

UPPMAX Introduction

150914
Martin Dahlö
martin.dahlo@scilifelab.uu.se

Enabler for Life Sciences

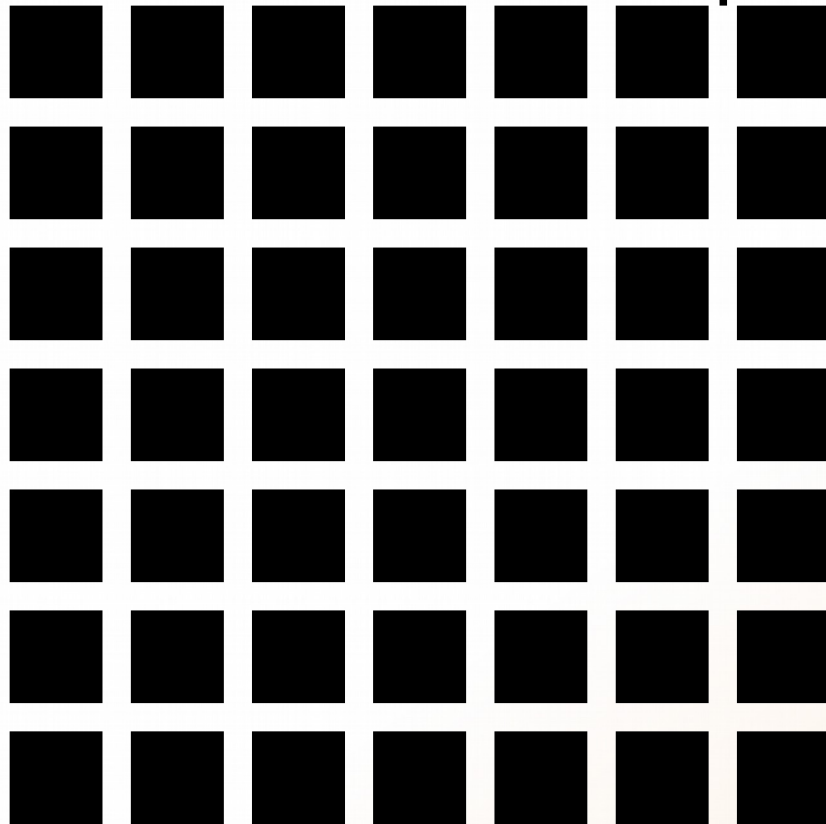
- Uppsala Multidisciplinary Center for Advanced Computational Science
- <http://www.uppmax.uu.se>
- 2 clusters
 - Tintin, 160 computer à 16 cores (64GB RAM)
 - Milou, 208 computers à 16 cores (128GB RAM)
 - 17 with 256, 17 with 512
- 1 high memory machine à 64 cores, 2TB RAM
- ~7 PB fast parallel storage

