High Performance Computing Cluster
Basic course

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30 October 2017

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Outline

- Introduction to the Agrogenomics HPC
- Connecting with Secure Shell to the HPC
- Introduction to the Unix/Linux command line
- Submitting and monitoring basic jobs on the HPC

Introduction to the Agrogenomics HPC

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Outline

- Some definitions
- Description of the Agrogenomics HPC

Some definitions

- High performance computing cluster
  - Group of interconnected computers (node) that work together and act like a single system

Some definitions

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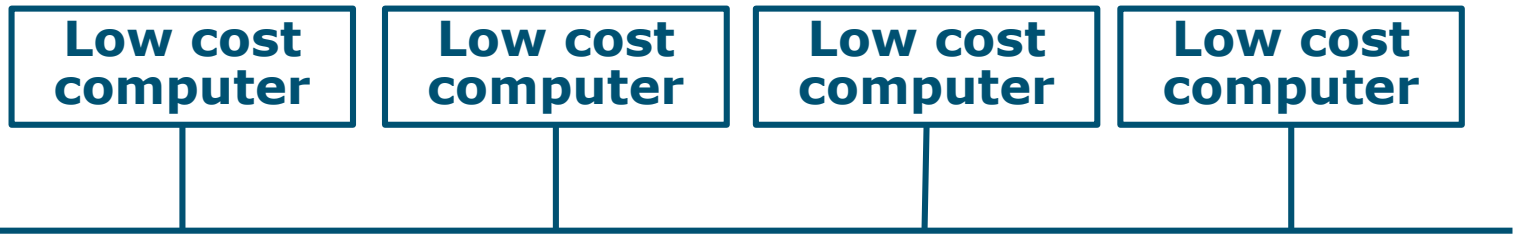
- CPU (Central processing unit)
  - Component within a computer that carries out the instructions of a computer program

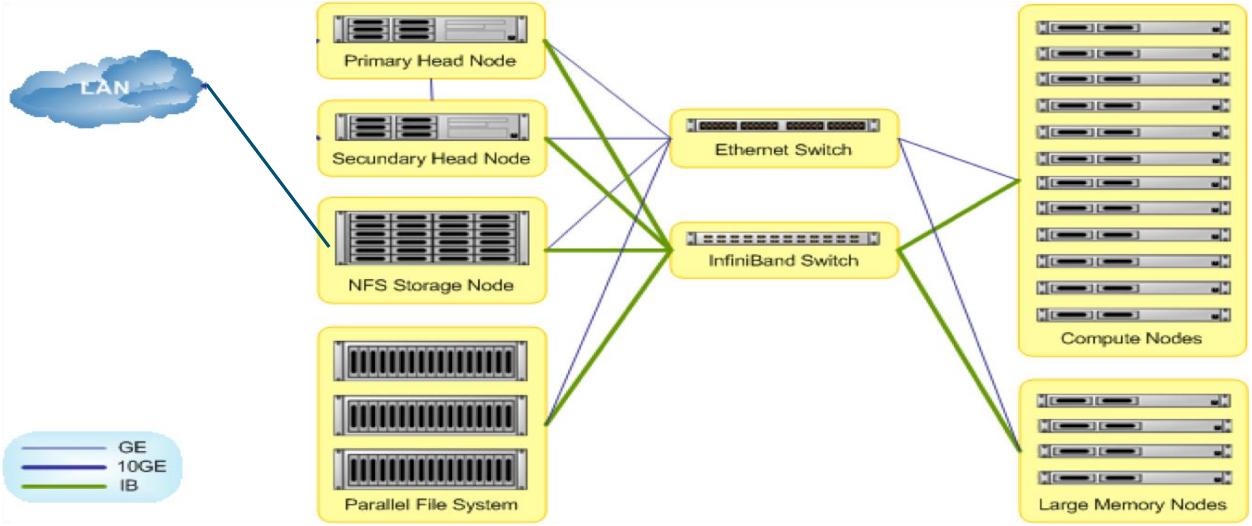
Some definitions

- High performance computing cluster
  - Group of interconnected computers (node) that work together and act like a single system
- CPU (Central processing unit)
  - Component within a computer that carries out the instructions of a computer program
- Core
  - Processing unit which reads and executes program instructions



Agrogenomics HPC

- 2 head nodes
- Compute nodes
  - 48 nodes (16 cores; 64GB RAM)
  - 2 fat nodes (64 cores; 1TB RAM)



Agrogenomics HPC – main storage

- Home directory
  - /home/[partner]/[username]
  - Directory where you are after logon
  - Quota of 200GB soft (210GB hard)

Agrogenomics HPC – main storage

- Lustre filesystem (faster storage)
  - backup
    - /lustre/backup/[partner]/[unit]/[username]
    - Extra cost for backup
  - nobackup
    - /lustre/nobackup/[partner]/[unit]/[username]
    - Some costs
  - scratch
    - /lustre/scratch/[partner]/[unit]/[username]
    - Free
    - Regularly cleaned up

Agrogenomics HPC – “rules”

- Home
  - Jobscripts
  - Small datasets (performance)
  - Not computational jobs
- Lustre
  - Big datasets
  - Intensive (computing) jobs
  - No job run outside SLURM

Agrogenomics HPC – useful information

- HPC wiki
  - https://wiki.hpcagrogenomics.wur.nl
- Bright HPC portal
  - https://portal.hpcagrogenomics.wur.nl/
- Contact person
  - Gwen Dawes
  - Jan van Lith

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Questions?

