# High Performance Computing Cluster
# Basic course

Jeremie Vandenplas, Gwen Dawes

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# Outline

- Introduction to the HPC Anunna
- Some “advanced” tools in Unix/Linux
- Submitting and monitoring basic jobs on Anunna

# Introduction to the HPC Anunna

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# Outline

- Some definitions
- Description of the HPC Anunna

# Some definitions

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

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  - Group of interconnected computers (node) that work together and act like a single system
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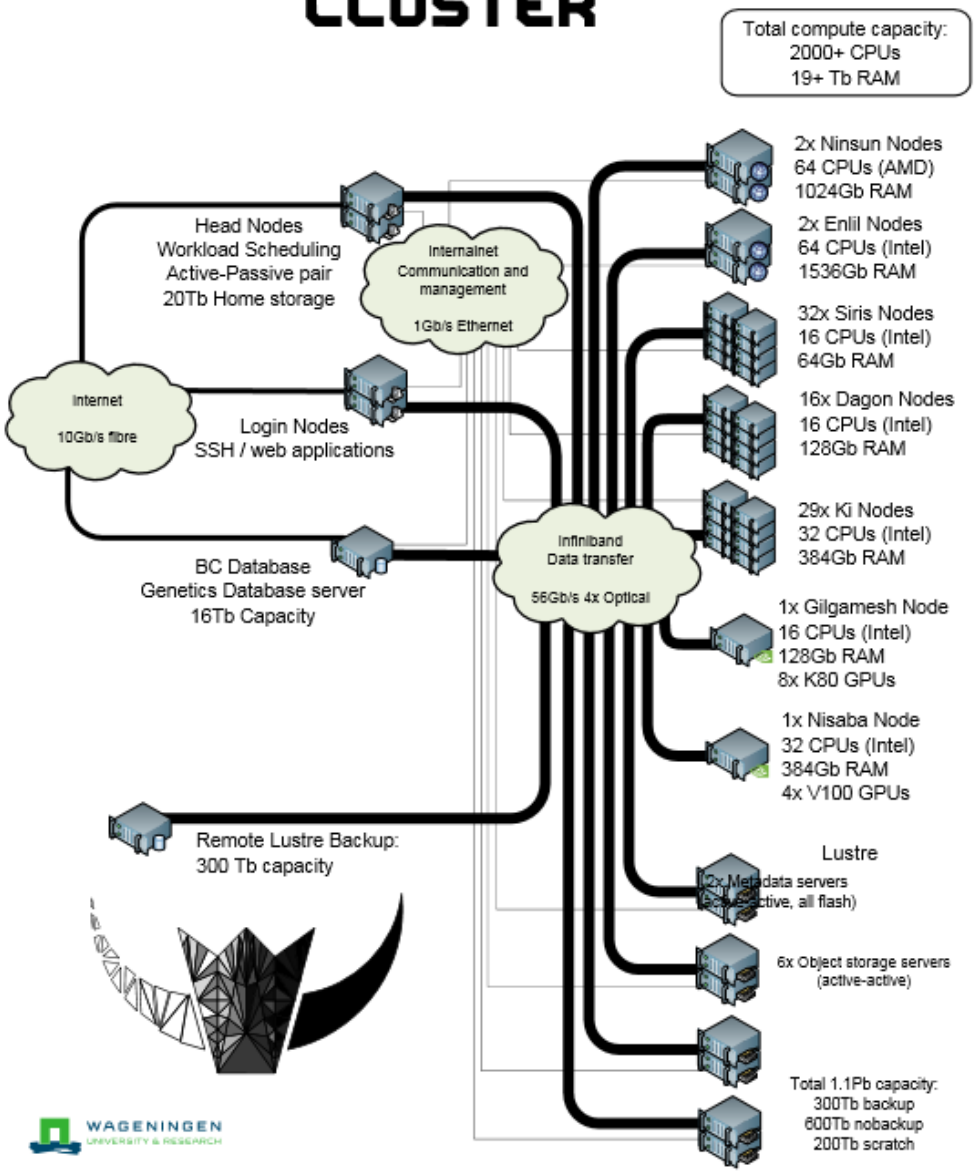
  - Component within a computer that carries out the instructions of a computer program