- The basic structure of supercomputer



Login nodes

- The basic structure of supercomputer

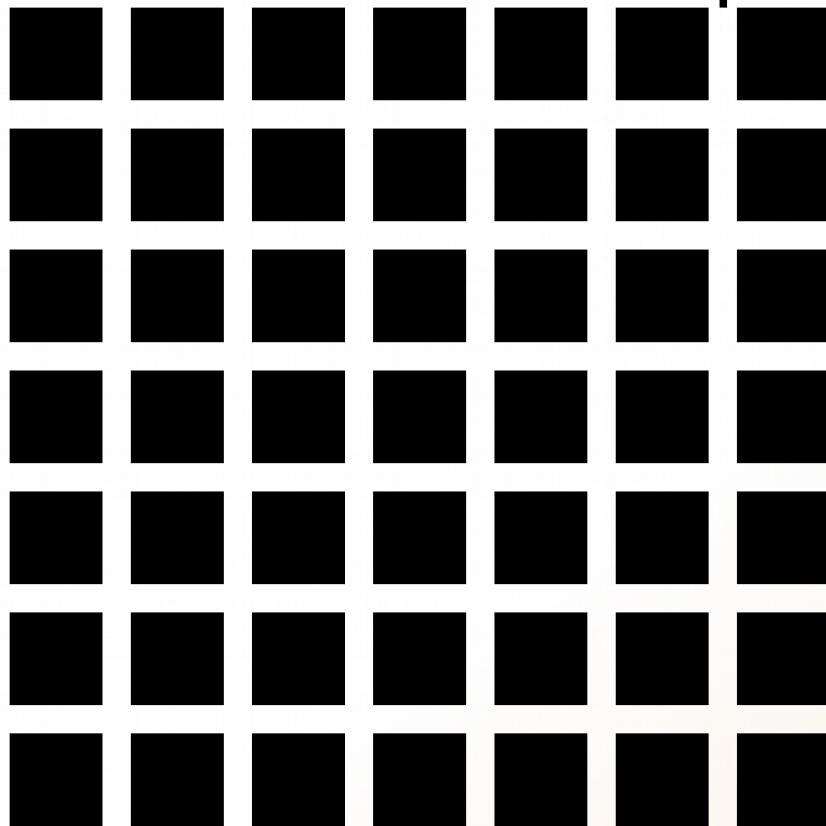


Calculation nodes

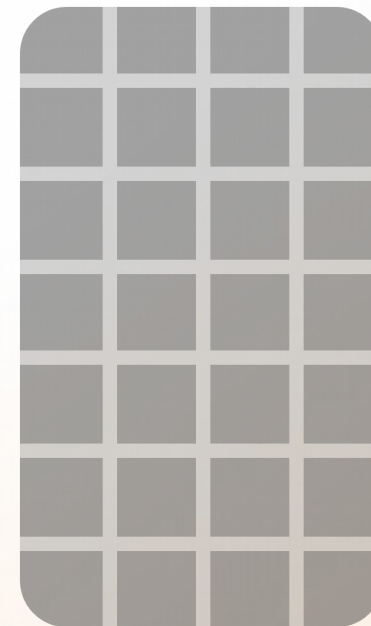


Login nodes

- The basic structure of supercomputer



Calculation nodes

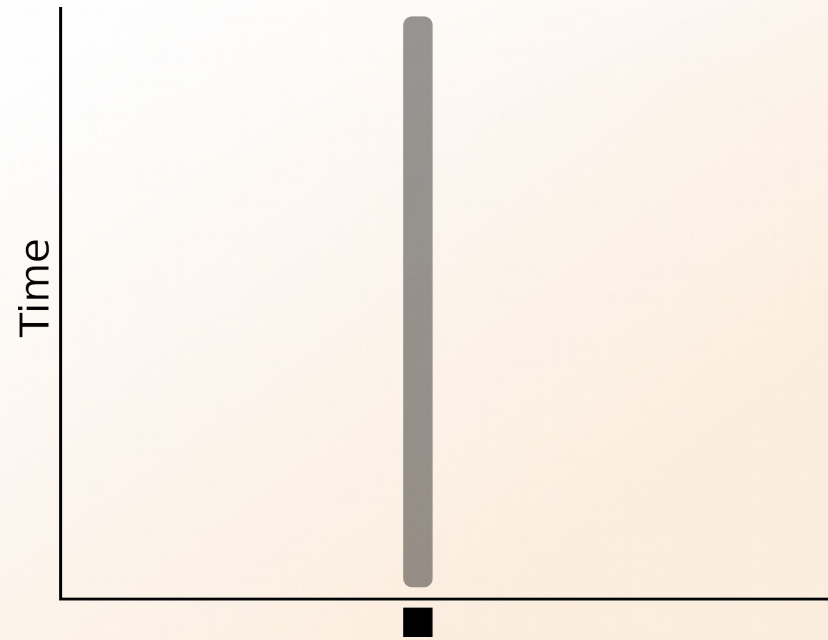


Storage



Login nodes

- The basic structure of a supercomputer
- Parallel computing is key
 - Not one super fast



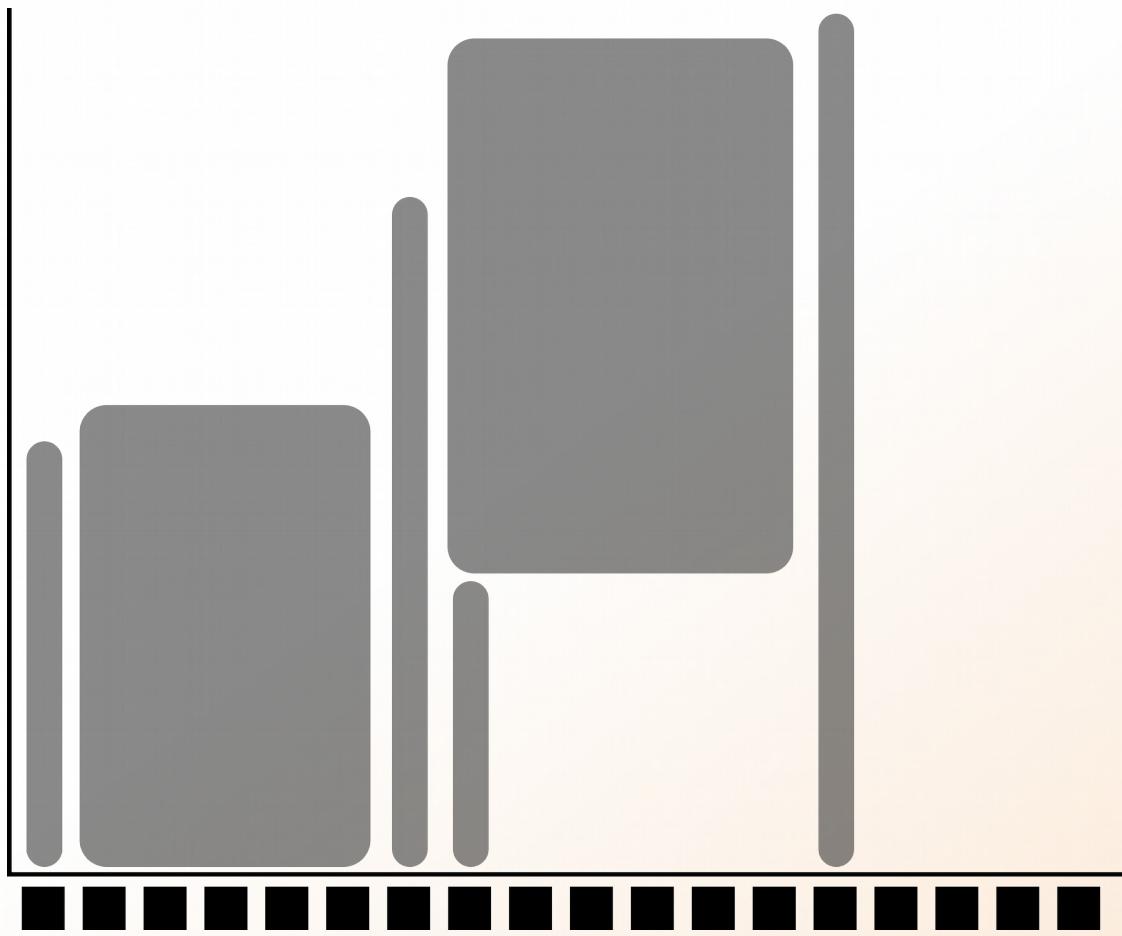
- The basic structure of a supercomputer
- Parallel computing is key
 - Not one super fast



