High Performance Computing Cluster Advanced course

Jeremie Vandenplas, Gwen Dawes

October 2021

WAGENINGEN UR
For quality of life

Outline

- Introduction to the HPC Anunna
- Submitting and monitoring jobs on the HPC
- Parallel jobs on the HPC
- Tips and tricks

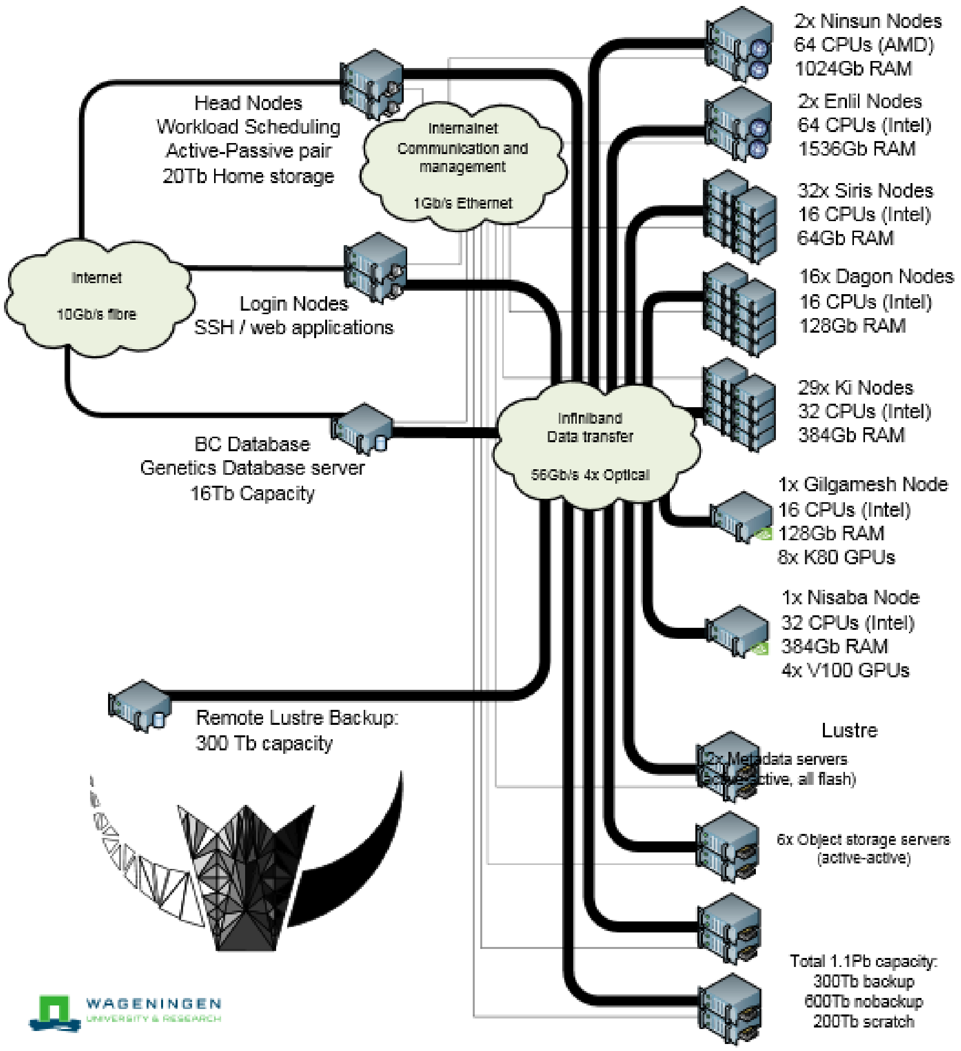
Introduction to the HPC Anunna

Jeremie Vandenplas, Gwen Dawes

ANUNNA

HIGH PERFORMANCE CLUSTER

Total compute capacity:
2000+ CPUs
19+ Tb RAM



Head Nodes
Workload Scheduling
Active-Passive pair
20Tb Home storage

Internalnet
Communication and management
1Gb/s Ethernet

Internet
10Gb/s fibre

Login Nodes
SSH / web applications

BC Database
Genetics Database server
16Tb Capacity

Infiniband
Data transfer
56Gb/s 4x Optical

Remote Lustre Backup:
300 Tb capacity

2x Ninsun Nodes
64 CPUs (AMD)
1024Gb RAM

2x Enlil Nodes
64 CPUs (Intel)
1536Gb RAM

32x Siris Nodes
16 CPUs (Intel)
64Gb RAM

16x Dagon Nodes
16 CPUs (Intel)
128Gb RAM

29x Ki Nodes
32 CPUs (Intel)
384Gb RAM

1x Gilgamesh Node
16 CPUs (Intel)
128Gb RAM
8x K80 GPUs

1x Nisaba Node
32 CPUs (Intel)
384Gb RAM
4x V100 GPUs

Lustre
2x Metadata servers
(active-active, all flash)

