SciLifeLab
UPPSALA

UPPMAX Introduction

150914

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Enabler for Life Sciences

SciLifeLab UPPSALA

UPPMAX

- 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

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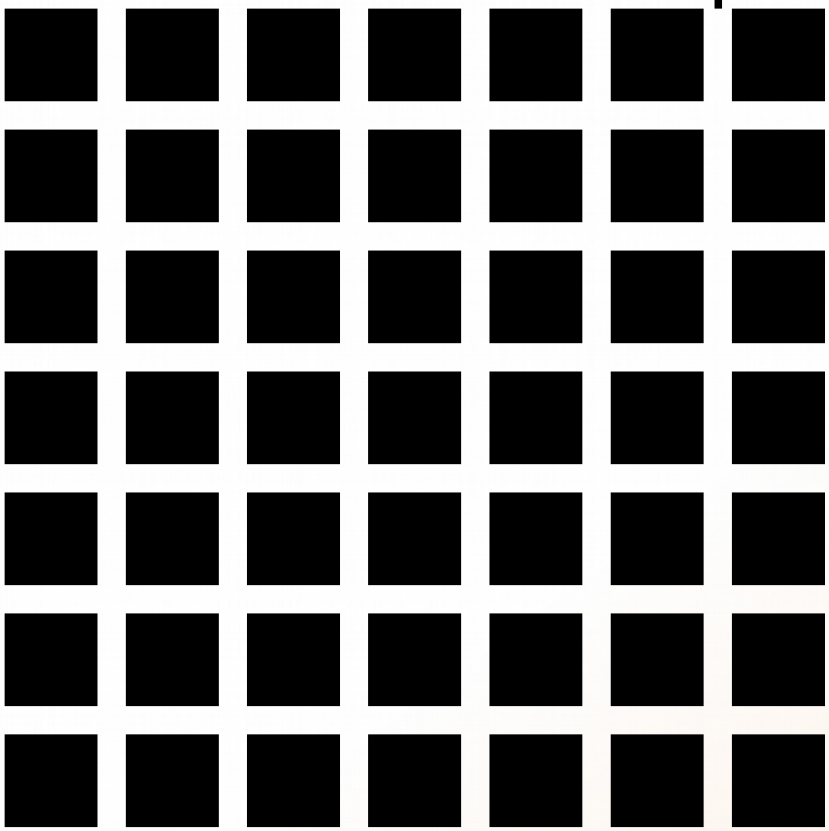
UPPMAX

- The basic structure of supercomputer



Calculation nodes

Login nodes

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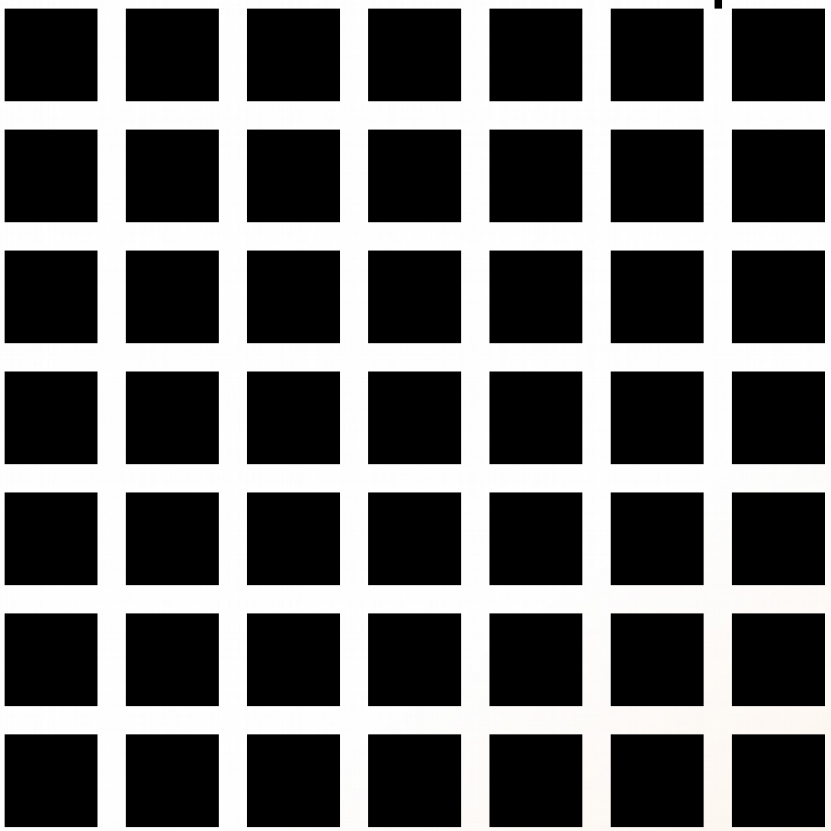
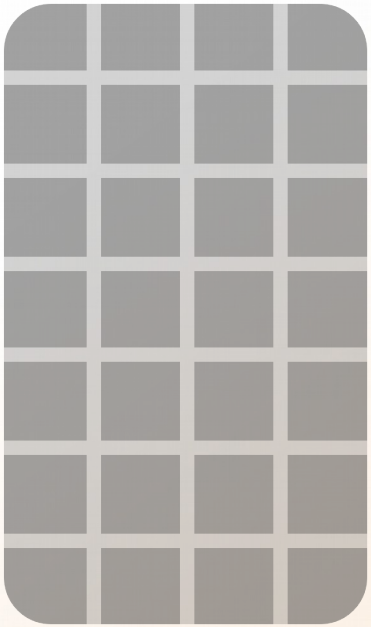
- The basic structure of supercomputer



