UPPMAX Introduction

160418
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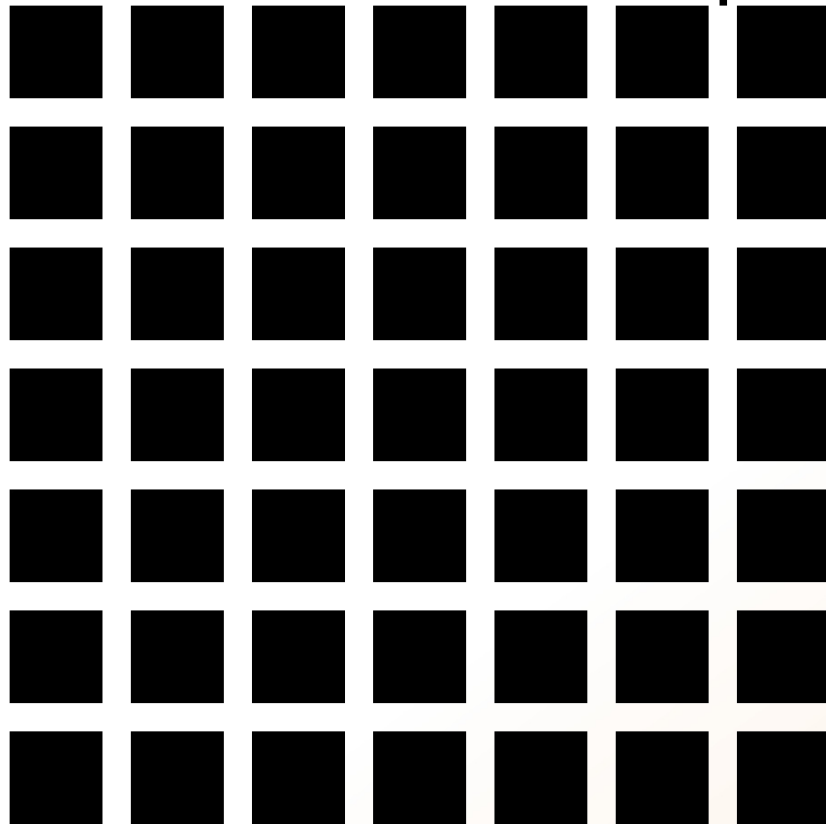- Uppsala Multidisciplinary Center for Advanced Computational Science

- http://www.uppmax.uu.se

- 2 clusters

  - Tintin, 160 nodes à 16 cores (64GB RAM)

  - Milou, 208 nodes à 16 cores (128GB RAM)

    - 17 with 256, 17 with 512

  - (Bianca, 100 nodes à 16 cores (128GB RAM))