6x Object storage servers
(active-active)

Total 1.1Pb capacity:
300Tb backup
600Tb nobackup
200Tb scratch

WAGENI
For q

WAGENINGEN
UNIVERSITY & RESEARCH

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
- 4x GPU nodes
  - NVIDIA Tesla V10
- 1000 TB Lustre parallel file system (15 GB/s)

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)
  - backup
    - /lustre/backup/[partner]/[unit]/[username]
  - nobackup
    - /lustre/nobackup/[partner]/[unit]/[username]
  - scratch
    - /lustre/scratch/[partner]/[unit]/[username]
    - Regularly cleaned up

HPC Anunna – “rules”

- Home
  - Jobscripts
  - Small datasets (performance)
  - No 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?

Submitting and monitoring basic jobs on the HPC

J. Vandenplas, G. Dawes

WAGENINGEN UR
For quality of life

Outline

- Running a job on the nodes of the HPC
  - Introduction to SLURM
  - Characteristics of a job
  - Writing and submitting a script
  - Monitoring and controlling a job
  - Tips and tricks
- Types of jobs
  - Sequential
  - Array
  - Shared memory
  - Distributed memory

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

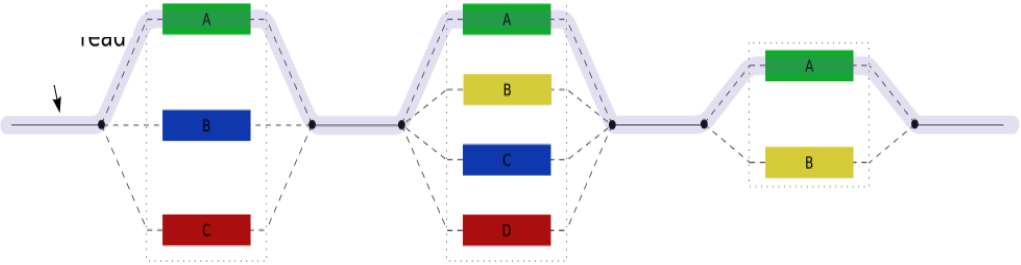
Job scheduler/Resource manager

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

- 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

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 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 job on the nodes of the HPC?

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

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

➔How can you know it?