Calculation nodes



Storage

Login nodes

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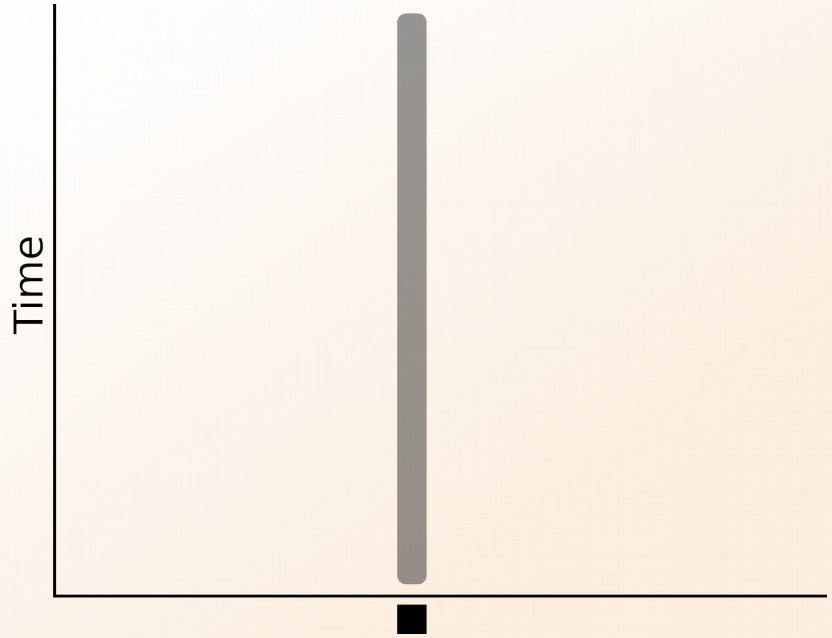
UPPMAX