Connecting with Secure Shell to the HPC

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30 October 2017

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SSH client usage - Windows

- Install **PuTTY** Windows MSI installer

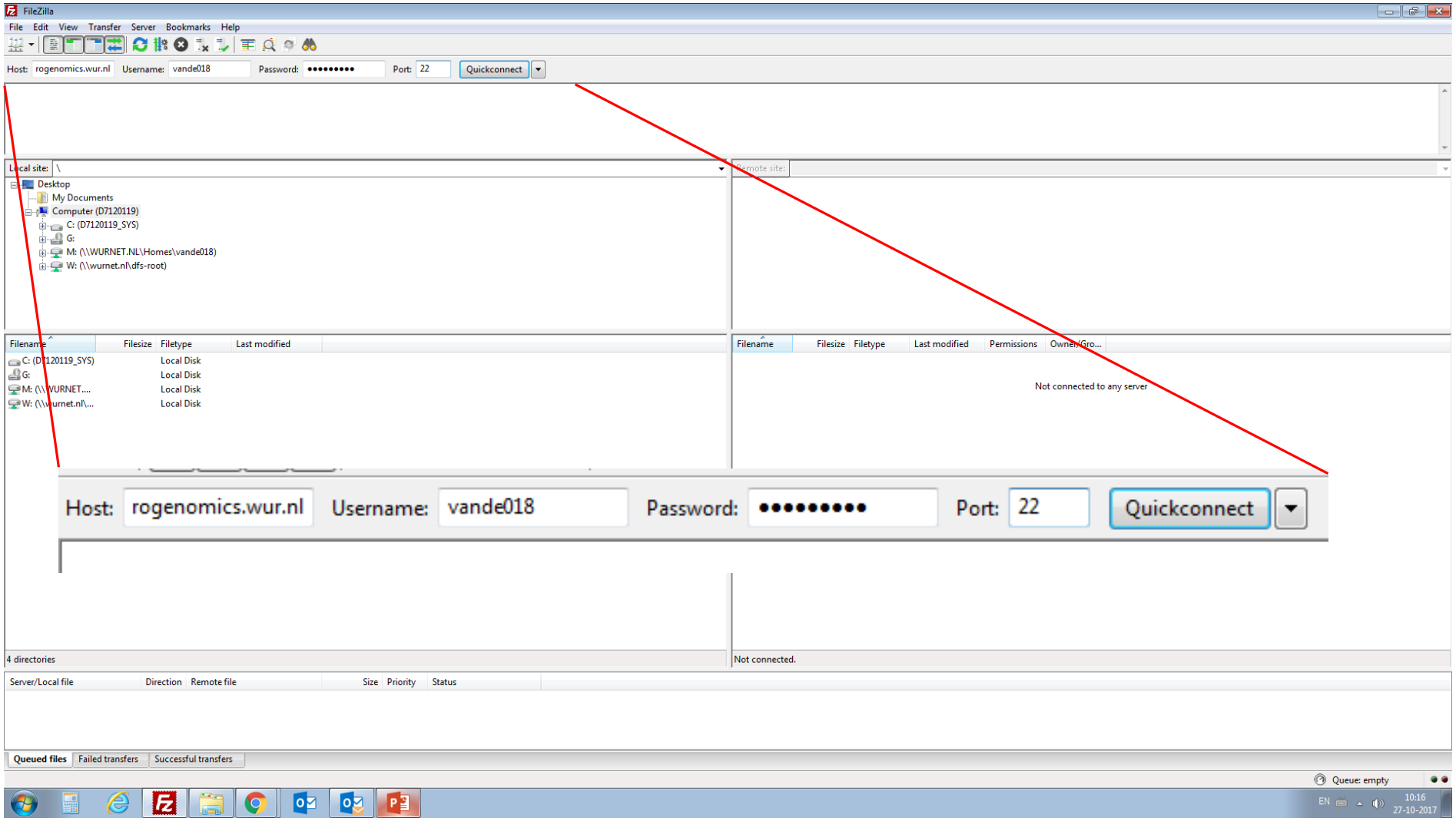
- PuTTY configuration
    - Session
        - Host Name: **nfs01.hpcagrogenomics.wur.nl**
    - Connection
        - Data
            - Auto-login username: *your_remote_username*

- More info

https://wiki.hpcagrogenomics.wur.nl/index.php/Log_in_to_B4F_cluster

SSH client usage - Windows

- Install **FileZilla** for transferring files



SSH client usage – Linux/MacOSX

- Use a Command Line Interface
- ssh [username]@nfs01.hpcagrogenomics.wur.nl
- More info

https://wiki.hpcagrogenomics.wur.nl/index.php/Log_in_to_B4F_cluster

Try it...

Questions?

Introduction to the command line

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6 June 2017

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The command line environment

- When you log in to your account using SSH:

[username@nfs01 ~]$

- The symbol *~ indicates that you are in your home directory.*

Listing files and directories

ls

The ***ls*** command provides a listing of a directory's contents.

More details:

ls -l

Navigating

- To determine which directory you are currently:

pwd

- To change to another directory:

cd path_to_other_directory

- To go back up one level:

cd ..

- To go to your home directory:

cd ~

Creating and removing directories

- To create a directory:

mkdir my_directory

- To remove an empty directory:

rmdir my_directory

Copying, moving and deleting files

- To copy a file:

cp file1 file2

- To move (rename) a file:

mv file1 file2

- To delete a file:

rm file1

(De)compressing files

- To compress a file:

gzip file1

- To decompress a file:

gunzip file1.gz

gzip –d file2.gz

- Other commands

bzip2, xz, zip,…

Transferring files using ***scp***

- To copy a file *from* an external machine:

scp username@hostname:~/file1 destination_name

- To copy a file *to* an external machine:

scp ~/file1 username@hostname:destination_name

Downloading files from the web

- To download a file from the web:

wget [options] [url]

Making a file executable

- To make a file executable

chmod u+x file1

- To execute a program/script/....

./program [options]

/path/to/the/program/program [options]

Environment variables

- ~data storage for Unix/Linux shell

- To assign an environment variable

MYVARIABLE=my_value

- To access the data stored within an environment variable:

echo ***$MYVARIABLE***

- To list all environment variables:

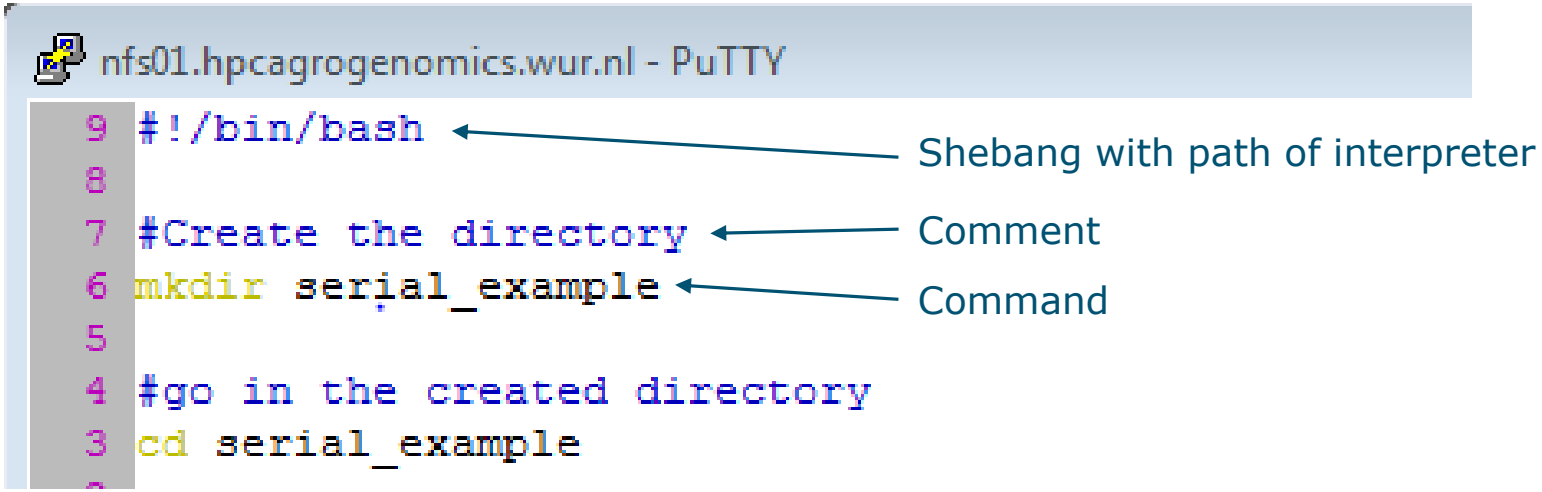
env

- Remove the existence of an environment variable:

unset MYVARIABLE

A bash (Shell) script

- Plain text file which contains a serie/mixture of commands.
- **Tip**
  - Anything you can run normally on the command line can be put into a script and it will do exactly the same thing.
- Convention: extension of **.sh** (e.g., script.sh).
- Example



Try it...