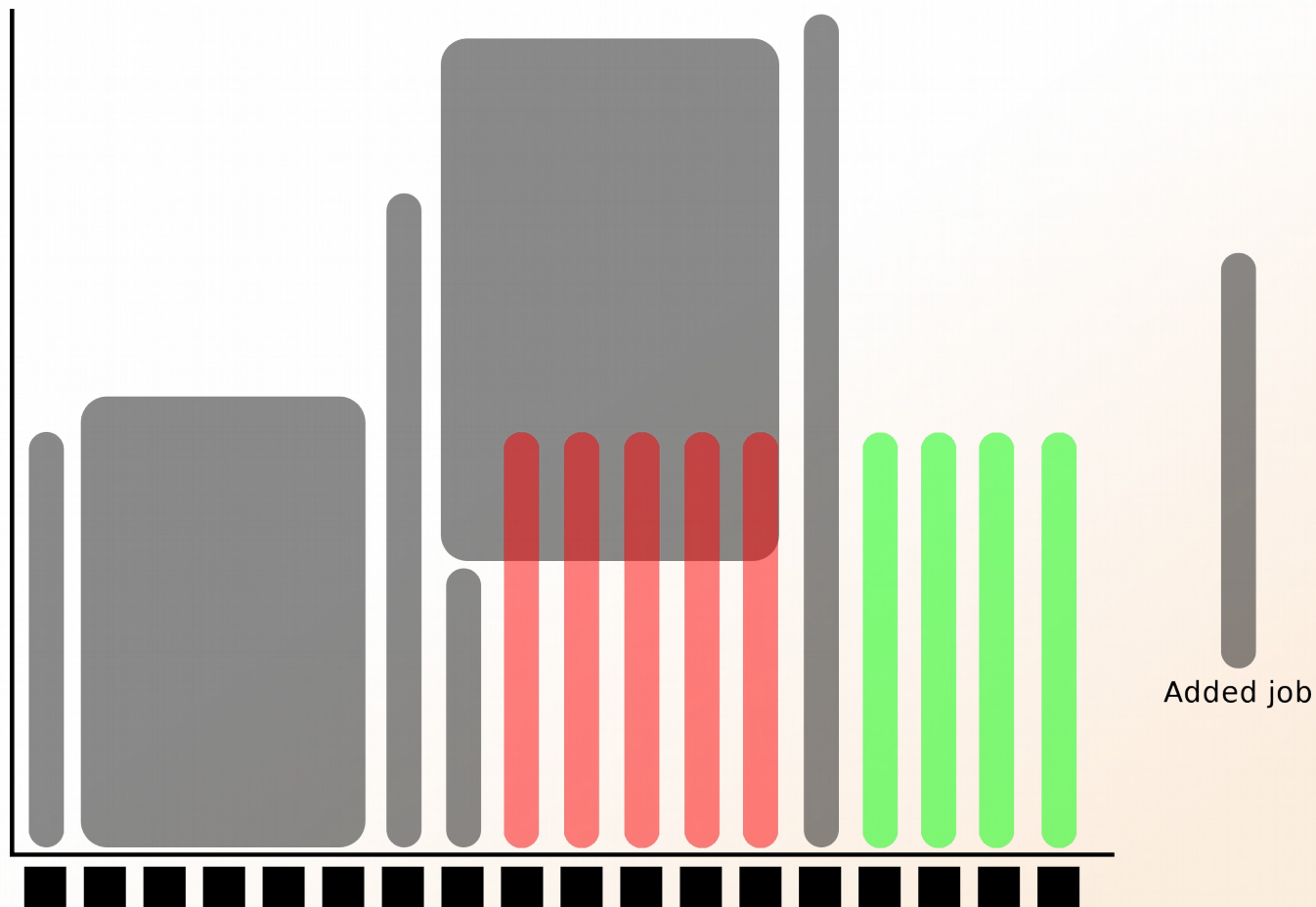
- More users than nodes
 - Need for a queue