# 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

# ANUNNA

## HIGH PERFORMANCE CLUSTER

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# HPC Anunna

- 48 Computes nodes
  - 16 cores (Intel), 64 GB or 128 GB RAM
- 29 Computes nodes
  - 32 cores (Intel), 328 GB RAM
- 2 Fat nodes
  - 64 cores (AMD), 1 TB RAM
- 2 Fat nodes
  - 64 cores (Intel), 1.5 TB RAM
- 4 GPU nodes
  - NVIDIA Tesla V10
- 1500 TB Lustre parallel file system (15 GB/s)

# HPC Anunna

- Software
  - Scientific Linux
  - Jobs scheduling with SLURM
  - Multiple compilers
  - R, SPARK, Octave, Jupyter, Matlab, Julia, ...
  - Multiple file formats (e.g., HDF5)
  - MPI

# HPC Anunna – main storage

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

- Archive
  - /archive/[partner]/[username]
  - Cheap
  - Only for storage and for WUR

# HPC Anunna – main storage

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

# HPC Anunna – "rules"

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

# HPC Anunna – useful information

- HPC Anunna wiki
  - https://wiki.anunna.wur.nl/index.php/Main_Page
- Linux User Group at WUR
  - https://lug.wur.nl/index.php/Main_Page
- Support
  - hpc.support@wur.nl

# Questions?

# Some “advanced” tools in Unix/Linux

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# (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 ***WinSCP***

- For MS Windows OS
- To install WinSCP:

***https://winscp.net/eng/download.php***

# 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:

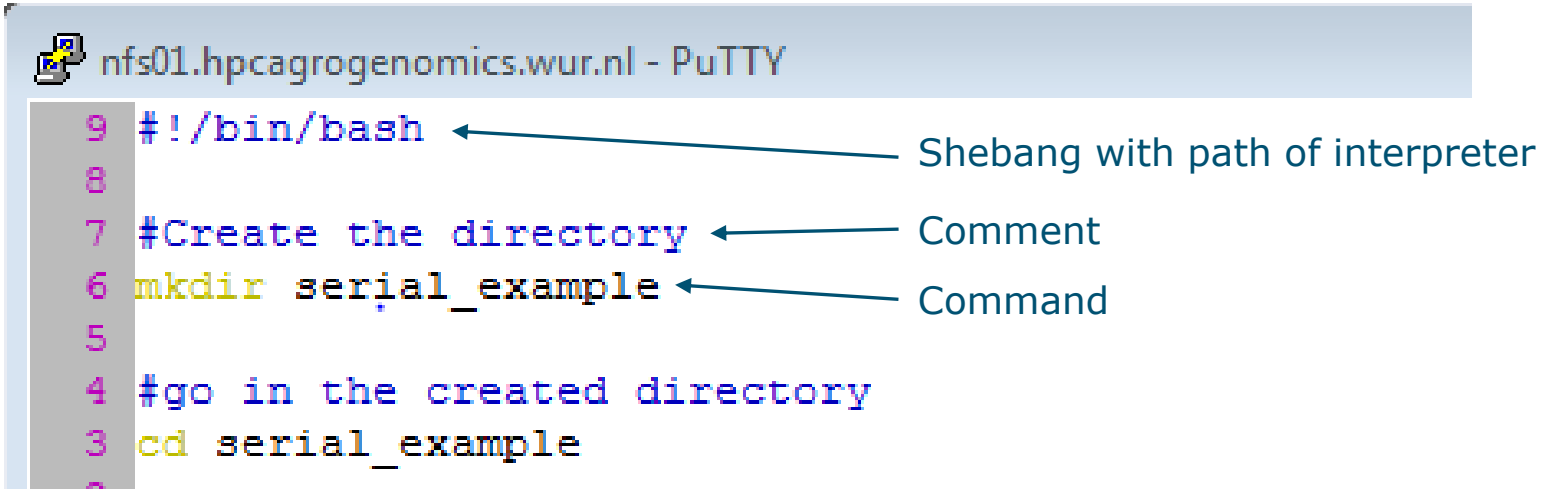
***unset MYVARIABLE***

# Environment modules

- Provides many software not installed by default
- module avail
- module list
- module load name
- module rm

# A bash (Shell) script

- Plain text file which contains a set/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 (***wget***) and decompress (***unzip***) it:

   https://git.wur.nl/dawes001/public-files/raw/master/QMSim-Linux.zip
3. Copy the parameter file /lustre/shared/training_slurm/autumn_2021/serial/training/ex_serial_qmsim.prm in your directory!