- The basic structure of a supercomputer

- Parallel computing is key
  - Not one super fast



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UPPMAX

- The basic structure of a supercomputer

- Parallel computing is key
  - Not one super fast

Queue System

- More users than nodes
  - Need for a queue

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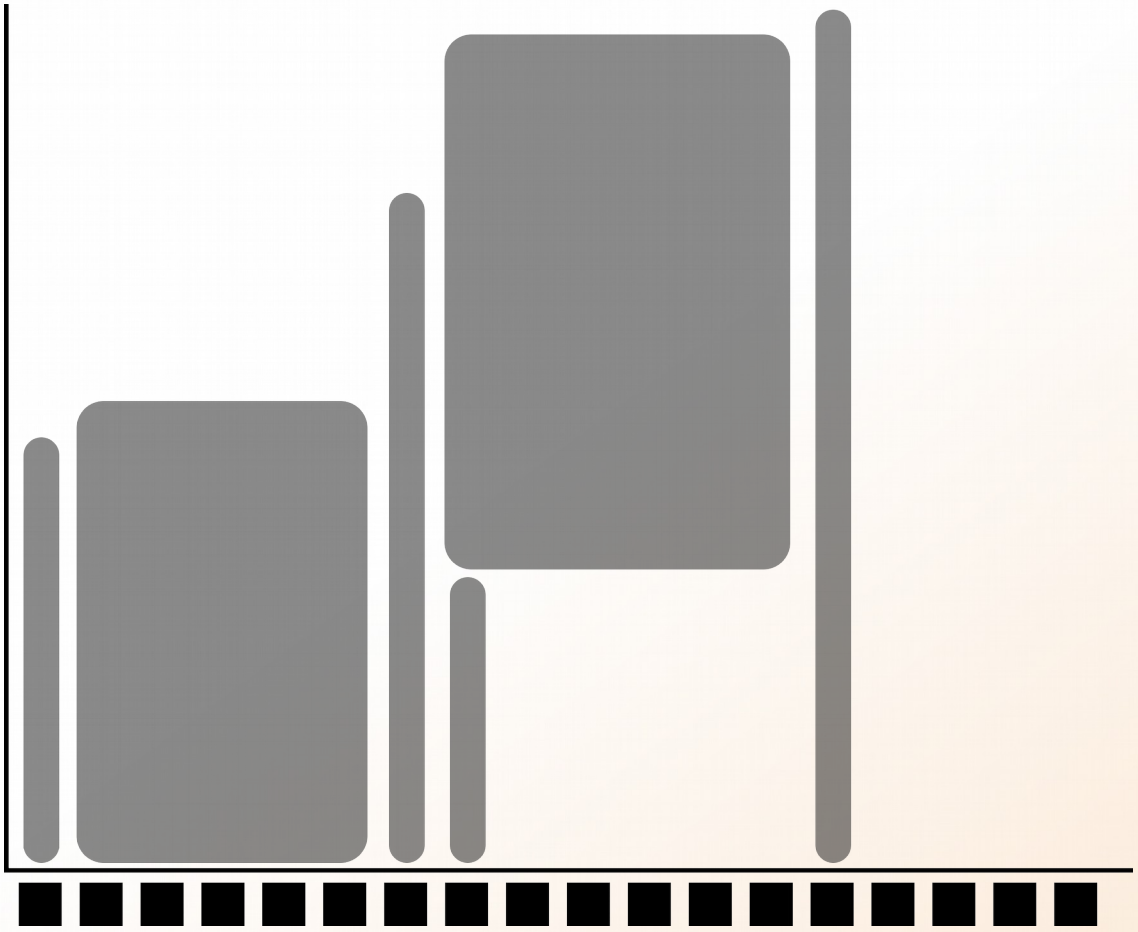

Queue System

- More users than nodes
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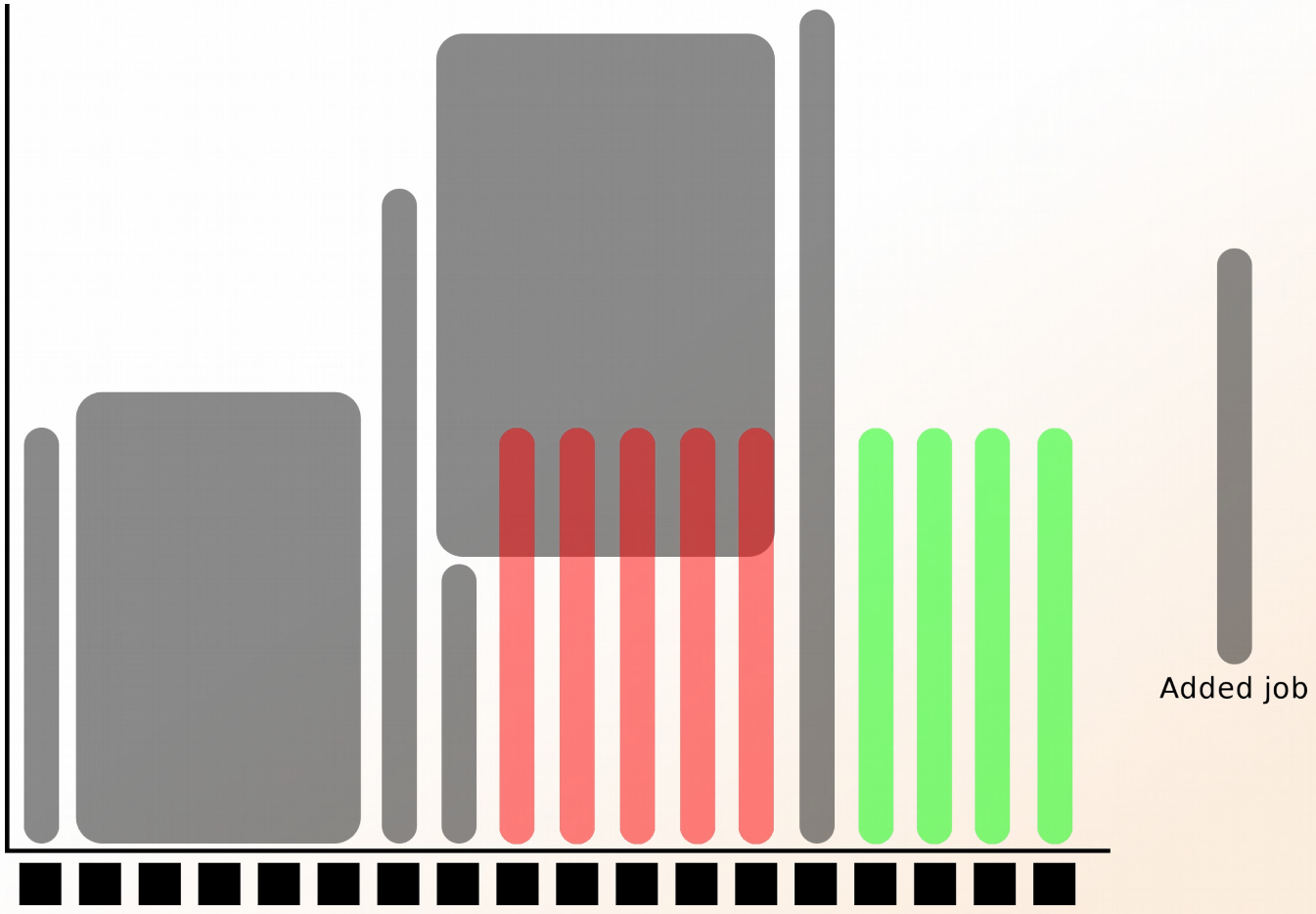