- ~7 PB fast parallel storage

- The basic structure of supercomputer

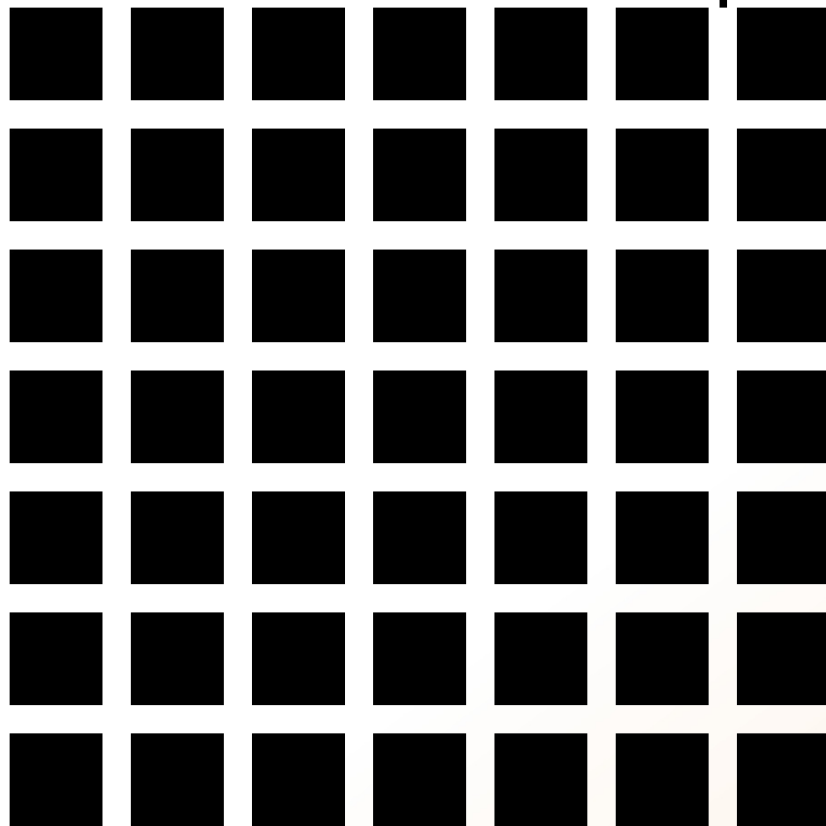Login nodes

- The basic structure of supercomputer

Calculation nodes

Login nodes

UPPMAX

SciLifeLab UPPSALA
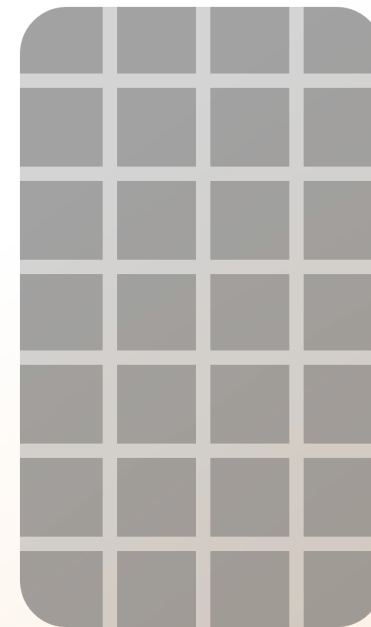
- The basic structure of supercomputer