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

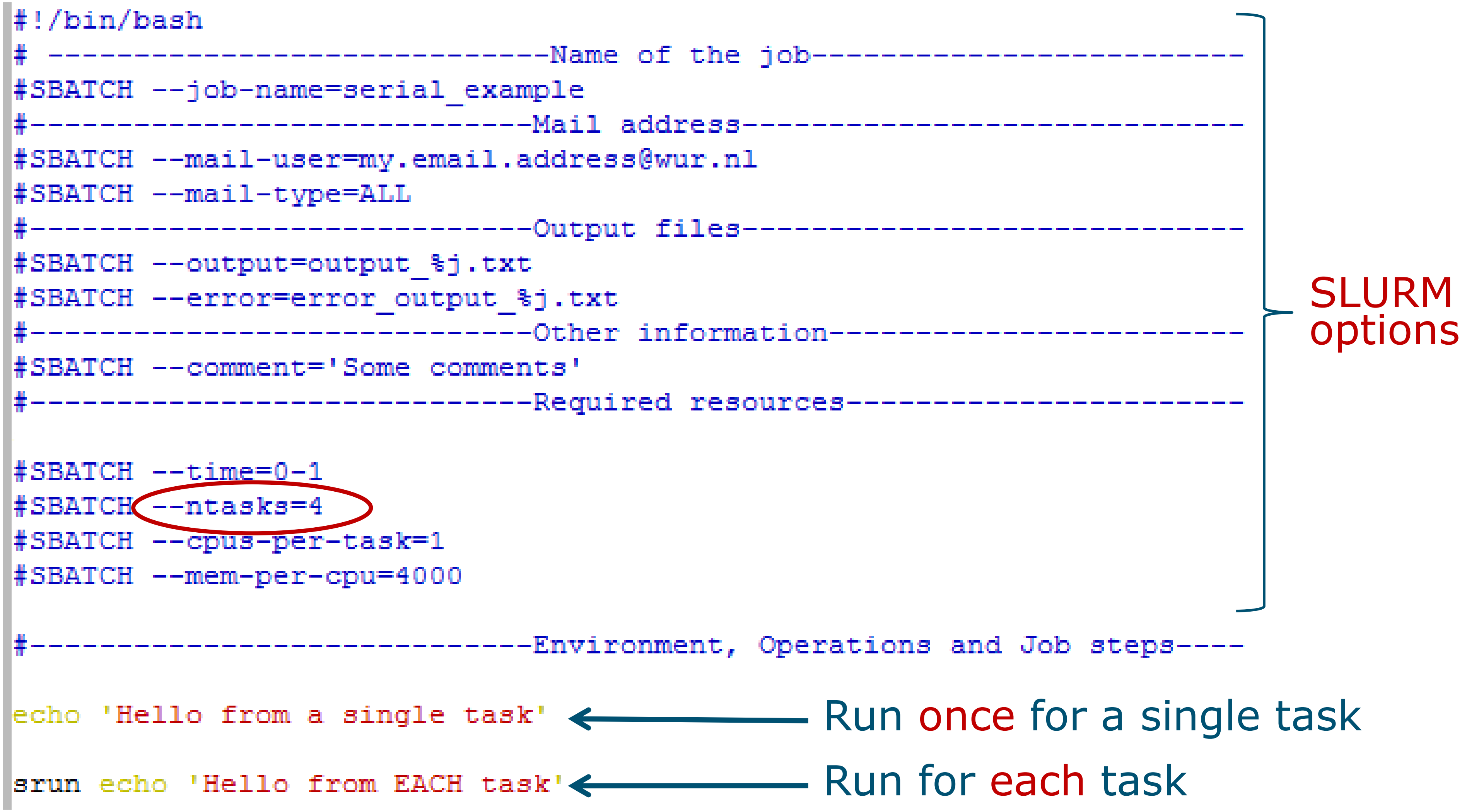
  ➔use ***sinteractive***!