Queue System

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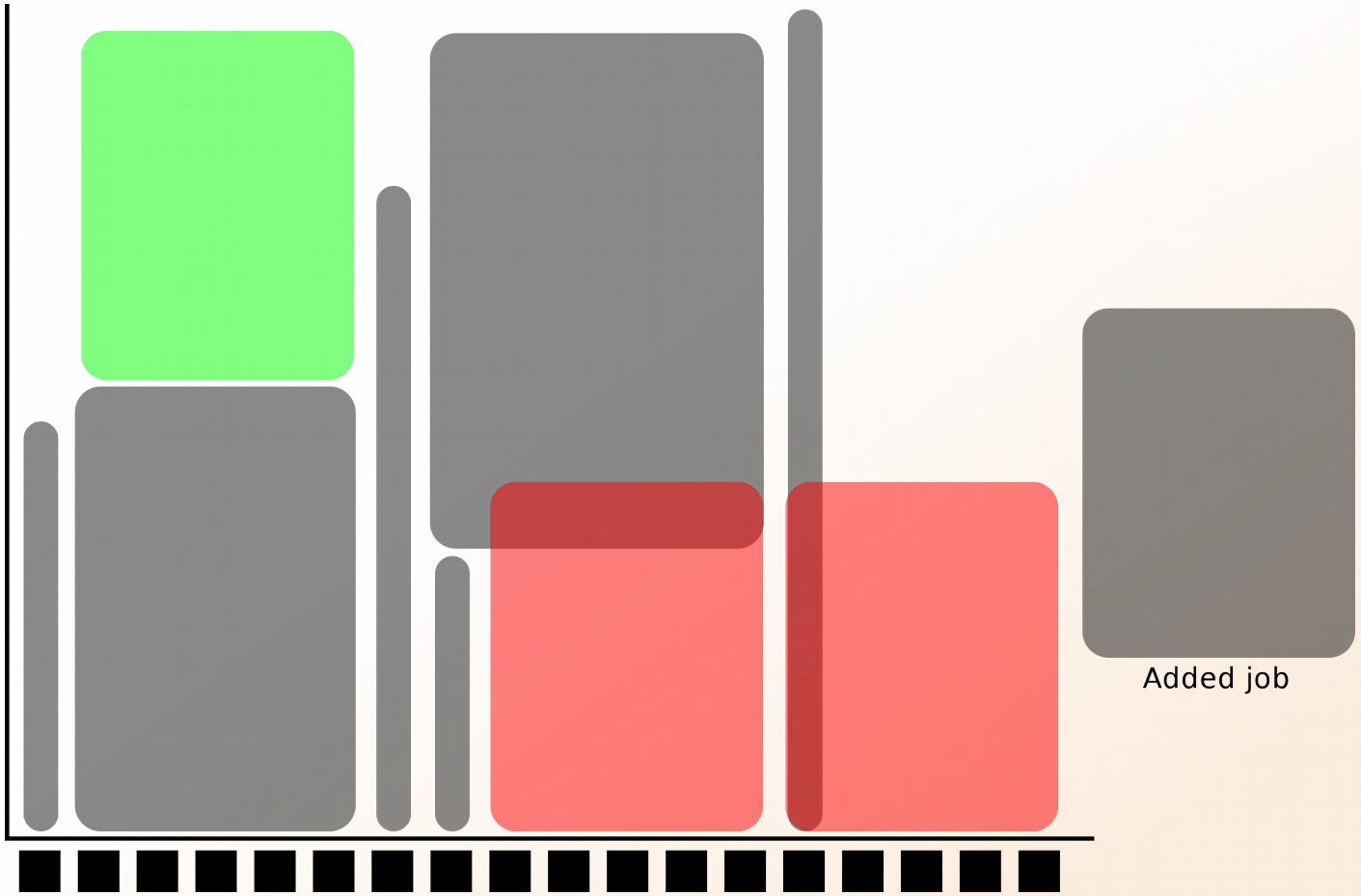
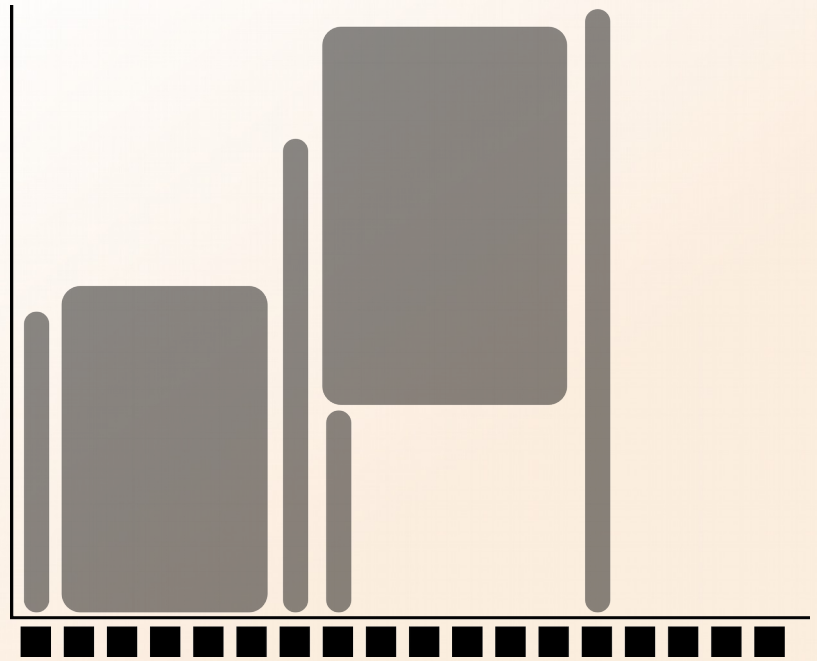