Calculation nodes

Storage

Login nodes

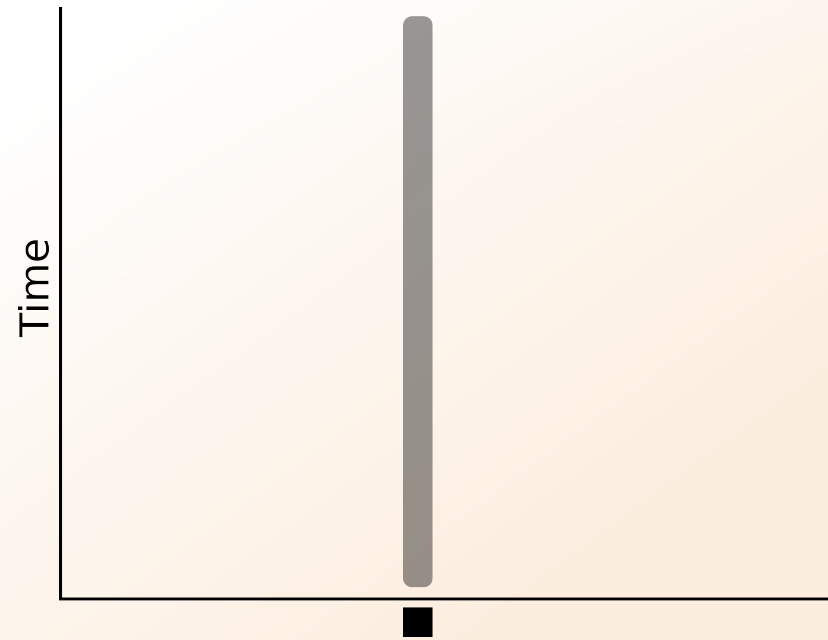- The basic structure of a supercomputer

- 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**
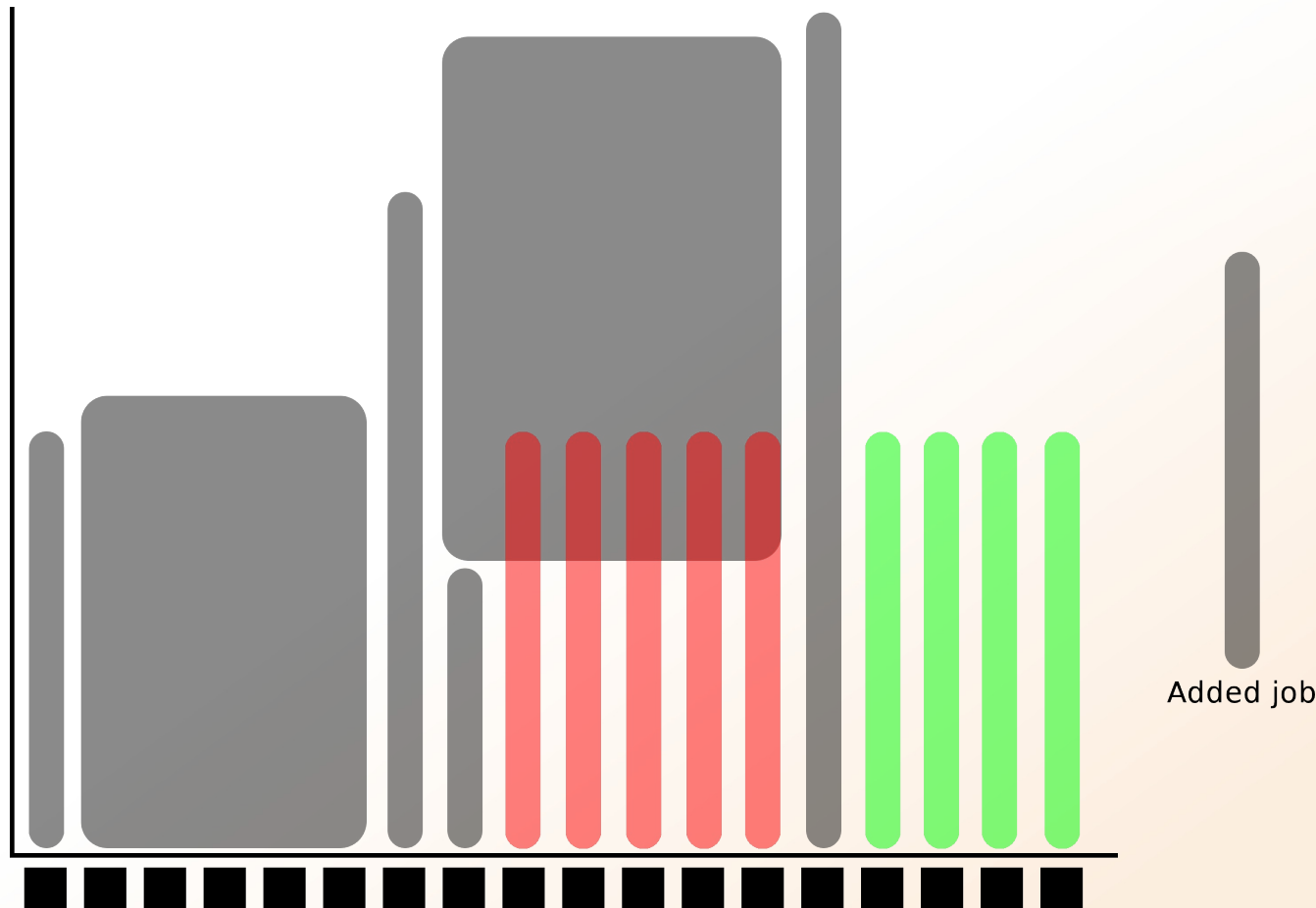
- More users than nodes
  - Need for a queue