1. Create a directory (e.g., 'example_1') in your Lustre scratch directory
2. Download QMSim from this URL and decompress (***unzip***) it: http://www.aps.uoguelph.ca/~msargol/qmsim/QMSim_Linux.zip
3. Copy the parameter file /lustre/shared/training_slurm/autumn_2017/serial/training/ex_serial_qmsim.prm in your directory!

- Extra: write a bash script to do all these steps!

Questions?

Solution

nfs01.hpcagrogenomics.wur.nl - PuTTY

```
#!/bin/bash
#Create the directory
mkdir example_1

#go in the created directory
cd example_1

 #Dowlowd the archive QMSim
 wget www.aps.uoguelph.ca/~msargol/qmsim/QMSim_Linux.zip

 #Decompress the archive
 unzip QMSim_Linux.zip

 #Copy the parameter file
 cp /lustre/shared/training_slurm/autumn_2017/serial/training/ex_serial_qmsim.prm .

 #Run QMSim16
 #QMSim_Linux/QMSim16 ex_serial_qmsim.prm

#go outside the created directory
```

Extra - Symbolic link

- To create a symbolic link to a file/directory, instead of copying it:

ln –s /path/to/file1 link

Submitting and monitoring basic jobs on the HPC

J. Vandenplas, G. Dawes

30 October 2017

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Outline

- Some definitions
- Running a basic job on the nodes of the HPC
  - Introduction to SLURM
  - Characteristics of a job
  - Writing and submitting a script
  - Monitoring and controlling a job
- Some exercises
- (Extra: Submitting a job array)

Some definitions

- Process
  - Instance of a computer program that is being executed

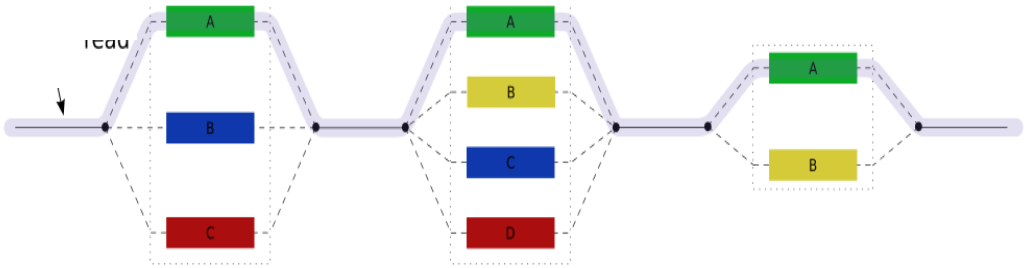
jvandenp@localhost:~ 92x46

```
top - 13:16:08 up 11 days, 18:06, 43 users,  load average: 7.13, 5.27, 4.28
Tasks: 860 total,   6 running, 852 sleeping,   2 stopped,   0 zombie
Cpu(s): 89.1%us,  2.8%sy,  0.0%ni,  8.0%id,  0.0%wa,  0.0%hi,  0.0%si,  0.0%st
Mem:  66059268k total, 62016800k used,  4042468k free,    88444k buffers
Swap: 63999992k total, 19730664k used, 44269328k free,  8198812k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
37014 vande018  20   0 14.2g  10g 2368 R 299.3 16.3   8:13.83 calc_grm
37291 vande018  20   0 22036 2036 1036 R  0.7  0.0   0:03.61 top
  936 vande018  20   0  130m  828  668 S  0.0  0.0   0:00.23 sshd
  938 vande018  20   0  112m 1968 1288 S  0.0  0.0   0:00.20 bash
 6515 vande018  20   0  127m  312  308 S  0.0  0.0   0:03.24 screen
 6516 vande018  20   0  112m  384  380 S  0.0  0.0   0:00.43 bash
 6520 vande018  20   0  112m  448  444 S  0.0  0.0   0:00.83 bash
13249 vande018  20   0  130m  984  808 S  0.0  0.0   0:00.43 sshd
13283 vande018  20   0  112m 2352 1508 S  0.0  0.0   0:00.39 bash
14627 vande018  20   0  112m 1216 1212 S  0.0  0.0   0:00.46 bash
14689 vande018  20   0  127m  456  452 S  0.0  0.0   0:04.53 screen
14690 vande018  20   0  112m  928  924 S  0.0  0.0   0:00.24 bash
14694 vande018  20   0  112m  928  924 S  0.0  0.0   0:00.17 bash
```