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

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

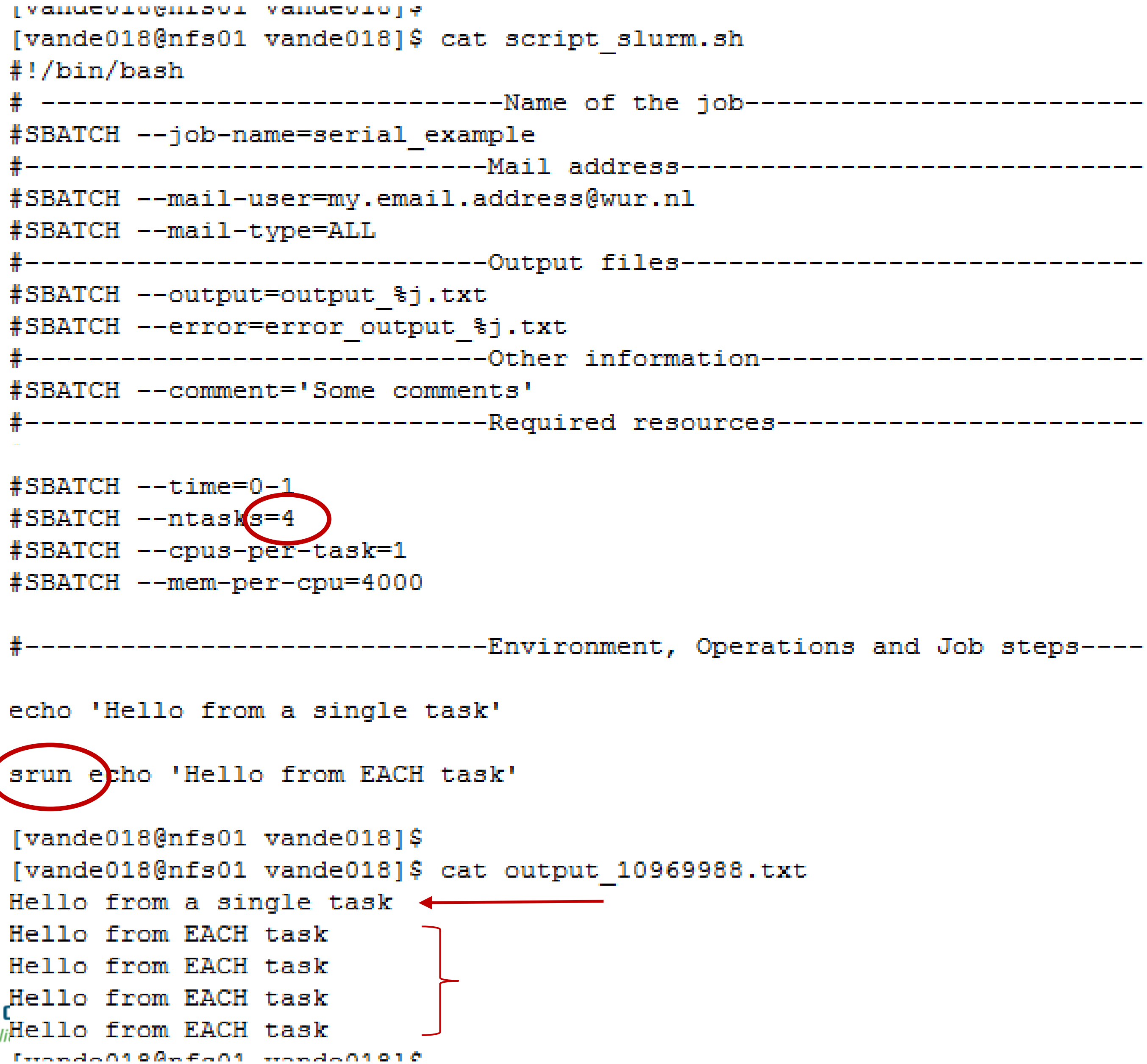
Run for each task

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]$
[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
#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'

[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 --mail-type=BEGIN|END|FAILED|ALL
To set the name of the **output files**	--output=output_%j.txt --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
12 hours	--time=0-12:00:00
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

WAGENINGEN UR
For quality of life

Some SLURM options: resource

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

Some SLURM options: quality of service

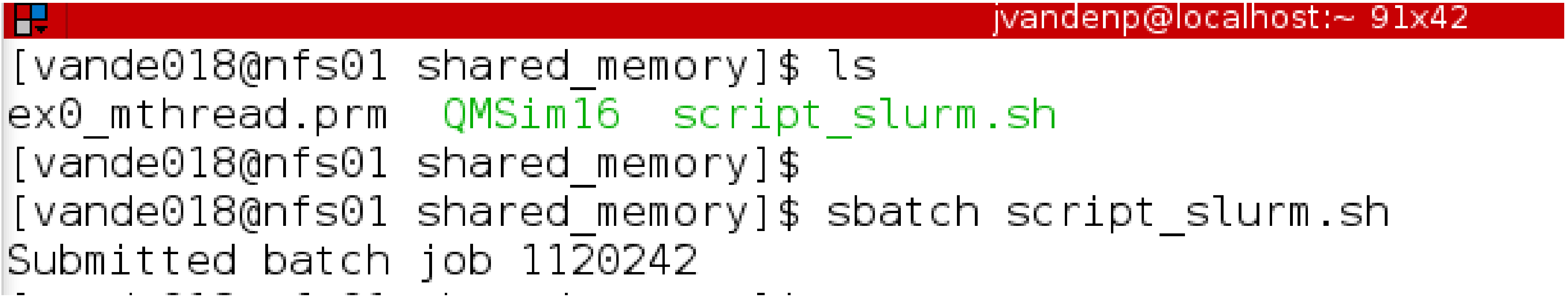
- low
  - 90 days
  - Very cheap
- std
  - 90 days
- high
  - 90 days+ extra costs
- Interactive
  - 1 day
  - Immediate running jobs
  - A few jobs only

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

3. Submitting a job

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



```
[vande018@nfs01 shared_memory]$ ls
ex0_mthread.prm  QMSim16  script_slurm.sh
[vande018@nfs01 shared_memory]$
[vande018@nfs01 shared_memory]$ sbatch script_slurm.sh
Submitted batch job 1120242
```

- 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
- See Gwen ‘s tips and tricks