Queue System

- 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)



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Queue System

- 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

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Queue System

- 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 resouces
  - Default project size: 2000 core hours
- -p = partition (node or core)
  - Default value: core

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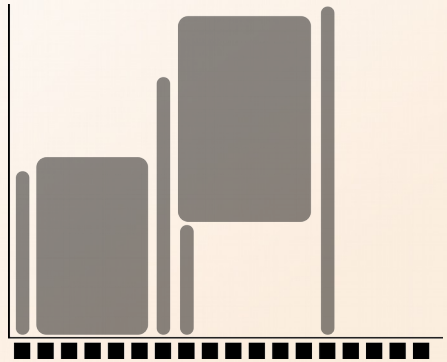
Queue System

- 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

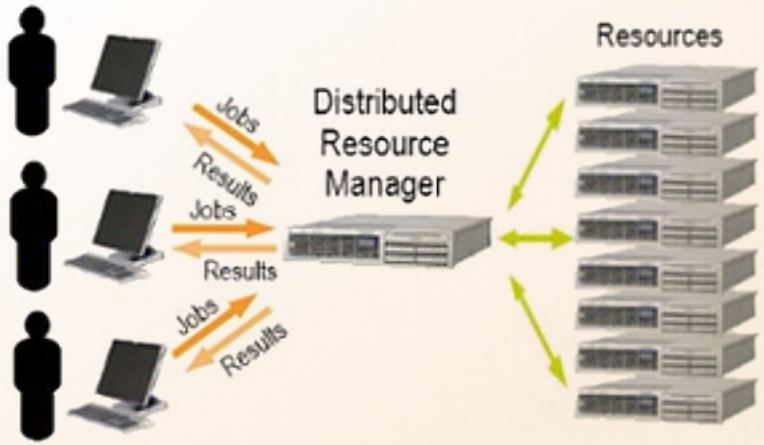
Queue System

- 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



A job?