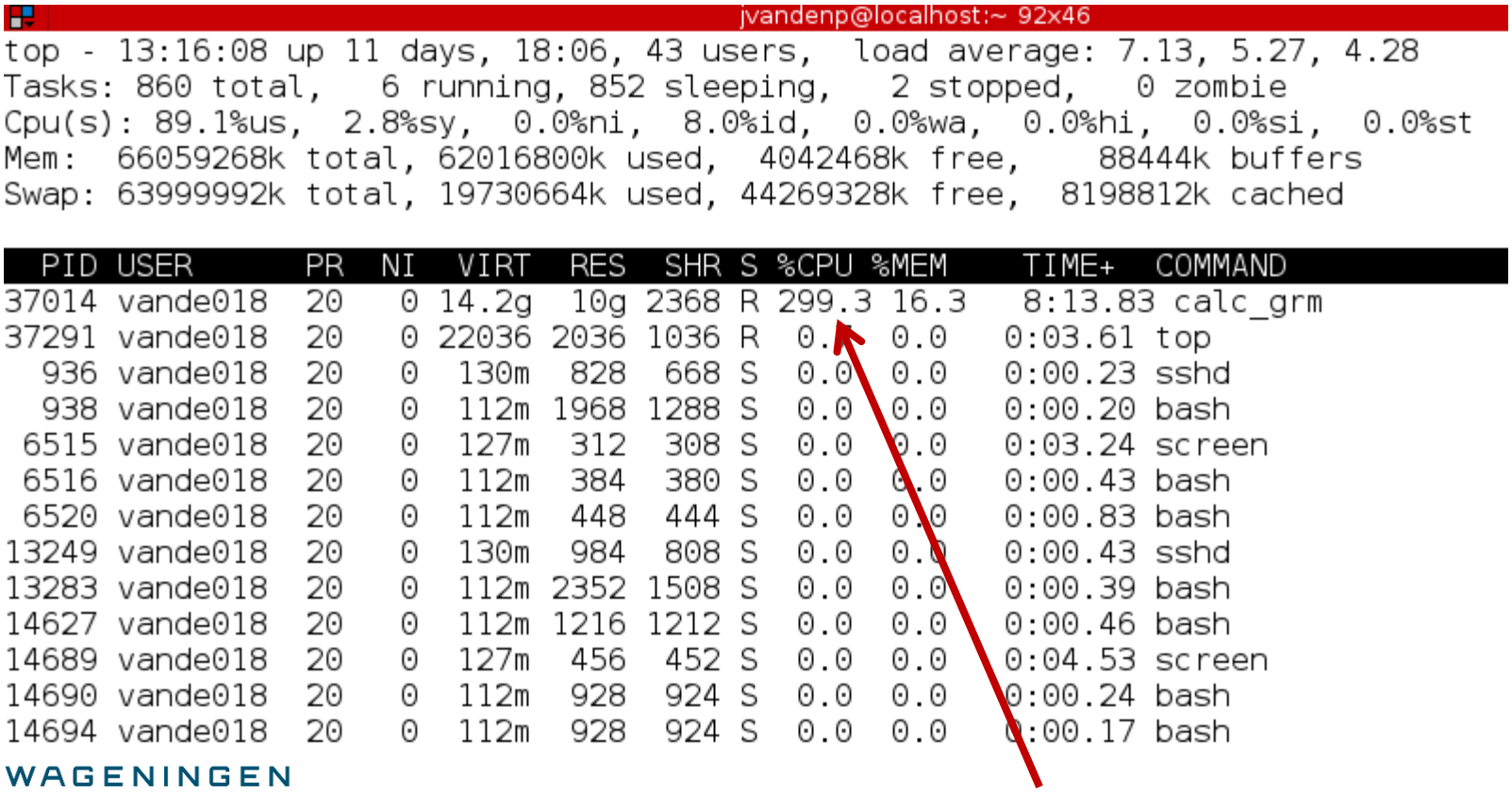
Some definitions

- Process
  - Instance of a computer program that is being executed
  - May be made up of multiple threads that execute instructions concurrently
- Thread
  - Smallest sequence of programmed instructions



Some definitions

- Process / Thread
  - Linux command: ***top***



Running a job on the nodes of the HPC?

Running a job on the nodes of the HPC?

- Job
  - An operation or a group of operations treated as a single and distinct unit
  - Two parts
    - Resource requests
    - Job steps
      - Tasks that must be done (e.g., software that must be run)

Running a job on the nodes of the HPC?

- Job
  - An operation or a group of operations treated as a single and distinct unit
  - Two parts
    - Resource requests
    - Job steps
      - Tasks that must be done (e.g., software that must be run)
- A job must be submitted to a job scheduler

  ➔Requires a (shell) submission script

Job scheduler/Resource manager

- Software which:
  - Manages and allocates resources (computer nodes)
  - Manages and schedules jobs on a set of allocated nodes
  - Sets up the environment for parallel and distributed computing

Job scheduler/Resource manager

- Software which:
  - Manages and allocates resources (compute nodes)
  - Manages and schedules jobs on a set of allocated nodes
  - Sets up the environment for parallel and distributed computing

- HPC's job scheduler: **SLURM** (Simple Linux Utility for Resource Management ; http://slurm.schedmd.com/slurm.html)

Some definitions for Slurm

- Task
  - In the Slurm context, it must be understood as a process.

Some definitions for Slurm

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- CPU
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Some definitions for Slurm

- Task
  - In the Slurm context, it must be understood as a process.
- CPU
  - In the Slurm context, it can be understood as a core or a hardware thread.
- Multithreaded program
  - One task using several CPUs
- Multi-process program
  - Several tasks

Running a basic job on the HPC nodes?

- A submission script is required...

```
#!/bin/bash
# ------------------------------Name of the job-------------------------
#SBATCH --job-name=example1
#------------------------------Mail address-----------------------------
#SBATCH --mail-user=jvandenplas@ulg.ac.be
#SBATCH --mail-type=ALL
#------------------------------Output files-----------------------------
#SBATCH --output=output_%j.txt
#SBATCH --error=error_output_%j.txt
#------------------------------Other information------------------------
#SBATCH --comment='Some comments'
#SBATCH --account=123456789
#------------------------------Required resources-----------------------
#SBATCH --partition=ABGC_Low
#SBATCH --time=0-1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=4000

#------------------------------Environment, Operations and Job steps----
export OMP_NUM_THREADS=1
echo 'Start calc_grm'
srun calc_grm --par param.par --pca  >out.calc_grm
~
```

➔... and it must be submitted!

Running a job on the HPC nodes?

Several steps

1. Characteristics of the jobs?
2. Writing a submission script
3. Submitting a job
4. Monitoring and controlling a job
5. Getting an overview of previous and current jobs

1. Characteristics of the job

- What is your job?
  - Sequential/parallel
  - Resource requests
    - Number of CPUs
    - Amount of RAM
    - Expected computing time
    - ...
  - Jobs steps
    - Job steps can be created with the command ***srun***

1. Characteristics of the job

- Try to fit to the real use as much as possible!

- Try to ask 4GB RAM per CPU for the compute node (15.6GB RAM per CPU for the large memory nodes)

1. Characteristics of the job

- What is your job?
  - Sequential/parallel
  - If parallel: multi-process vs multi-threaded?

➔How can you tell?