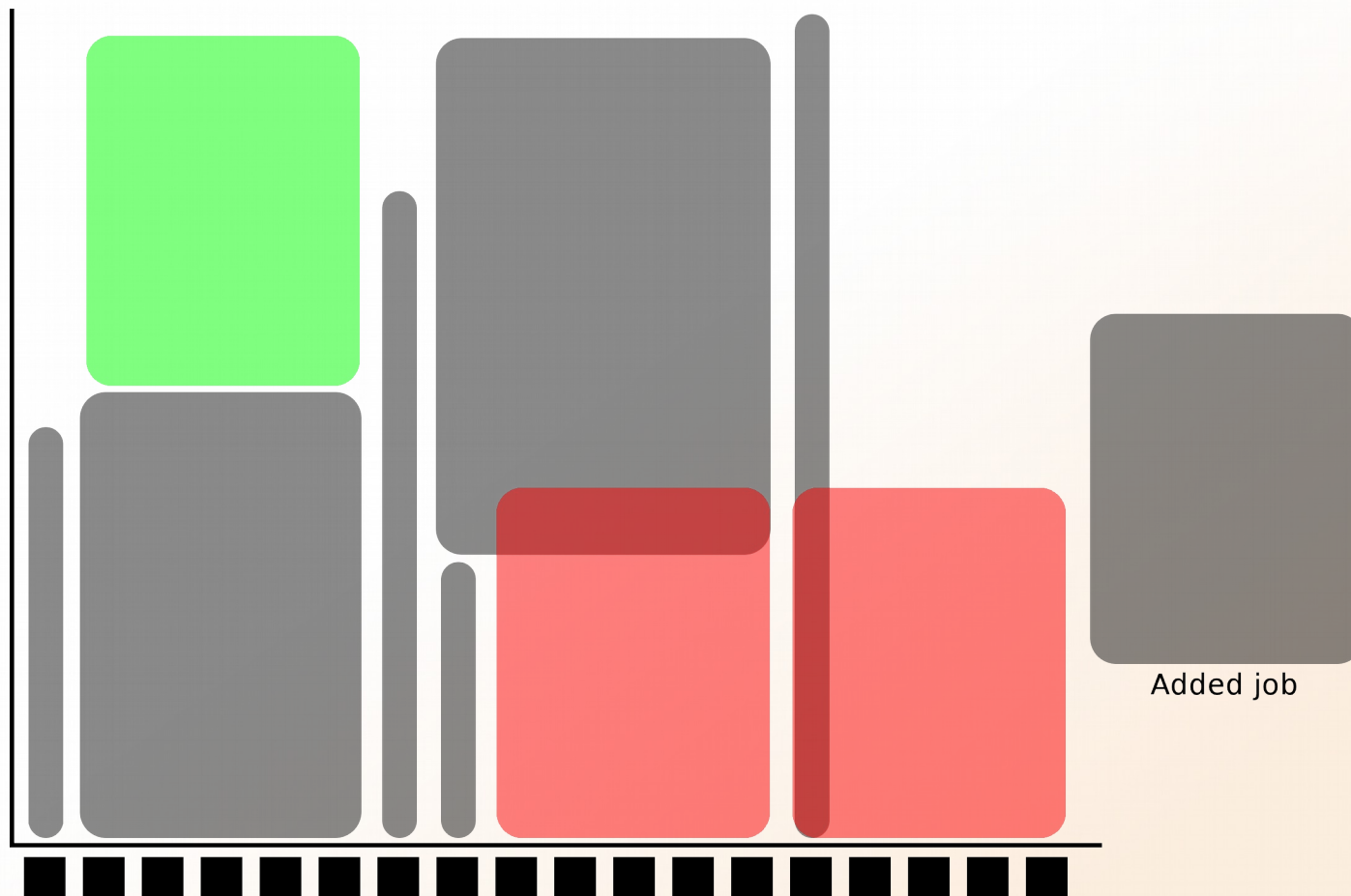
- More users than nodes
 - Need for a queue



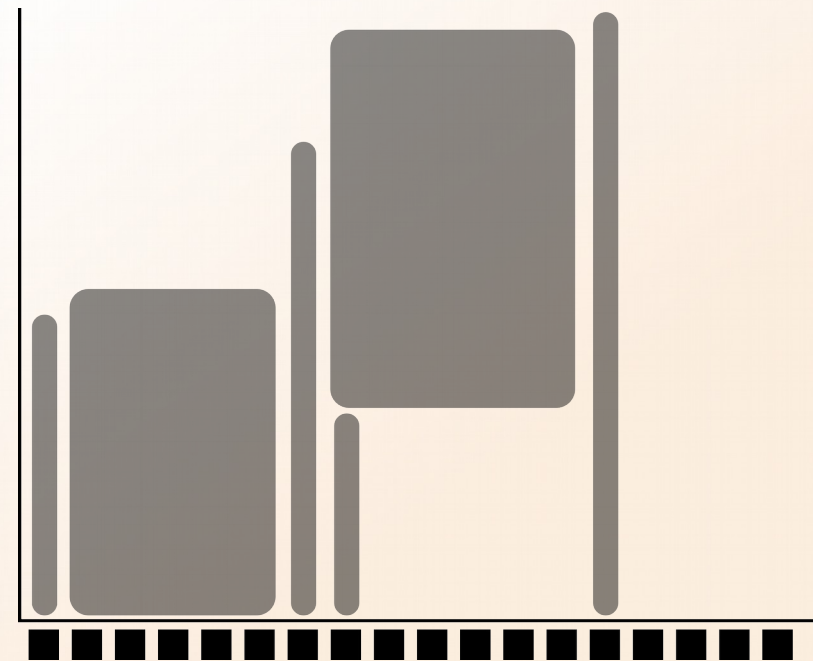
- More users than nodes
 - Need for a queue



- More users than nodes
 - Need for a queue



- 1 mandatory setting for jobs:
 - Who pays for it? (-A)
- 3 settings you really should set: (default values NOT good)
 - Where should it run? (-p)
 - (How wide is it? (-n))
 - How long is it? (-t)