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

# Questions?

# Solution

```
1   #!/bin/bash
  1
  2 #Environment variable
  3 namedir='example_1'
  4
  5 #delete the directory if it exists
  6 if [ -d $namedir ]; then rm -r $namedir; fi
  7
  8 #Create the directory
  9 mkdir $namedir
 10
 11 #go in the created directory
 12 cd $namedir
 13
 14  #dowload the archive QMSim
 15  wget https://git.wur.nl/dawes001/public-files/raw/master/QMSim-Linux.zip
 16
 17  #decompress the archive
 18  unzip QMSim-Linux.zip
 19
 20  #copy the parameter file
 21  cp /lustre/shared/training_slurm/ autumn_2019  /serial/training/ex_serial_qmsim.prm .
 22
 23  #list the content of the directory
 24  ls
~
```

# 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 Anunna

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# Outline

- Some definitions
- Running a basic job on the nodes of Anunna
  - 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
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13283 vande018  20   0  112m 2352 1508 S  0.0  0.0   0:00.39 bash
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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
```

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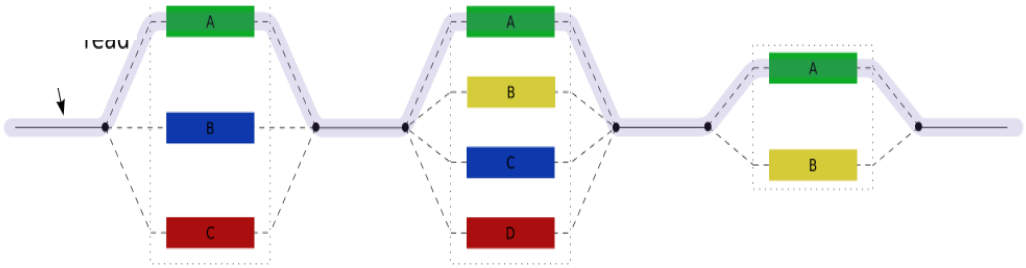
# Some definitions

- 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***

jvandenp@localhost:~ 92x46

```
top - 13:16:08 up 11 days, 18:06, 43 users,  load average: 7.13, 5.27, 4.28
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Mem:  66059268k total, 62016800k used,  4042468k free,    88444k buffers
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# Running a job on the nodes of Anunna?

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- 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 Anunna?

- 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 (compute 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.

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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'

#------------------------------Required resources-----------------------

#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?

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
  - 4 GB RAM per CPU for nodes with 64 GB
  - 8 GB RAM per CPU for nodes with 128 GB
  - 10.2 GB RAM per CPU for nodes with 328 GB
  - 15.6 GB RAM per CPU for nodes with 1 TB
  - 23.4 GB RAM per CPU for nodes with 1.5 TB