4. Monitoring and controlling a job

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

- More details in Gwen’s presentation

4. Monitoring and controlling a job

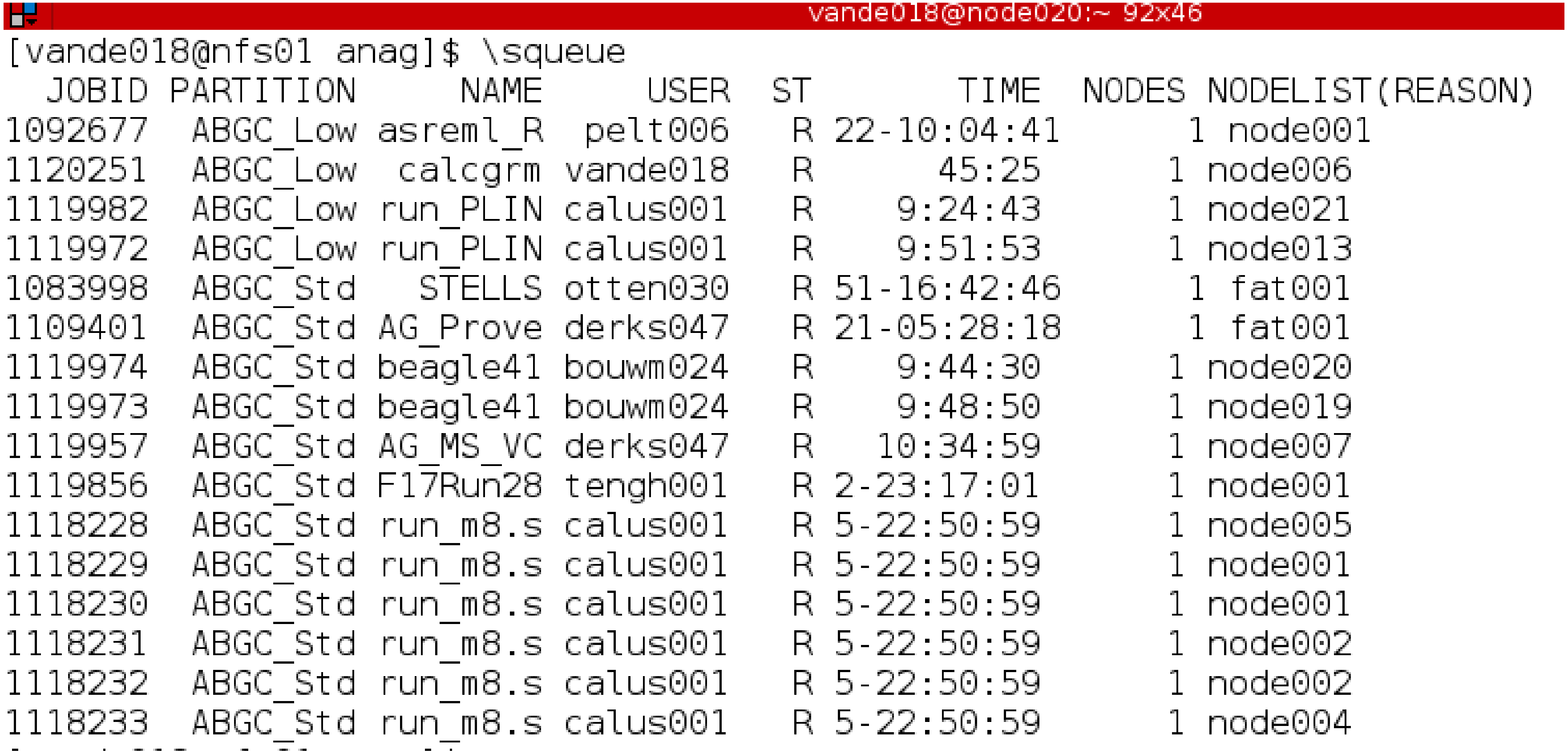
squeue

- ***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@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
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**