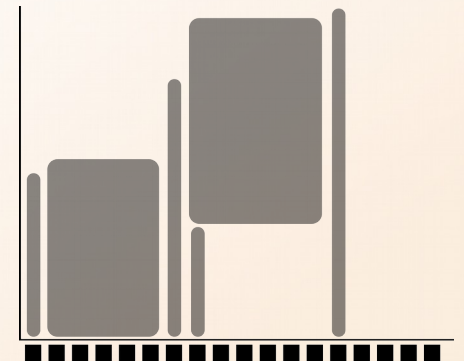


- Who pays for it? (-A)
 - Only projects can be charged
 - You have to be a member
 - This course's project ID: g2015031
- -A = account (the account you charge)
 - No default value, mandatory

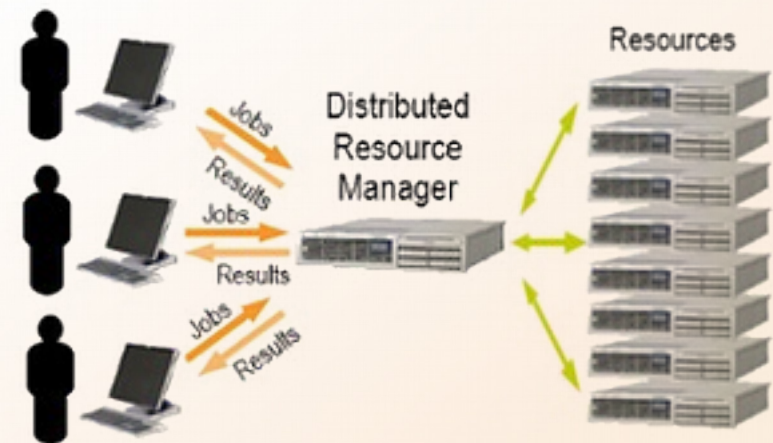
- Where should it run? (-p)
 - Use a whole node or just part of it?
 - 1 node = 16 cores
 - 1 hour walltime = 16 core hours = expensive
 - Waste of resources
 - Default project size: 2000 core hours
- -p = partition (node or core)
 - Default value: core

- How wide is it? (-n)
 - How much of the node should be booked?
 - 1 node = 16 cores
 - Any number of cores
 - 1, 2, 5, 13, 15 etc
- -n = number of cores
 - Default value: 1
 - Usually used together with -p core

- How long is it? (-t)
 - Always overestimate ~50%
 - Jobs killed when timelimit reached
 - Only charged for time used
- -t = time (hh:mm:ss)
 - 78:00:00 or 3-6:00:00
 - Default value: 7-00:00:00



- Job = what happen during the booked time
 - Script file
 - Start programs
 - Move files
 - and more



- How to submit a job
 - Write a script (bash)
 - Queue options
 - Rest of the 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!
```

- How to submit a job
 - Write a script (bash)
 - Queue options
 - Rest of the 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
```

- How to submit a job
 - Script written, now what?

```
[dahlo@kalkyl1 temp]$ ls -l
total 16
-rw-r--r-- 1 dahlo uppmax 169 Jan 28 15:45 test.sbatch
[dahlo@kalkyl1 temp]$ cat test.sbatch
#!/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!"
[dahlo@kalkyl1 temp]$ sbatch test.sbatch
Submitted batch job 1745244
[dahlo@kalkyl1 temp]$
```

- Prints to a file instead of terminal
 - slurm-<job id>.out

```
[dahlo@biologin glob]$ ll
total 16
-rw-r--r-- 1 dahlo uppmx 1025 Sep 22 19:46 my_script.sb
[dahlo@biologin glob]$
```

- Prints to a file instead of terminal
 - slurm-<job id>.out

```
[dahlo@biologin glob]$ ll
total 16
-rw-r--r-- 1 dahlo uppmx 1025 Sep 22 19:46 my_script.sb
[dahlo@biologin glob]$
[dahlo@biologin glob]$ sbatch my_script.sb
Submitted batch job 2226951
[dahlo@biologin glob]$
[dahlo@biologin glob]$ ll
total 32
-rw-r--r-- 1 dahlo uppmx 1025 Sep 22 19:46 my_script.sb
-rw-r--r-- 1 dahlo uppmx   87 Sep 22 19:56 slurm-2226951.out
[dahlo@biologin glob]$
```

- Prints to a file instead of terminal
 - slurm-<job id>.out

```
[dahlo@biologin glob]$ ll
total 16
-rw-r--r-- 1 dahlo uppmx 1025 Sep 22 19:46 my_script.sb
[dahlo@biologin glob]$
[dahlo@biologin glob]$ sbatch my_script.sb
Submitted batch job 2226951
[dahlo@biologin glob]$
[dahlo@biologin glob]$ ll
total 32
-rw-r--r-- 1 dahlo uppmx 1025 Sep 22 19:46 my_script.sb
-rw-r--r-- 1 dahlo uppmx   87 Sep 22 19:56 slurm-2226951.out
[dahlo@biologin glob]$
[dahlo@biologin glob]$ cat slurm-2226951.out
Example of error with line number and message
slurm script: 40: An error has occurred.
[dahlo@biologin glob]$
```