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  - Need for a queue

Added job

- More users than nodes
  - Need for a queue

Added job
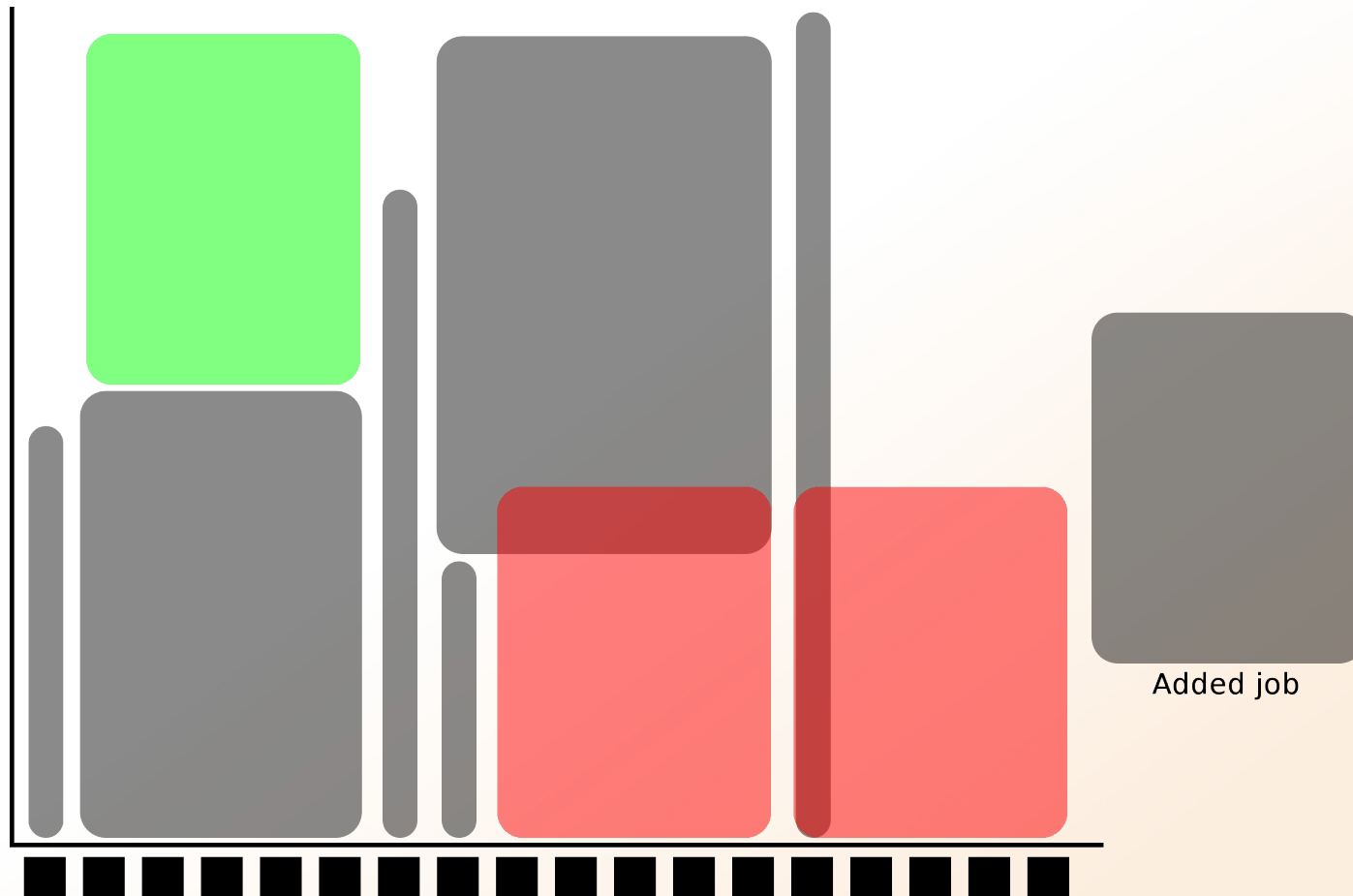
- 1 mandatory setting for jobs:
  - Who pays for it?   (-A)