# 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!

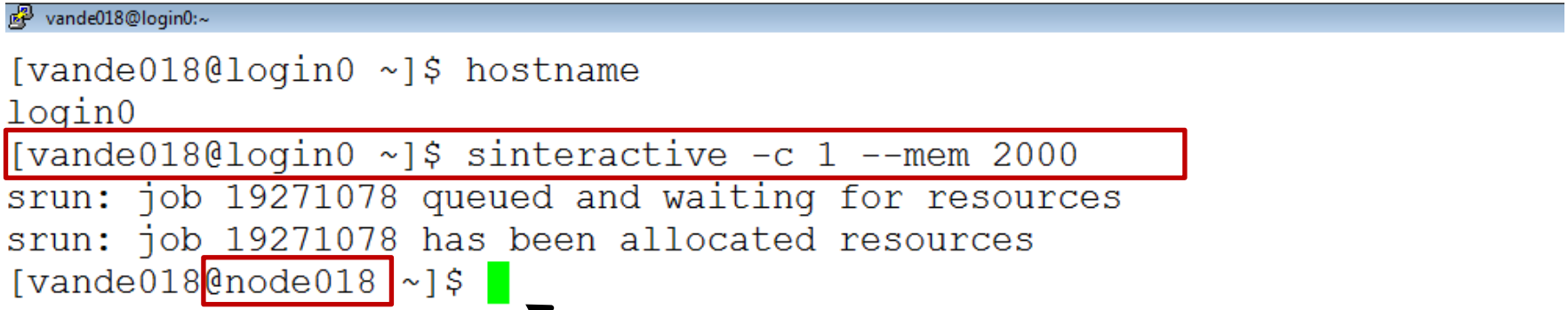
    ➔use ***sinteractive***!

# 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*** –c <cpus> --mem <MB>

# 1. Characteristics of the job




Shell now on node018
with resources contained
➔just like a real script!

# Try it...

1. Create a directory (e.g., ‘example_1’) in your Lustre scratch directory
2. Download QMSim from this URL and decompress it: https://git.wur.nl/dawes001/public-files/raw/master/QMSim-Linux.zip
3. Copy the parameter file /lustre/shared/training_slurm/autumn_2021/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=serial_example
#-----------------------------Mail address-----------------------------
#SBATCH --mail-user=my.email.address@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'
#-----------------------------Required resources---------------------

#SBATCH --time=0-1
#SBATCH --ntasks=4
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=4000

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

echo 'Hello from a single task'

srun echo 'Hello from EACH task'
```

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***

```
[vande018@nfs01 vande018]$ cat script_slurm.sh
#!/bin/bash
# ----------------------------Name of the job-------------------------
#SBATCH --job-name=serial_example
#----------------------------Mail address-----------------------------
#SBATCH --mail-user=my.email.address@wur.nl
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#----------------------------Environment, Operations and Job steps----

echo 'Hello from a single task'

srun echo 'Hello from EACH task'