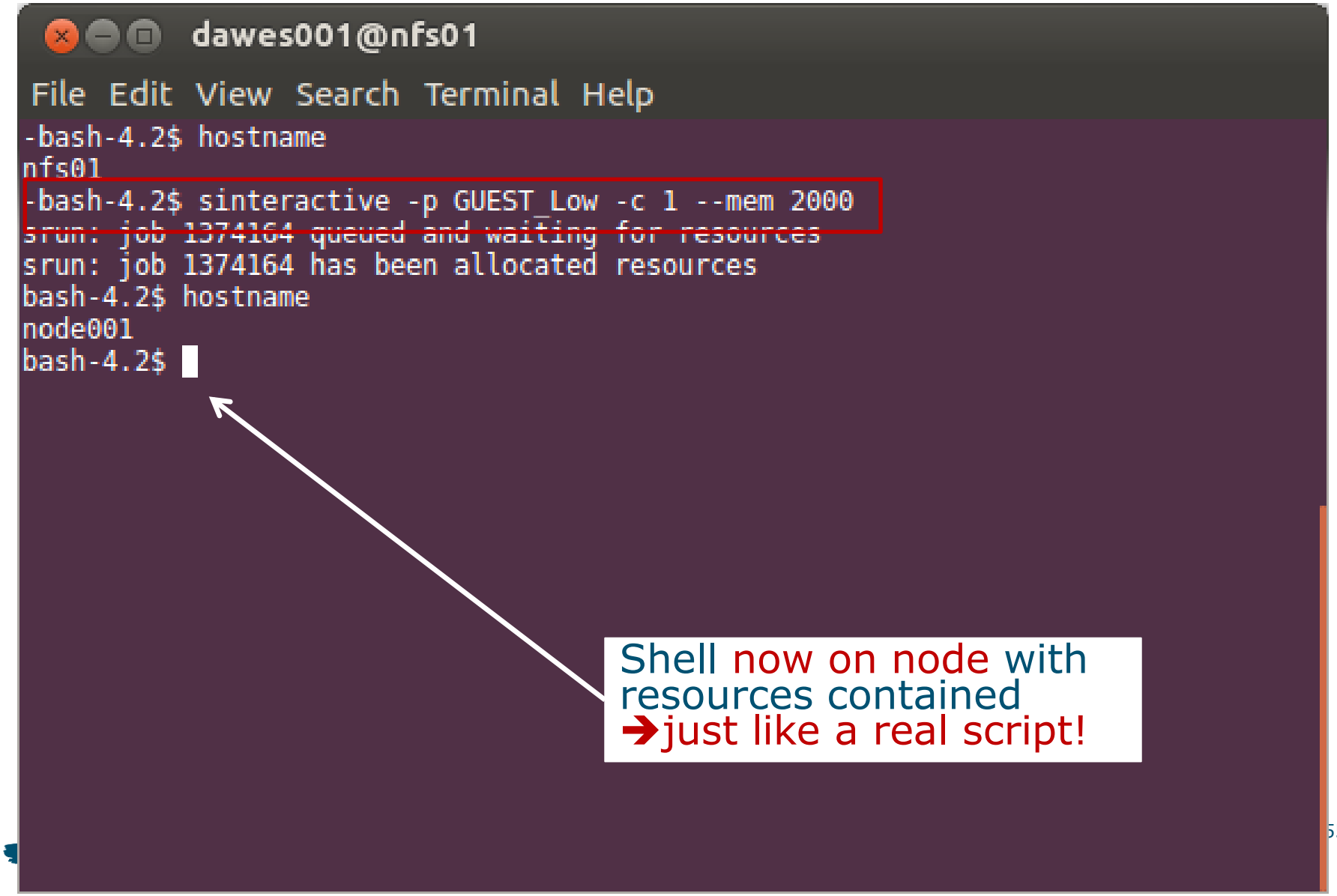
  - RTFM!
  - Read the source code (if available)
  - Just run it!

    ➔use ***sinteractive***!

1. Characteristics of the job

- Run the job using Sandbox environment – interactive jobs
  - ***sinteractive***
    - Wrapper on ***srun***
    - Request immediate interactive shell on node(s)
  - ***sinteractive*** –p GUEST_LOW –c <cpus> --mem <MB>

1. Characteristics of the job



Try it...

1. Create a directory (e.g., 'example_1') in your Lustre scratch directory
2. Download QMSim from this URL and decompress it: http://www.aps.uoguelph.ca/~msargol/qmsim/QMSim_Linux.zip
3. Copy the parameter file
   /lustre/shared/training_slurm/autumn_2017/serial/training/ex_serial_qmsim.prm
   in your directory!
4. Try to find the requirements (e.g., memory) of **QMSim16** using **sinteractive**

   (The parameter file must be mentioned in the command line)

Questions?

2. Writing a submission script

```
#!/bin/bash
# ----------------------------Name of the job-----------------------
#SBATCH --job-name=example1
#----------------------------Mail address----------------------------
#SBATCH --mail-user=jvandenplas@ulg.ac.be
#SBATCH --mail-type=ALL
#----------------------------Output files----------------------------
#SBATCH --output=output_%j.txt
#SBATCH --error=error_output_%j.txt
#----------------------------Other information-----------------------
#SBATCH --comment='Some comments'
#SBATCH --account=123456789
#----------------------------Required resources----------------------
#SBATCH --partition=ABGC_Low
#SBATCH --time=0-1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=4000

#----------------------------Environment, Operations and Job steps----
export OMP_NUM_THREADS=1
echo 'Start calc_grm'
srun calc_grm --par param.par --pca  >out.calc_grm
~
```

SLURM options

Run once for a single task

Run for each task

The Slurm command ***srun***

- ***srun*** [options] executable [args]
  - Run a parallel job on cluster
  - Useful options

Option	Report
-c=<ncpus>	Request that ncpus allocated per process
-n=<number>	Specify the number of tasks to run

The Slurm command ***srun***

```
jvandenp@localhost:~ 78x27
[vande018@nfs01 srun_example]$ more script_slurm.sh
#!/bin/bash
# -----------------------------Name of the job-----------------------
#SBATCH --job-name=srunexample
#------------------------------Mail address-----------------------------
#SBATCH --mail-user=jeremie.vandenplas@wur.nl
#SBATCH --mail-type=ALL
#------------------------------Output files-----------------------------
#SBATCH --output=output.txt
#SBATCH --error=error_output.txt
#------------------------------Other information-----------------------
#SBATCH --comment='Some comments'
#SBATCH --account=4414801570
#------------------------------Required resources----------------------
#SBATCH --partition=ABGC_Low
#SBATCH --time=0-1
#SBATCH --ntasks=4
#SBATCH --mem-per-cpu=4000

#------------------------------Environment, Operations and Job steps----
srun echo "Hello"
[vande018@nfs01 srun_example]$ more output.txt
Hello
Hello
Hello
Hello
[vande018@nfs01 srun_example]$
```

Some SLURM options

You want	SLURM option
To set a **job name**	--job-name="job1"
To get **emails**	--mail-user=name.name@wur.nl --mail-type=BEGIN|END|FAILED|ALL
To set the name of the **output files**	--output=output_%j.txt --error=error_output_%j.txt
To set the name of an **account**	--account=12345678
To attach a **comment** to the job	--comment="abcd"

Some SLURM options: resource

You want	SLURM option
To choose a **partition**	--partition=ABGC_Low|Std|High
To choose a **specific feature** (e.g., a regular compute node)	--constraint=normalmem|largemem
3 **independent processes**	--ntasks=3
3 **independent processes** to spread across **2 nodes**	--ntasks=3 --ntasks-per-node=2
3 **processes** that can use each **2 cores**	--ntasks=3 --cpus-per-task=2
4000MB per cpu	--mem-per-cpu=4000

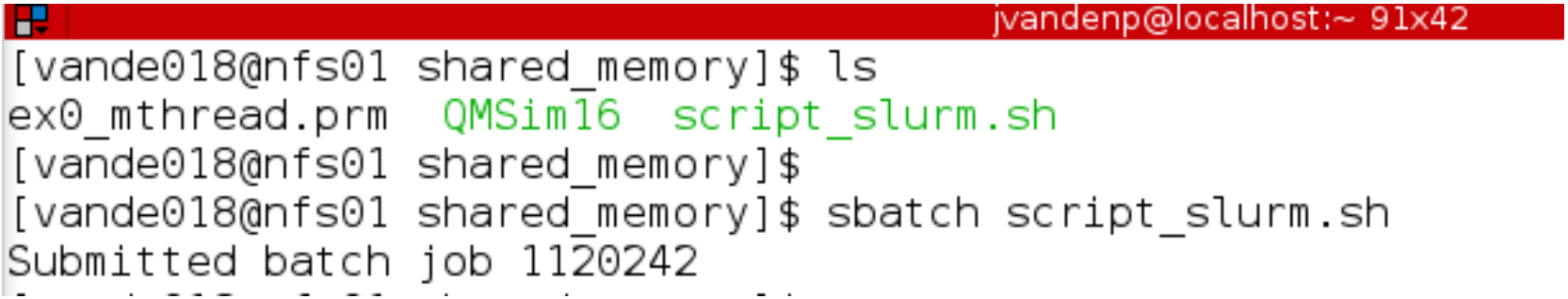
Some SLURM options: partitions

- xxxx_Low
  - Limited time (8h)
  - Very cheap
- xxxx_Std
  - No limit
- xxxx_High
  - No limit + extra costs

- xxxx = ABGC/ESG/GUEST/EDUCATION/...