- Shows information about your jobs

`queue -u <user>`

```
[dahlo@kalkyl4 work]$ queue -u dahlo
  JOBID PARTITION   NAME     USER  ST      TIME  NODES NODELIST(REASON)
2215978      core   My_job   dahlo  PD      0:00      1 (Resources)
[dahlo@kalkyl4 work]$
```

- Shows information about your jobs

`queue -u <user>`

```
[dahlo@kalkyl4 work]$ queue -u dahlo
  JOBID PARTITION   NAME     USER  ST      TIME  NODES NODELIST(REASON)
2215978     core  My job   dahlo  R      0:13     1 q148
[dahlo@kalkyl4 work]$
```

- Shows information about your jobs

`queue -u <user>`

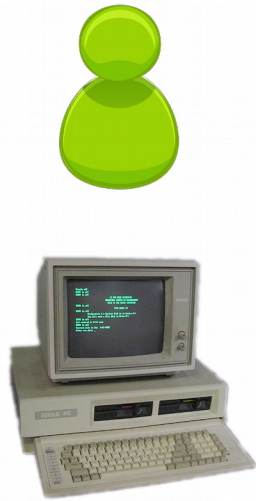
```
[dahlo@kalkyl4 work]$ queue -u dahlo
  JOBID PARTITION   NAME     USER  ST      TIME  NODES NODELIST(REASON)
 2215978      core  My job   dahlo  R       0:13     1 q148
[dahlo@kalkyl4 work]$
```

- `jobinfo -u <user>`

- Connects to a node

ssh -X <node name>

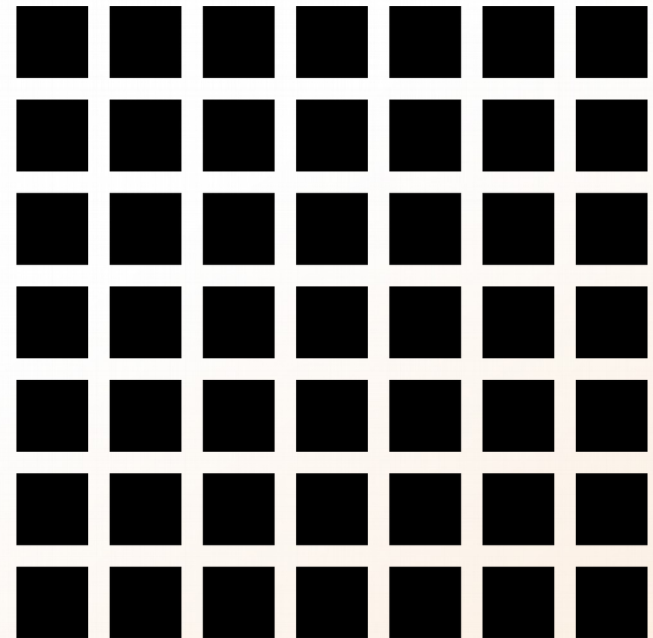
```
[dahlo@kalkyl4 work]$ queue -u dahlo
  JOBID PARTITION   NAME     USER  ST      TIME  NODES NODELIST(REASON)
2215978     core  My_job   dahlo  R       0:13     1 q148
[dahlo@kalkyl4 work]$
[dahlo@kalkyl4 work]$ ssh -X q148
[dahlo@q148 work]$
```