- 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)
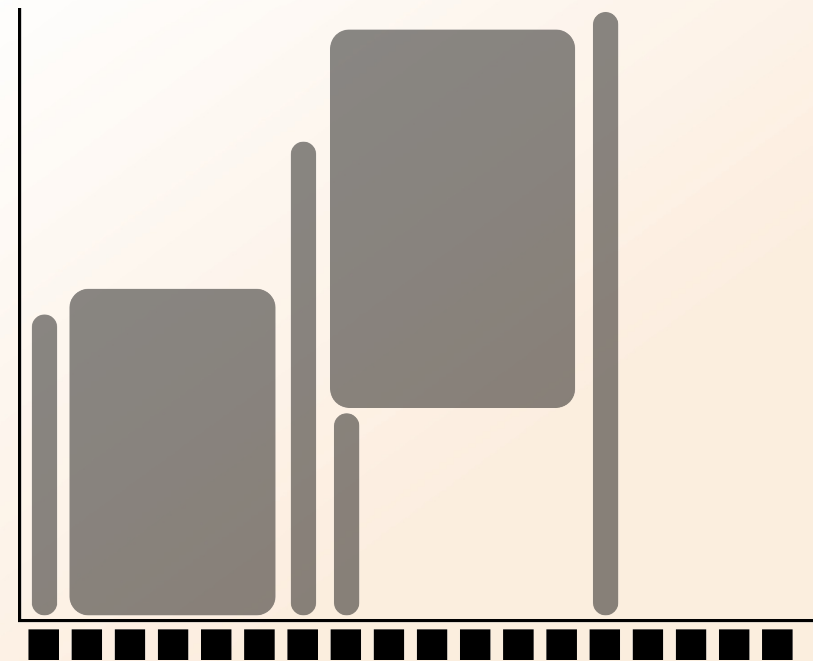
- Who pays for it?   (-A)

  - Only projects can be charged

    - You have to be a member

  - This course's project ID: g2016008

- -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 resouces

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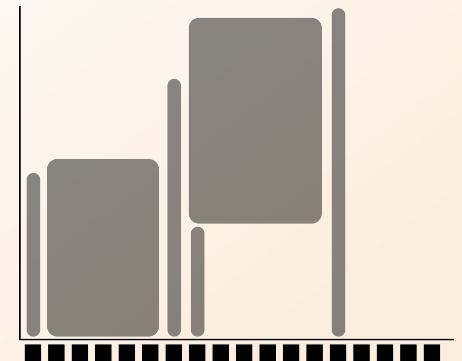
- Job = what happen during the booked time
    - Script file
        - Start programs
        - Move files
        - and more

- ## 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!
```

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- 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 uppmax 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 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]$
```

- 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]$
```

- 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]$
```

- 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]$
```

- 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>

- Connects to a node

ssh -Y <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 -Y q148
[dahlo@q148 work]$
```