3. Submitting a job

- The scripts are submitted using the ***sbatch*** command



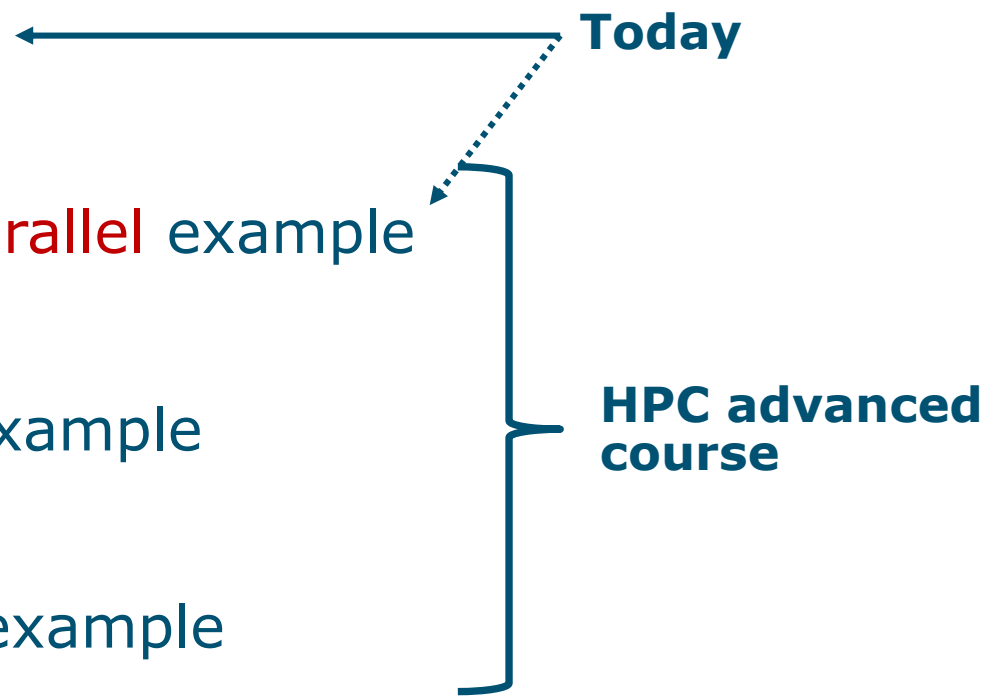
  - Slurm gives an ID to the job ($JOBID)
  - Options may be passed from the command line
    - E.g., sbatch --ntasks=3 script_slurm.sh
    - Will override value in script

Some jobs and their option requirements

- Serial example
- Embarrassingly parallel example
- Shared memory example
- Message passing example

Some jobs and their option requirements

- Serial example
- Embarrassingly parallel example
- Shared memory example
- Message passing example



A serial example

- You run one (several) program(s) serially
- There is no parallelism

A serial example: resource

You want	SLURM options
To chose a partition	--partition=ABGC_Std
8 hours	--time=00-08:00:00
1 independent process	--ntasks=1
4000MB per CPU	--mem-per-cpu=4000
You use	(srun) ./myprog

A serial example: script

```
#!/bin/bash
# ------------------------------Name of the job-------------------------
#SBATCH --job-name=multiple_datafiles
#------------------------------Mail address-----------------------------
#SBATCH --mail-user=jvandenplas@ulg.ac.be
#SBATCH --mail-type=ALL
#------------------------------Output files-----------------------------
#SBATCH --output=output_%j.txt
#SBATCH --error=error_output_%j.txt
#------------------------------Other information------------------------
#SBATCH --comment='Some comments'
#SBATCH --account=4414801570
#------------------------------Required resources-----------------------
#SBATCH --partition=ABGC_Low
#SBATCH --time=0-1
#SBATCH --ntasks=1
#SBATCH --mem-per-cpu=4000

#------------------------------Environment, Operations and Job steps----
srun ./QMSim16 ex0.prm

~
```

4. Monitoring and controlling a job

scancel

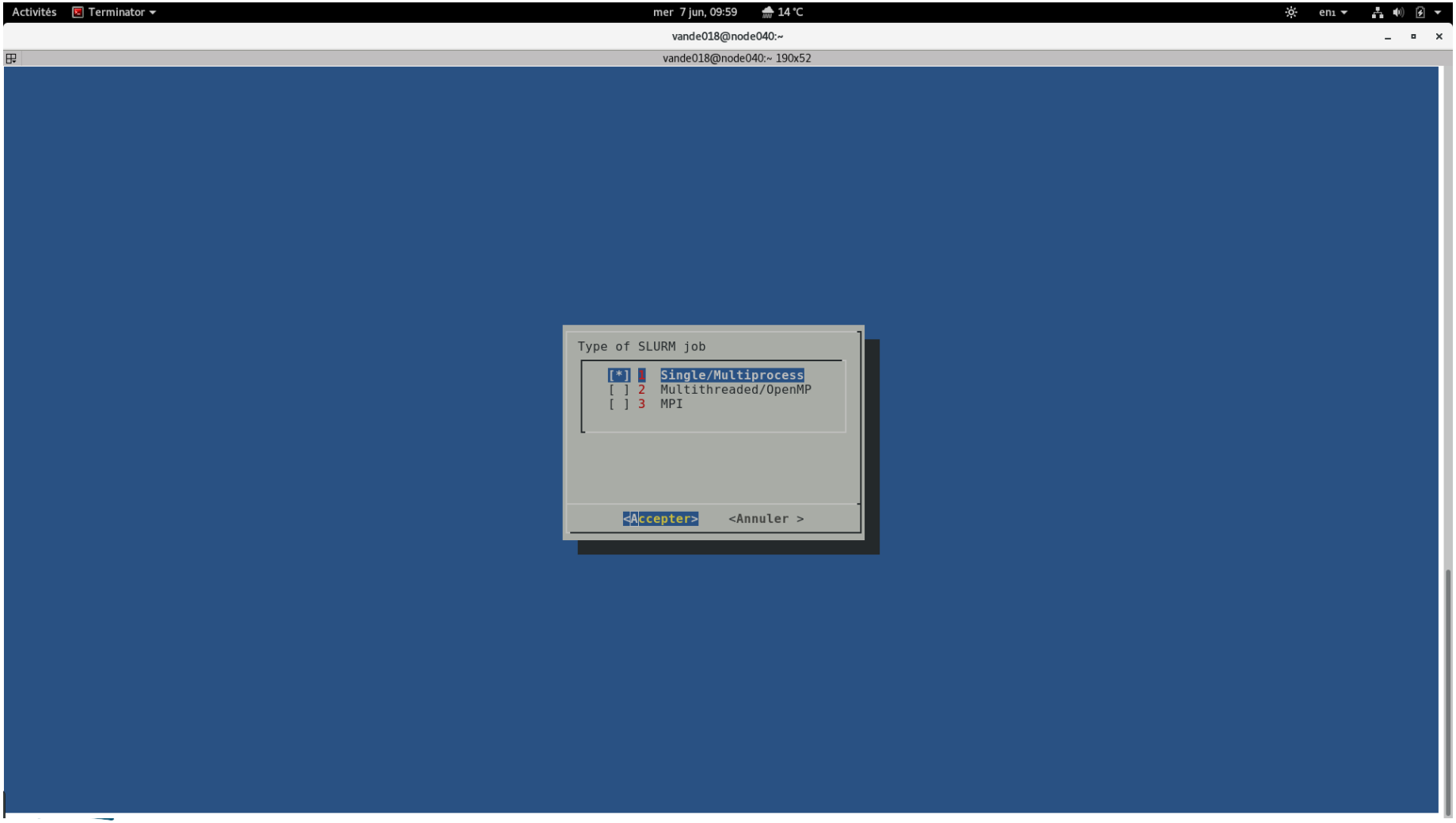
- ***scancel*** [options] [job_id[.step_id]...]
  - Cancel jobs or job steps

