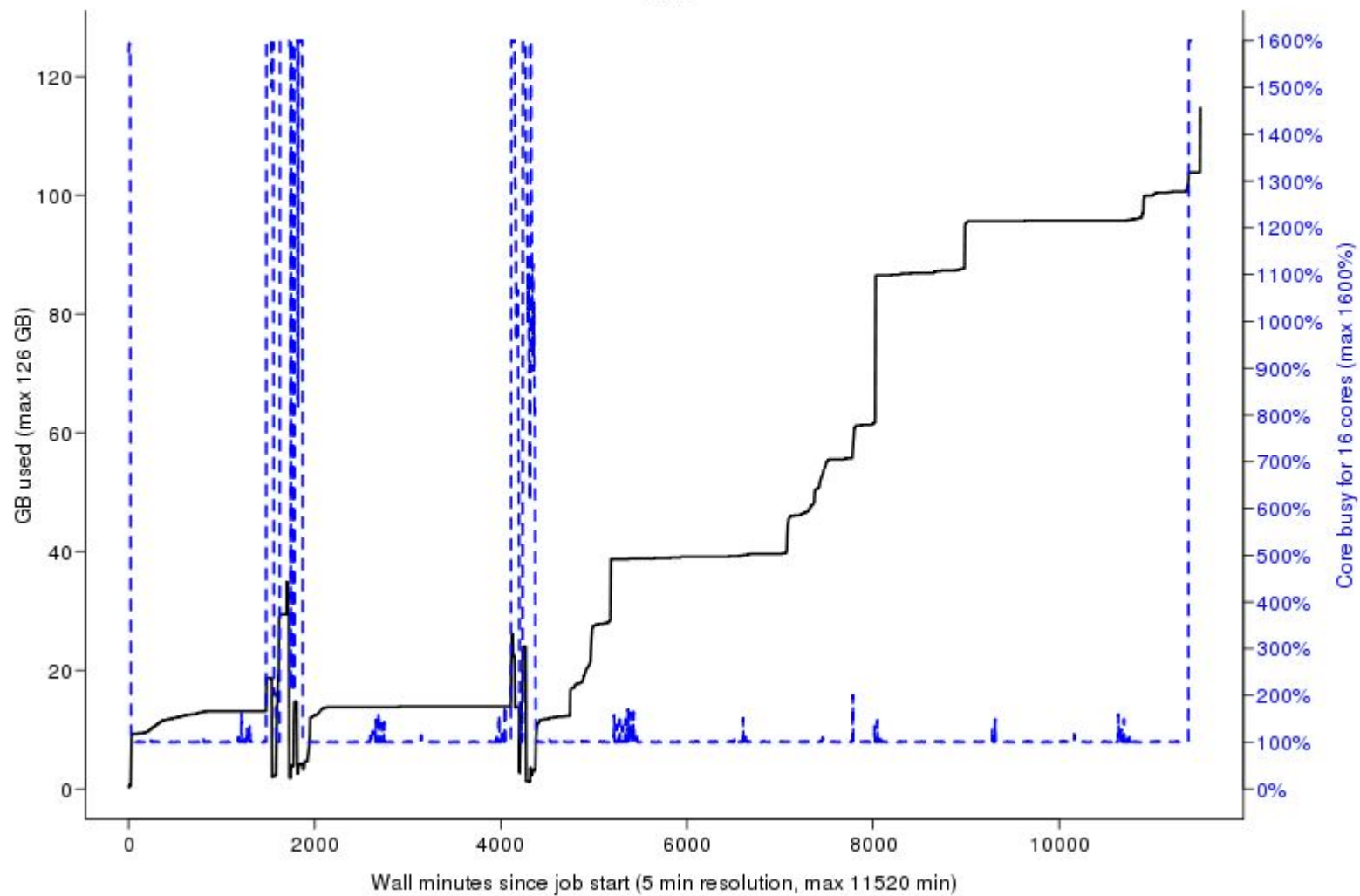
Flags: mem_underused:504.7:7.9 node_type_misbooked:mem512GB:mem128GB



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

Flags: none

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)

<https://scilifelab.github.io/courses/ngsintro/1811/labs/uppmax-intro>