[vande018@nfs01 vande018]$
[vande018@nfs01 vande018]$ cat output_10969988.txt
Hello from a single task
Hello from EACH task
Hello from EACH task
Hello from EACH task
Hello from EACH task
[vande018@nfs01 vande018]$
```

# Some SLURM options

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

# Some SLURM options: resource

| You want | SLURM option |
|---|---|
| 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: features

- 128g/384g/1019g/1536g/normalmem/largemem/moremem
  - Nodes with specific RAM
- 16cpus/32cpus/64cpus
  - Nodes with a specific total number of CPUs
- 4gpercpu/8gpercpu/16gpercpu/24gpercpu
- nvidia/K80/V100
  - Nodes with GPUs
- Amd/avx512/intel
  - Nodes with specific processors
- dagon/enlil/gilgamesh/ki/ninsun/siris/gen2

# Some SLURM options: resource

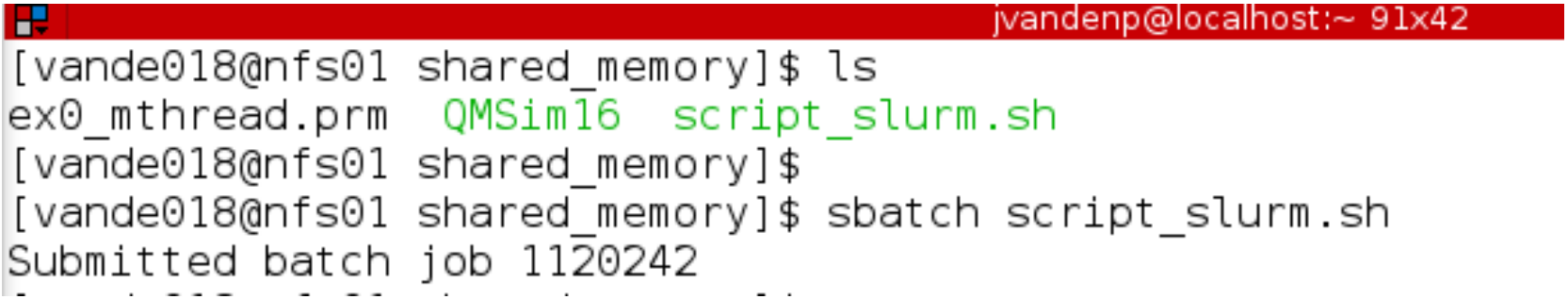
| You want | SLURM option |
| --- | --- |
| To choose a **partition** | --partition=main\|gpu<br>*Default: main* |
| To choose a **Quality of Service** | --qos=low\|std\|high\|interactive<br>*Default: std* |

# Some SLURM options: quality of service

- low
  - 90 days
  - Very cheap
- std
  - 90 days
- high
  - 90 days+ extra costs
- Interactive
  - 1 day
  - Immediate running jobs
  - A few jobs only

# 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

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- Serial example
- Embarrassingly parallel example
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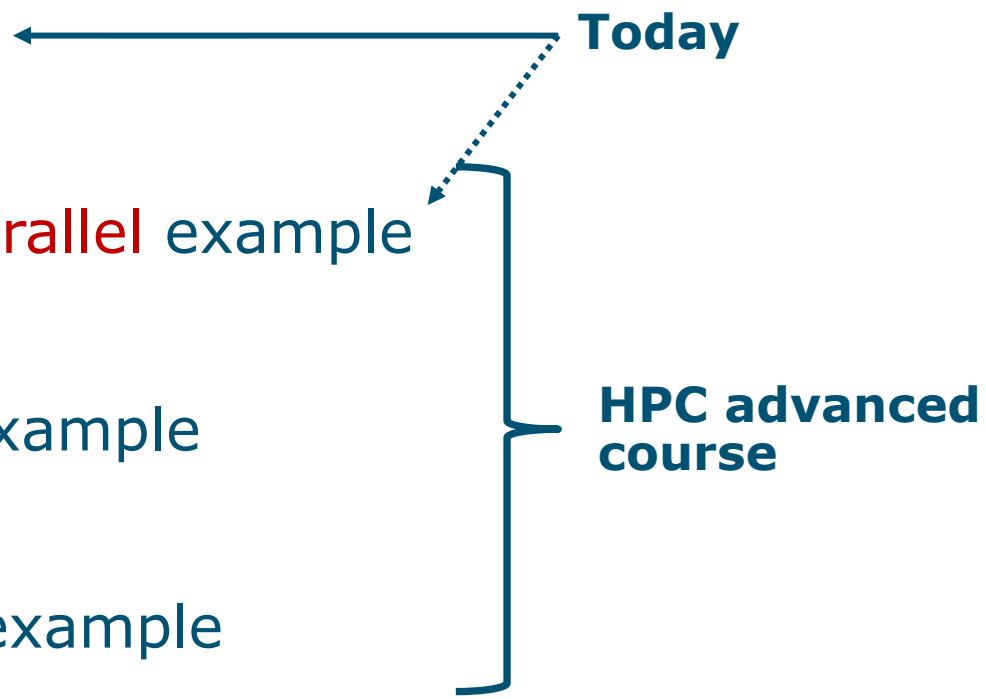


# A serial example


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

# A serial example: resource

| You want | SLURM options |
|---|---|
| 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=serial_example
#-----------------------------Mail address-----------------------------
#SBATCH --mail-user=my.email.address@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'
#-----------------------------Required resources---------------------
:
#SBATCH --time=0-1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=4000

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


srun echo 'Hello'
```