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



Queue System

- 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!
```

Queue System

- 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
```

Queue System

- 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]$
```

SLURM Output

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

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

SLURM Output

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

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

SLURM Output

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

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

Squeue

- Shows information about your jobs

squeue -u <user>

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

Squeue

- Shows information about your jobs

squeue -u <user>

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

Squeue

- Shows information about your jobs

squeue -u <user>

```
[dahlo@kalkyl4 work]$ squeue -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>

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SSH

- Connects to a node

ssh -X <node name>

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

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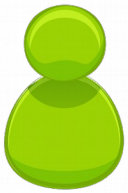
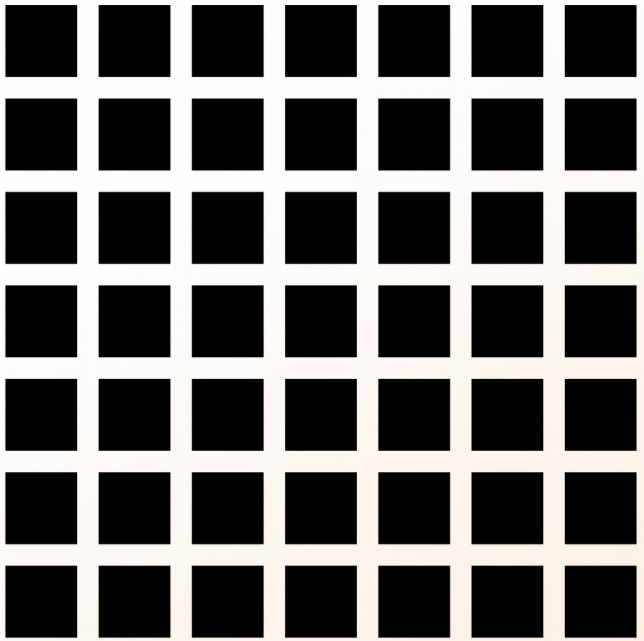
SSH



Local computer

Login nodes



Computation nodes

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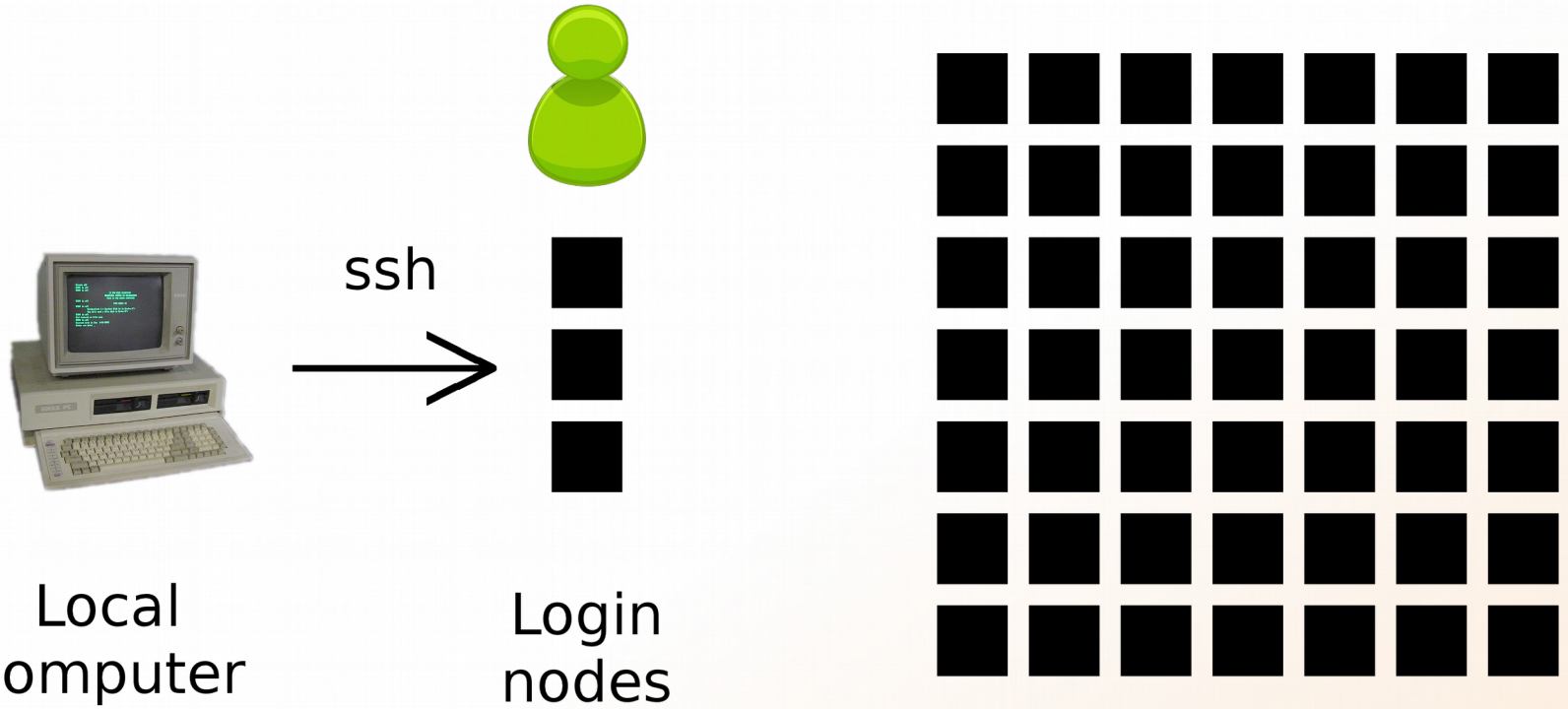
SSH