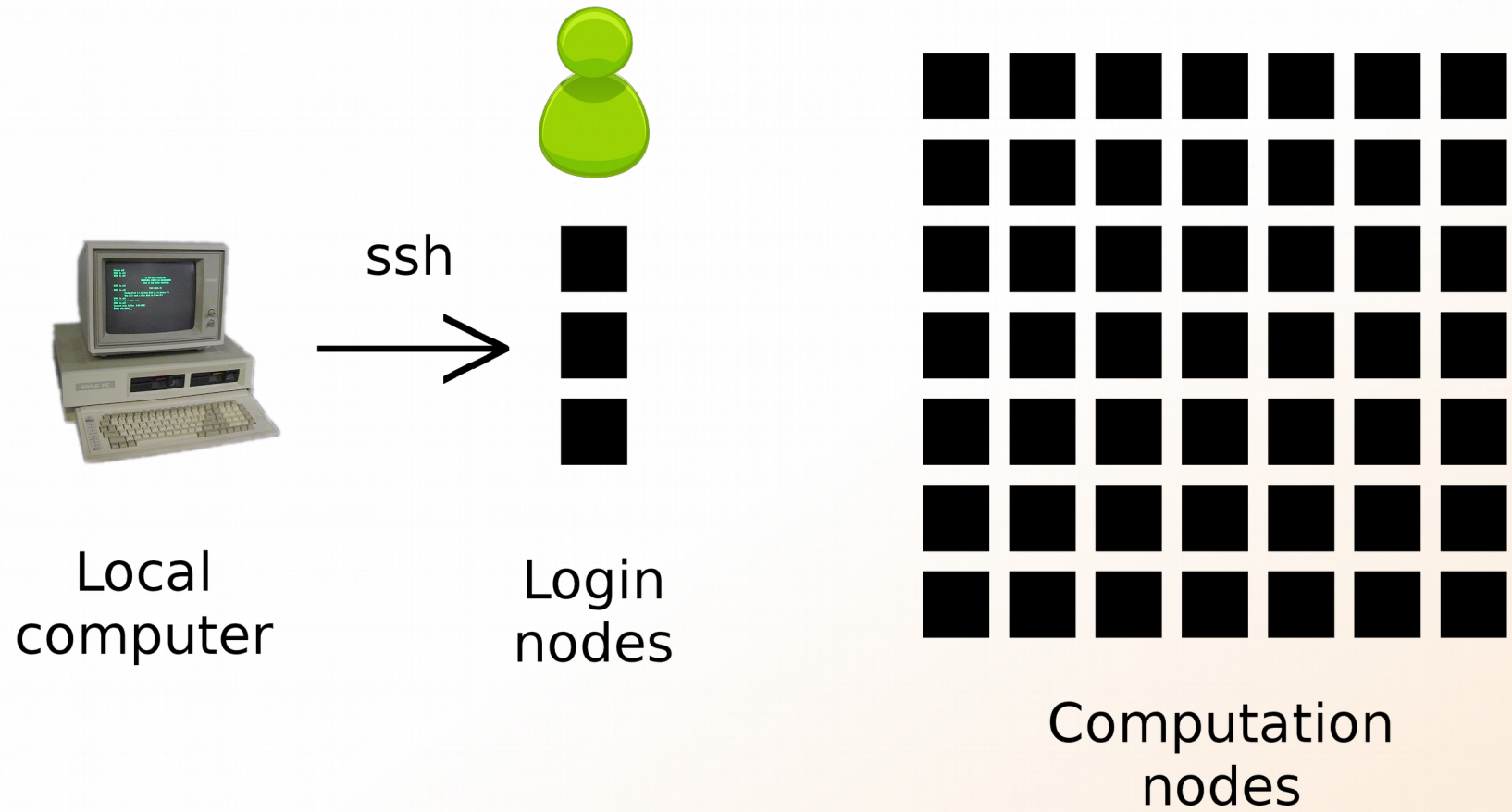
Local
computer

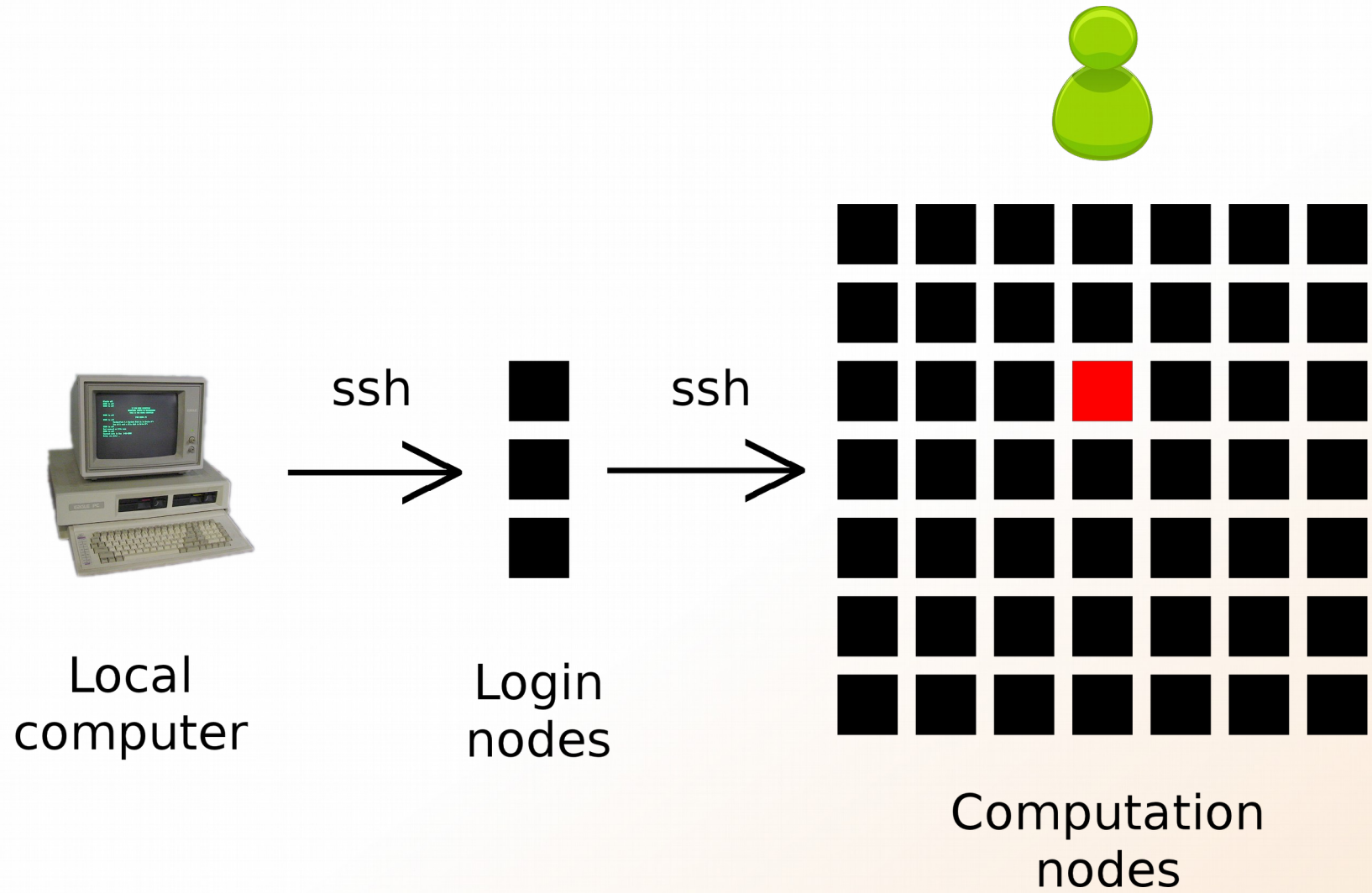


Login
nodes



Computation
nodes





- Books a node and connects you to it

interactive -A <proj id> -p <core or node> -t <time>

```
[dahlo@kalkyl3 work]$ interactive -A g2012205 -t 00:15:00 -p core
```