SSH
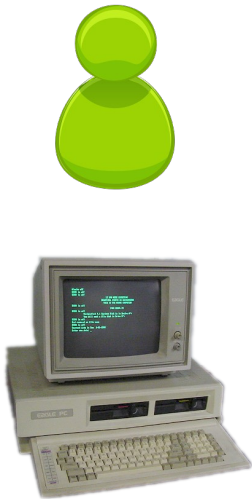
Local
computer

Login
nodes

Computation
nodes
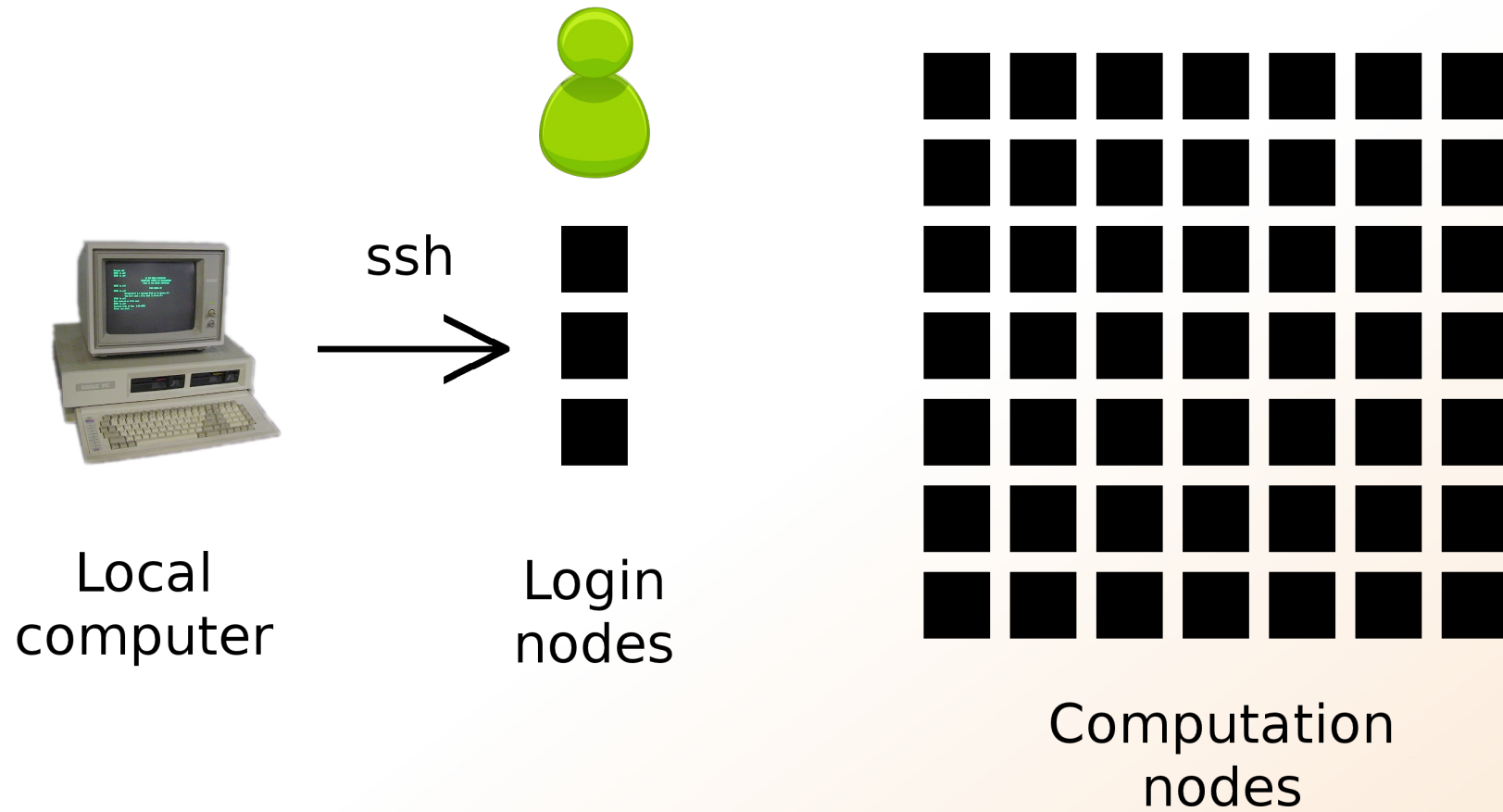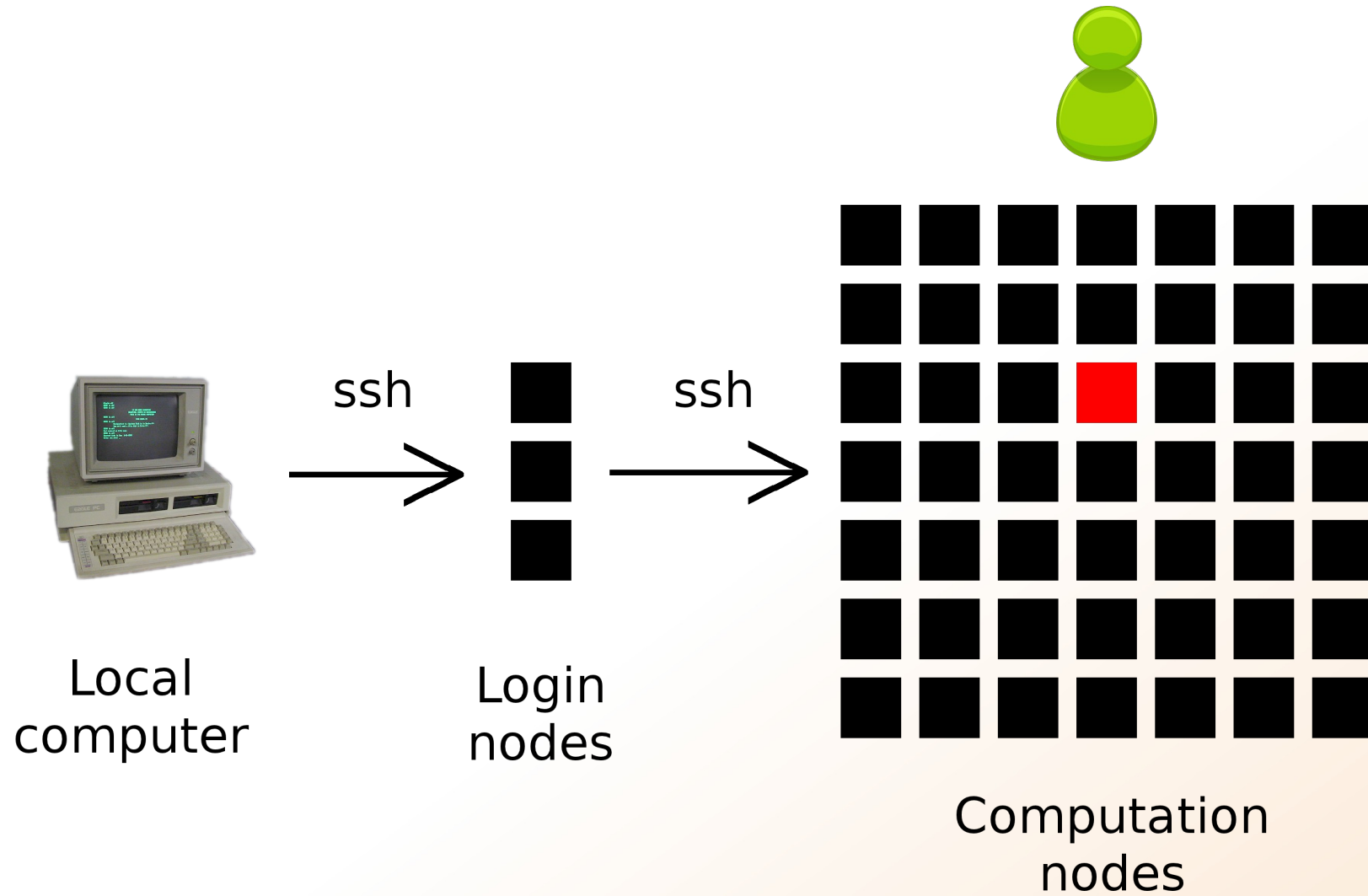
SSH