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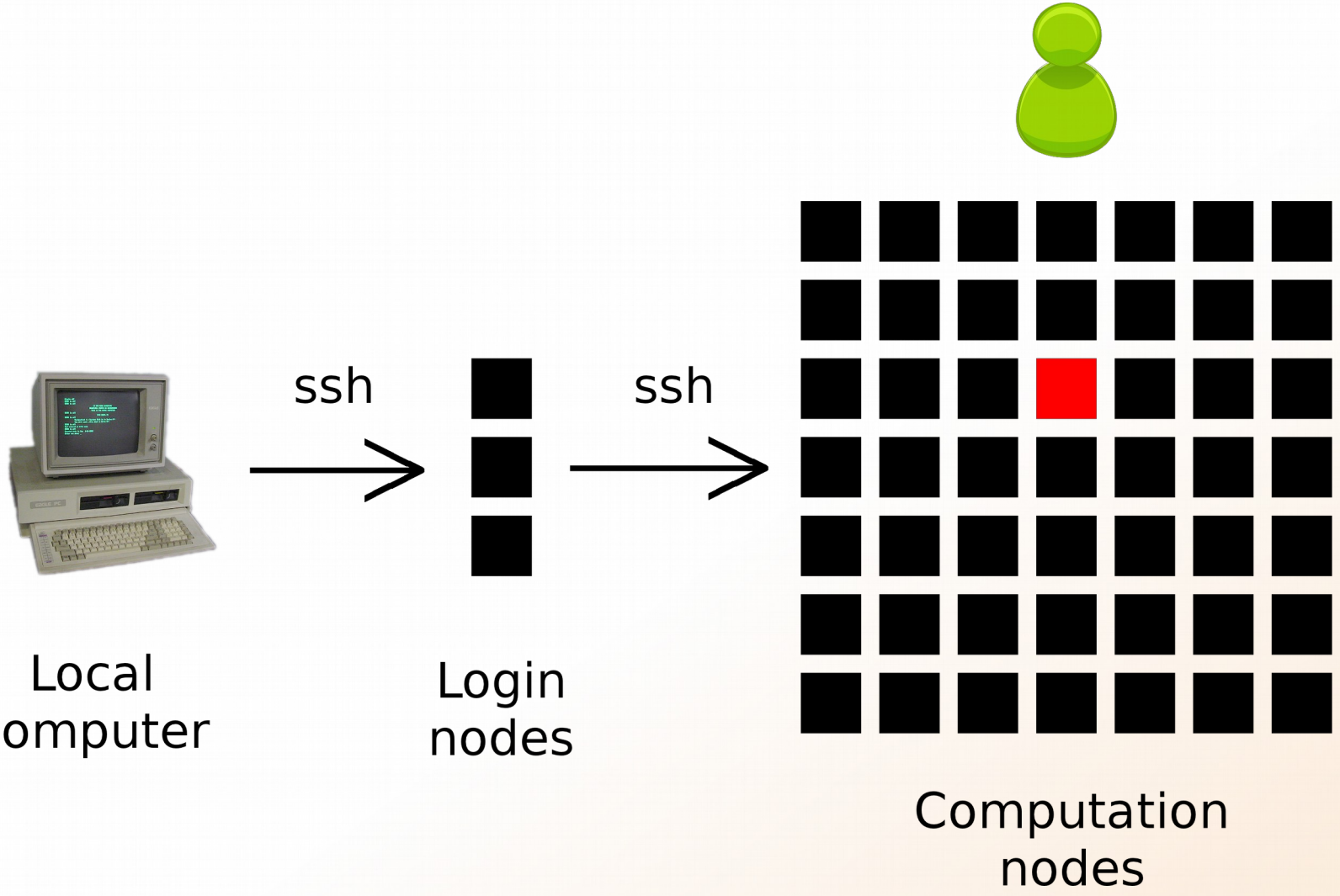
SSH