Try it...

- Write a Slurm script to run **QMSim16** with the required memory and submit it!

Helpful tool

/cm/shared/apps/accounting/sbatch-generator



4. Monitoring and controlling a job

- Commonly used commands to monitor and control a job
  - ***squeue***
  - ***scontrol***
  - ***scancel***
  - ***sprio***

4. Monitoring and controlling a job

squeue

- ***squeue*** [options]
  - View information about jobs located in the SLURM scheduling queue
  - Useful options

Option	Report
-j <job_id_list>	Report for a list of **specific jobs**
-l	Report **time limit**
--start	Report the **expected start time** of pending jobs
-u <user_id_list>	Report for a list of **users**

4. Monitoring and controlling a job

squeue

vande018@node020:~ 92x46

```
[vande018@nfs01 anag]$ \squeue
  JOBID PARTITION     NAME     USER  ST       TIME  NODES NODELIST(REASON)
1092677  ABGC_Low asreml_R  pelt006   R 22-10:04:41      1 node001
1120251  ABGC_Low  calcgrm vande018   R      45:25      1 node006
1119982  ABGC_Low run_PLIN calus001   R    9:24:43      1 node021
1119972  ABGC_Low run_PLIN calus001   R    9:51:53      1 node013
1083998  ABGC_Std   STELLS otten030   R 51-16:42:46      1 fat001
1109401  ABGC_Std AG_Prove derks047   R 21-05:28:18      1 fat001
1119974  ABGC_Std beagle41 bouwm024   R    9:44:30      1 node020
1119973  ABGC_Std beagle41 bouwm024   R    9:48:50      1 node019
1119957  ABGC_Std AG_MS_VC derks047   R   10:34:59      1 node007
1119856  ABGC_Std F17Run28 tengh001   R 2-23:17:01      1 node001
1118228  ABGC_Std run_m8.s calus001   R 5-22:50:59      1 node005
1118229  ABGC_Std run_m8.s calus001   R 5-22:50:59      1 node001
1118230  ABGC_Std run_m8.s calus001   R 5-22:50:59      1 node001
1118231  ABGC_Std run_m8.s calus001   R 5-22:50:59      1 node002
1118232  ABGC_Std run_m8.s calus001   R 5-22:50:59      1 node002
1118233  ABGC_Std run_m8.s calus001   R 5-22:50:59      1 node004
```

4. Monitoring and controlling a job

scontrol

- ***scontrol*** [options] [command]
  - View Slurm configuration and state
  - Update job resource request
  - Work only for running jobs

  - Useful option

    scontrol show job *JOB_ID*

    ➔***Lots of information***

4. Monitoring and controlling a job

scontrol

```
jvandenp@localhost:~ 91x42
[vande018@nfs01 anag]$ scontrol show jobid 1120249
JobId=1120249 Name=calcgrm
   UserId=vande018(17240402) GroupId=domain users(16777729)
   Priority=1 Account=4414801570 QOS=normal
   JobState=RUNNING Reason=None Dependency=(null)
   Requeue=1 Restarts=0 BatchFlag=1 ExitCode=0:0
   RunTime=00:01:29 TimeLimit=2-00:00:00 TimeMin=N/A
   SubmitTime=2016-03-29T18:48:38 EligibleTime=2016-03-29T18:48:38
   StartTime=2016-03-29T18:48:38 EndTime=2016-03-31T18:48:38
   PreemptTime=None SuspendTime=None SecsPreSuspend=0
   Partition=ABGC_Low AllocNode:Sid=nfs01:10205
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=node006
   BatchHost=node006
   NumNodes=1 NumCPUs=16 CPUs/Task=16 ReqS:C:T=*:*:*
   MinCPUsNode=16 MinMemoryCPU=4000M MinTmpDiskNode=0
   Features=(null) Gres=(null) Reservation=(null)
   Shared=OK Contiguous=0 Licenses=(null) Network=(null)
   Command=/lustre/scratch/WUR/ABGC/vande018/apy1/popsbi/anag/lance.sh
   WorkDir=/lustre/scratch/WUR/ABGC/vande018/apy1/popsbi/anag
```

4. Monitoring and controlling a job

scancel

- ***scancel*** [options] [job_id[.step_id]...]
  - Cancel jobs or job steps

4. Monitoring and controlling a job

sprio

- ***sprio*** [options]
  - View the components of a job's scheduling priority
  - Rule: a job with a lower priority can start before a job with a higher priority IF it does not delay that jobs's start time
  - Useful options

Option	Report
-j <job_id_list>	Report for a list of **specific jobs**
-l	Report **more information**
-u <user_id_list>	Report for a list of **users**

5. Getting an overview of jobs

- Previous and running jobs
  - ***sacct***
- Running jobs
  - ***scontrol***
  - ***sstat***
- *Previous jobs*
  - *Contents of emails (--mail-type=END|ALL)*

5. Getting an overview of jobs

sacct

- ***sacct*** [options]
  - Display accounting data for all jobs/steps
  - Some information are available only at the end of the job
  - Useful options

Option	Report
-j <job_id_list>	Report for a list of **specific jobs**
--format	Comma separated **list of fields**