# 4. Monitoring and controlling a job

## *scancel*

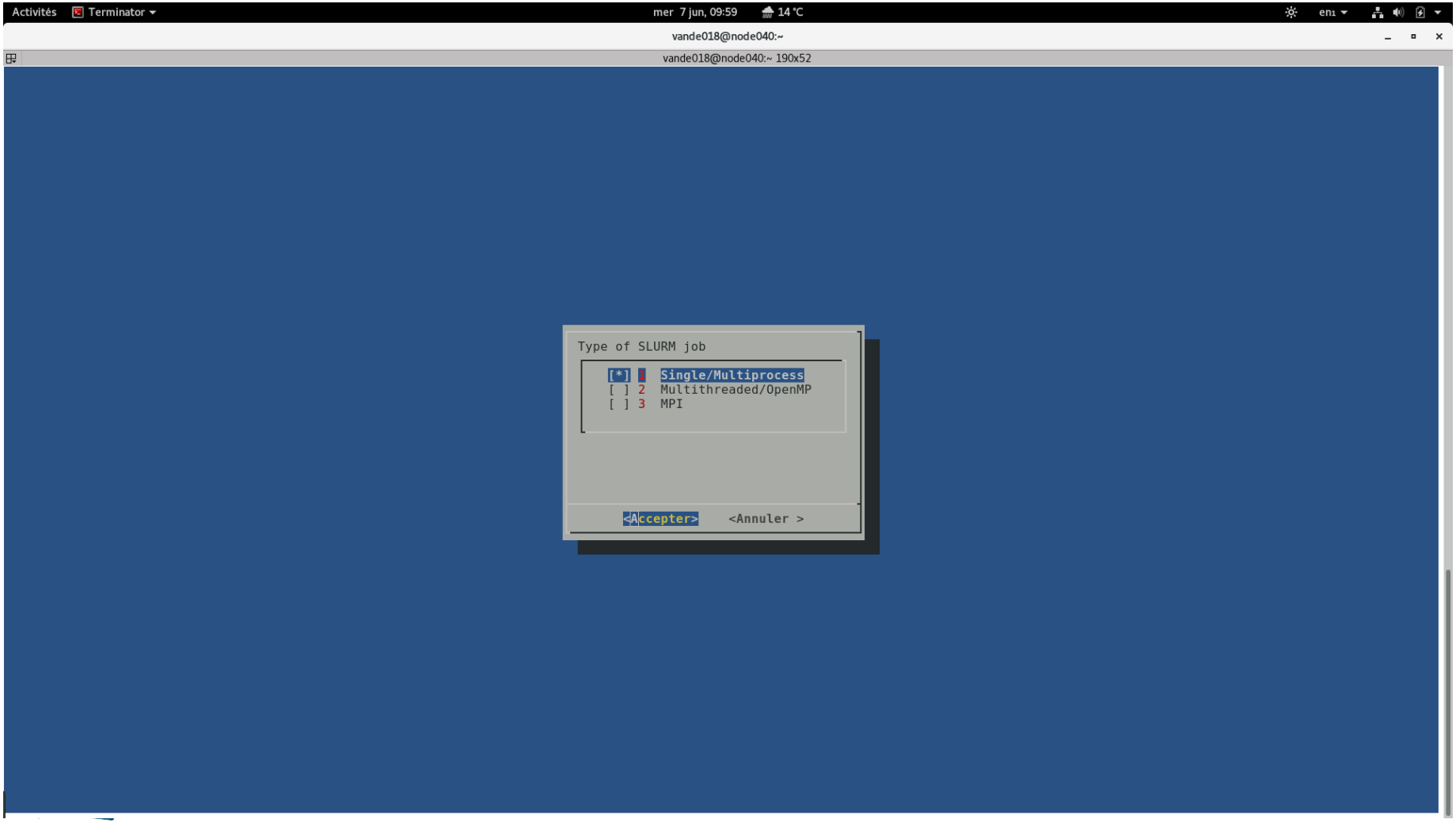
- ***scancel*** [options] [job_id[.step_id]...]
  - Cancel jobs or job steps

# 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 options

    ***scontrol show job*** *JOB_ID*

    ***scontrol show nodes***

  ➔***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

# Information on the HPC

## /cm/shared/apps/accounting/node_reserve_usage_graph

# Information on the HPC Anunna

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

# 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 |
|---|---|
| 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<br>(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'

#-----------------------------Required resources---------------------

#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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