Local
computer

ssh

Login
nodes

Computation
nodes

SSH

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Local computer → ssh → Login nodes → ssh → 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                    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]$
```
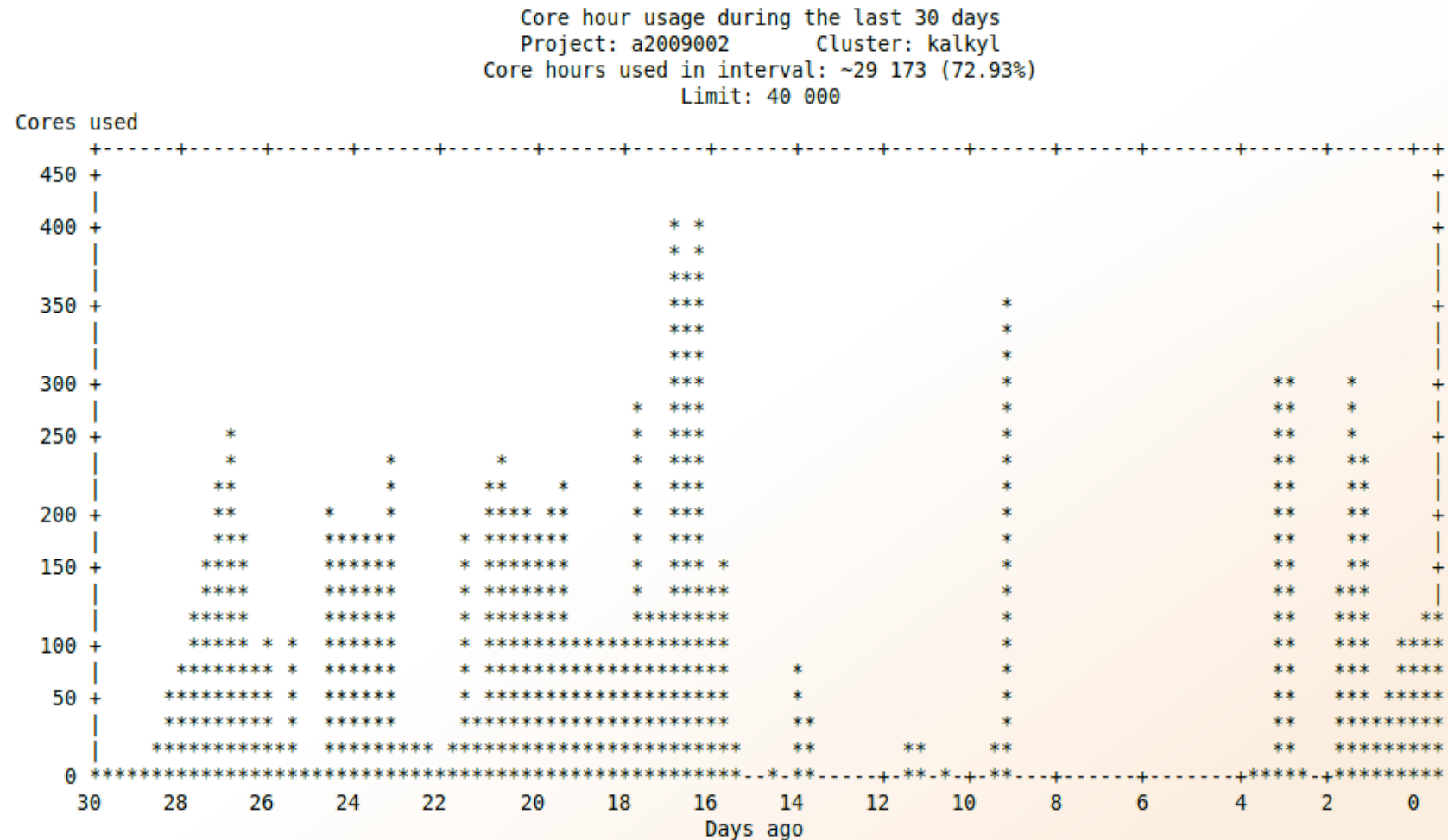
UPPMAX Commands

- projplot -A <proj-id>   (-h for more options)

- ## 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)