Interactive

- 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
```

Interactive

- 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.
```

Interactive

- Books a node and connects you to it

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

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

Interactive

- 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

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                             -
```

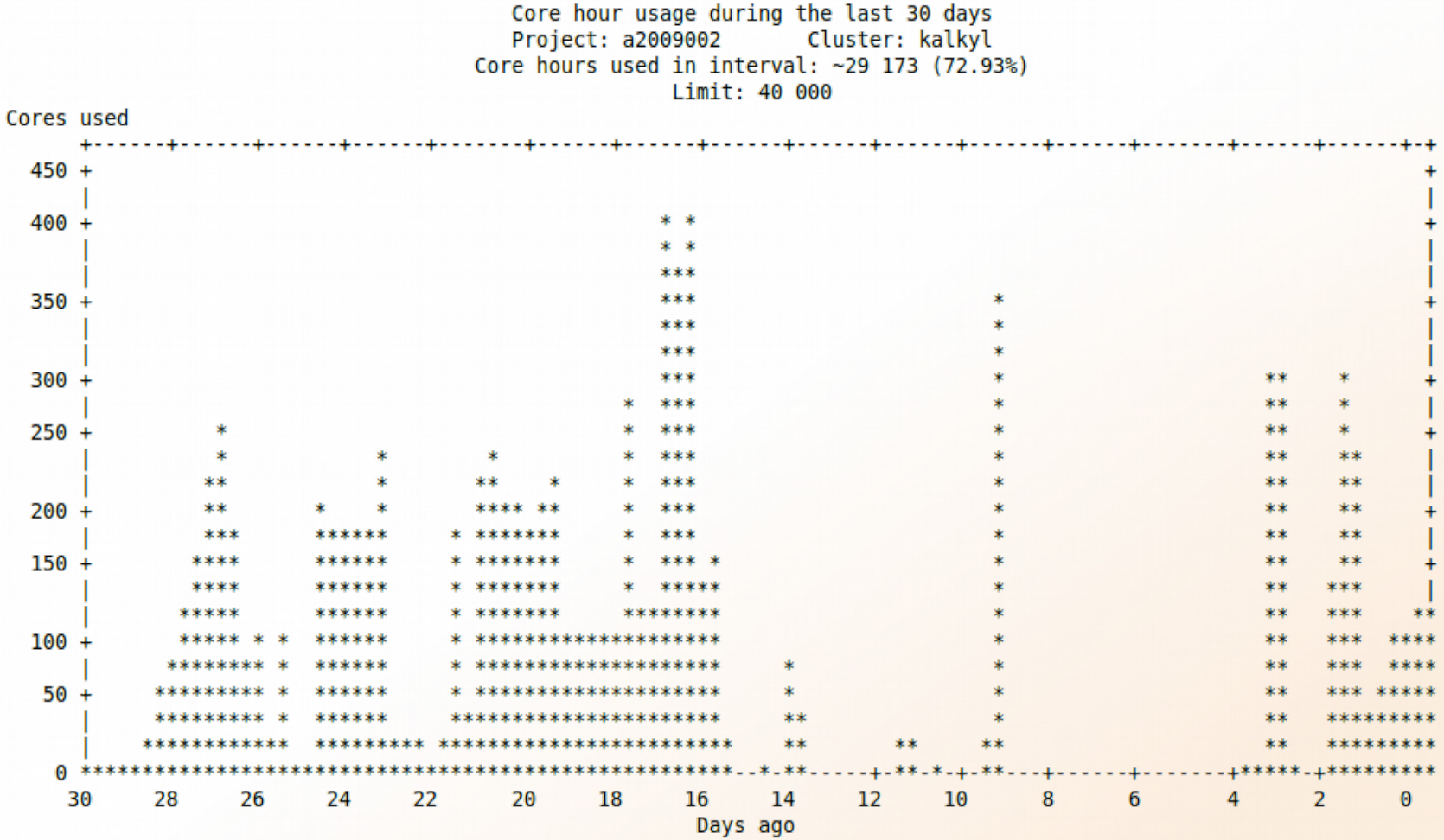
UPPMAX Commands

- 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]$
```

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- 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)