- Books a node and connects you to it

```
interactive -A <proj id> -p <core or node> -t <time>
```

```
[dahlo@kalkyl3 work]$ interactive -A g2012205 -t 00:15:00 -p core  
Your job is assigned a high interactive priority.
```

```
Please note that you must not use more than three GB of memory.  
Waiting for job 2216477 to start...  
Starting job now -- you waited for 3 seconds.
```

- Books a node and connects you to it

```
interactive -A <proj id> -p <core or node> -t <time>
```

```
[dahlo@q229 work]$
```

- Books a node and connects you to it

```
interactive -A <proj id> -p <core or node> -t <time>
```

```
[dahlo@q229 work]$
```

- Add -n to get more cores if you need more memory

- 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

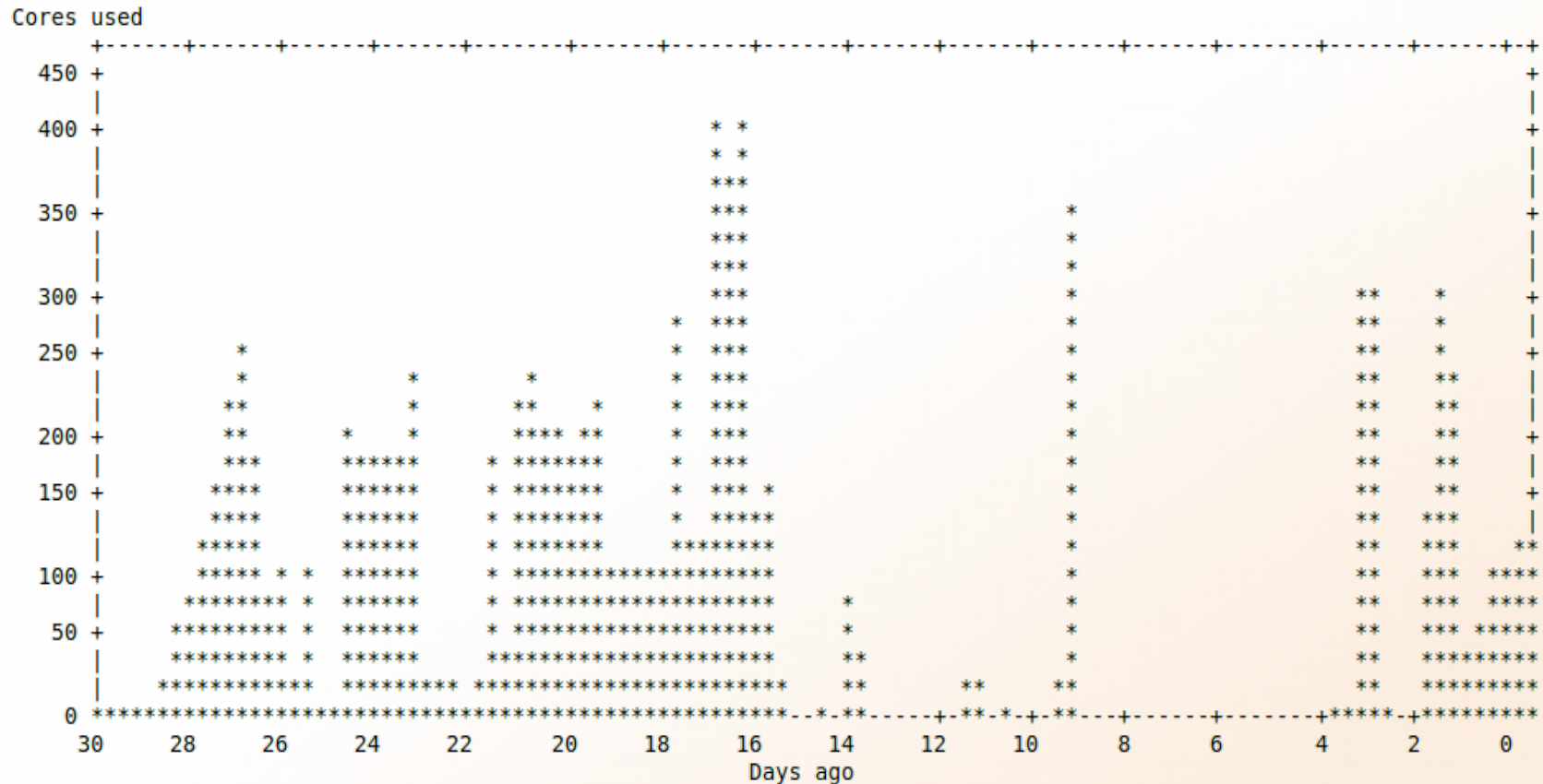
g2012083	0.00	2000

g2012157	0.12	2000
dahlo	0.12	

```
[dahlo@kalkyl4 work]$
```


- 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



- 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>

- **Laboratory time!** (again)