5. Getting an overview of jobs

sacct

jvandenp@localhost:~

```
[vande018@nfs01 anag]$ jobid=1120217
[vande018@nfs01 anag]$ sacct  -j $jobid --format=JobID%-20,Submit,Eligible,Start,End
              JobID             Submit           Eligible               Start                 End
-------------------- ------------------- ------------------- ------------------- -------------------
1120217              2016-03-29T16:30:12 2016-03-29T16:30:12 2016-03-29T16:30:12 2016-03-29T16:30:14
1120217.batch        2016-03-29T16:30:12 2016-03-29T16:30:12 2016-03-29T16:30:12 2016-03-29T16:30:14
[vande018@nfs01 anag]$ sacct  -j $jobid --format=JobID%-20,AveVMSize,AveRSS,MaxVMSize,MaxRSS
              JobID  AveVMSize     AveRSS  MaxVMSize     MaxRSS
-------------------- ---------- ---------- ---------- ----------
1120217
1120217.batch          555872K     83432K    555872K     83432K
```

5. Getting an overview of running jobs

sstat

- ***sstat*** [options]
  - Display various status information of a running job/step
  - Work only if srun if used
  - Useful options

Option	Report
-j <job_id_list>	Report for a list of **specific jobs**
--format	Comma separated **list of fields**

5. Getting an overview of running jobs

sstat

```
jvandenp@localhost:~ 92x46
[vande018@nfs01 anag]$ sstat -j 1120251
       JobID  MaxVMSize  MaxVMSizeNode  MaxVMSizeTask  AveVMSize     MaxRSS MaxRSSNode MaxRS
STask     AveRSS MaxPages MaxPagesNode   MaxPagesTask   AvePages     MinCPU MinCPUNode MinCP
UTask     AveCPU   NTasks AveCPUFreq ConsumedEnergy
------------ ---------- -------------- -------------- ---------- ---------- ---------- -----
----- ---------- -------- ------------ -------------- ---------- ---------- ---------- -----
----- ---------- -------- ---------- --------------
1120251.0     90449472K        node006              0  90449472K  62096348K    node006
    0  62096348K      31K      node006              0        31K  58:12.000    node006
    0  58:12.000        1     972295                0
[vande018@nfs01 anag]$ sstat --format=JobID,AveCPU,AveRSS,MaxRSS -j 1120251
       JobID     AveCPU     AveRSS     MaxRSS
------------ ---------- ---------- ----------
1120251.0     58:55.000  62096348K  62096348K
[vande018@nfs01 anag]$
```

5. Getting an overview of jobs

emails

- Displays time, memory and CPU data

5. Ge

ema

- Displ

From: root <root@master1.hpcagrogenomics.wur.nl>
To: Vandenplas, Jeremie
Cc:
Subject: SLURM Job_id=1452680 Name=snpblup Failed, Run time 00:43:24, FAILED, ExitCode 1

Final State: FAILED

Time data:

JobID	Submit	Eligible	End	Timelimit	Elapsed
1452680	2017-06-01T11:05:46	2017-06-01T11:05:46	2017-06-01T15:57:28	1-00:00:00	00:43:24
1452680.batch	2017-06-01T15:14:04	2017-06-01T15:14:04	2017-06-01T15:57:28		00:43:24

Memory data:

JobID	ReqMem	AveVMSize	AveRSS	MaxVMSize	MaxRSS
1452680	4000Mc				
1452680.batch	4000Mc	79868064K	48562480K	79868064K	48562480K

CPU data:

JobID	NCPUS	NTasks	CPUTime	UserCPU	SystemCPU	TotalCPU	AveCPU	MinCPU
1452680	16		11:34:24	39:07.705	04:10.573	43:18.279		
1452680.batch	16	1	11:34:24	39:07.705	04:10.573	43:18.279	00:42:53	00:42:53

Accounting Data:
Current resource costs:

TYPE	COST	TIME
Std	0.049	2017-01-01 00:00:00
High	0.099	2017-01-01 00:00:00
Low	0.025	2017-01-01 00:00:00

home	400.0	2017-01-01 00:00:00
scratch	0.0	2014-12-12 15:52:06
backup	400.0	2017-01-01 00:00:00
nobackup	200.0	2017-01-01 00:00:00

USER: vande018
Disk costs
backup: 0.0 EUR
home: 0.0 EUR
nobackup: 0.0 EUR
scratch: 0.0 EUR
TOTAL: 0.0 EUR

Total number of jobs: 39
Compute costs by Partition
Low: 0.0 EUR

WAG
UNIVER

Information on the HPC

/cm/shared/apps/accounting/node_reserve_usage_graph

Information on the HPC

- ***/cm/shared/apps/accounting/node_reserve_usage_graph***
- ***/cm/shared/apps/accounting/get_my_bill***
- ***sinfo***
- ***scontrol show nodes***

- **https://wiki.hpcagrogenomics.wur.nl/index.php/Log_in_to_B4F_cluster**

Extra information – job array

An embarrassingly parallel example

- Parallelism is obtained by launching the same program multiple times simultaneously
- Everybody does the same thing
- No inter-process communication
- Useful cases
  - Multiple input/data files
  - Random sampling
  - ...

An embarrassingly parallel example
Multiple input/data files

- The program processes input/data from one file

  ➔Launch the same program multiple times on distinct input/data files

- It could be submit several times manually
- Or use job arrays!

An embarrassingly parallel example

Resource

You want	SLURM options
To chose a partition	--partition=ABGC_Std
8 hours	--time=00-08:00:00
3 processes to launch 3 completely independent jobs	--array=1-3
1 process per array	--ntasks=1
4000MB per CPU	--mem-per-cpu=4000
You use	$SLURM_ARRAY_TASK_ID (srun) ./myprog

```
[vande018@nfs01 one_parameter_file]$ more script_slurm.sh
#!/bin/bash
# -----------------------------Name of the job-----------------------
#SBATCH --job-name=multiple_datafiles
#-----------------------------Mail address-----------------------------
#SBATCH --mail-user=jernplas@wur.nl
#SBATCH --mail-type=ALL
#-----------------------------Output files-----------------------------
#SBATCH --output=output_%j.txt
#SBATCH --error=error_output_%j.txt
#-----------------------------Other information-----------------------
#SBATCH --comment='Some comments'
#SBATCH --account=44570
#-----------------------------Required resources-----------------------
#SBATCH --partition=ABGC_Low
#SBATCH --time=0-1
#SBATCH --array=1-3
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=4000

#-----------------------------Environment, Operations and Job steps----

echo "Processing the array $SLURM_ARRAY_TASK_ID"
mkdir simulation_$SLURM_ARRAY_TASK_ID && cd simulation_$SLURM_ARRAY_TASK_ID
../QMSim16 ../ex0.prm >out.qmsim

[vande018@nfs01 one_parameter_file]$
```

3 array jobs
(from 1 to 3)

SLURM script

Try it...

- Write a Slurm script to run **4 times** the program **QMSim16** with **1 thread** and a total of **4 GB RAM**.

Thank you!

Questions?

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Helpful tool

http://www.ceci-hpc.be/scriptgen.html