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***

5. Getting an overview of jobs

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

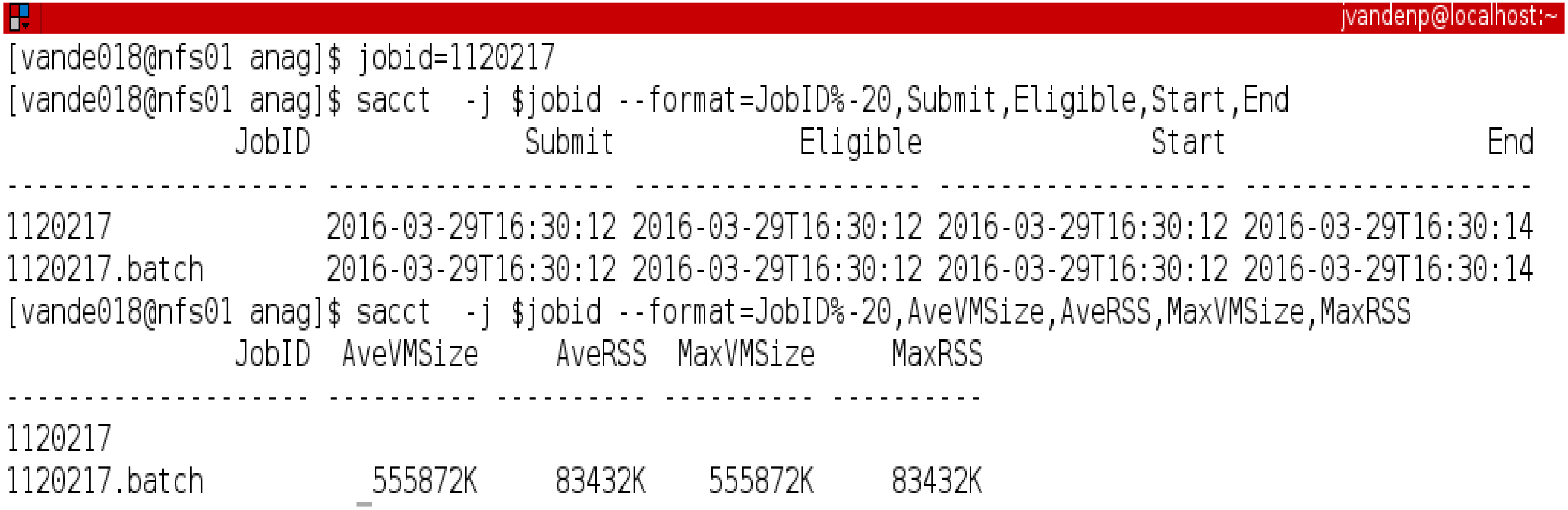
5. Getting an overview of jobs
sacct

- ***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



```
[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
```

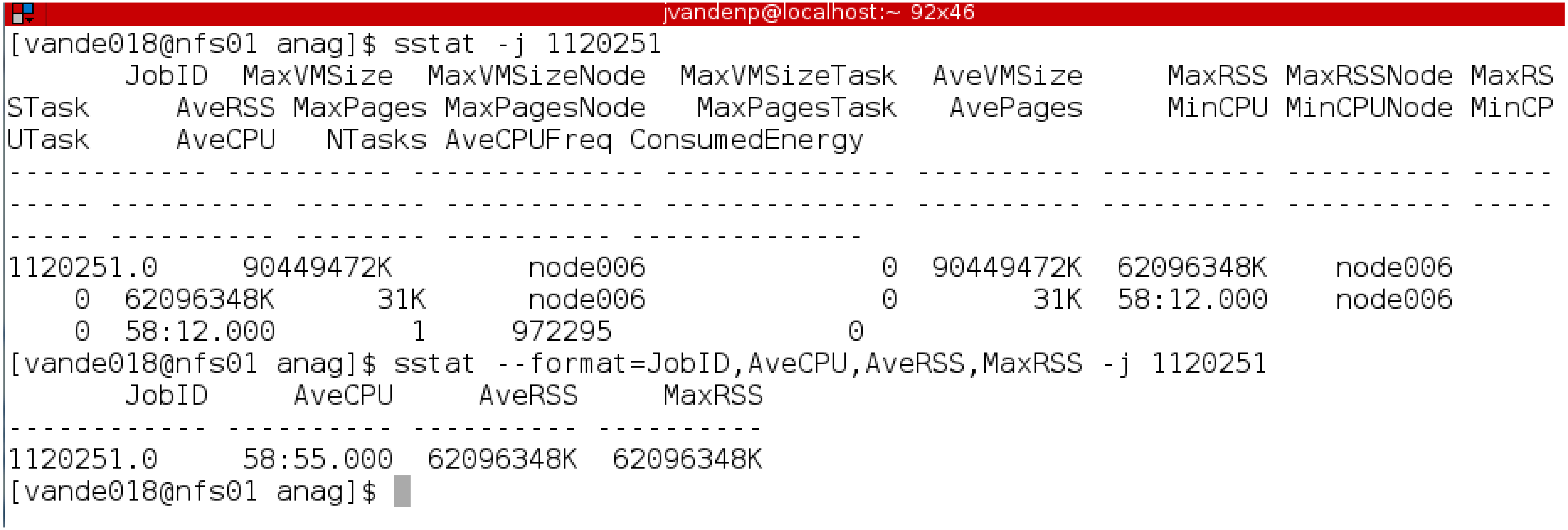
5. Getting an overview of running jobs
sstat

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



```
[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]$ 
```

WAGENINGEN UR
For quality of life

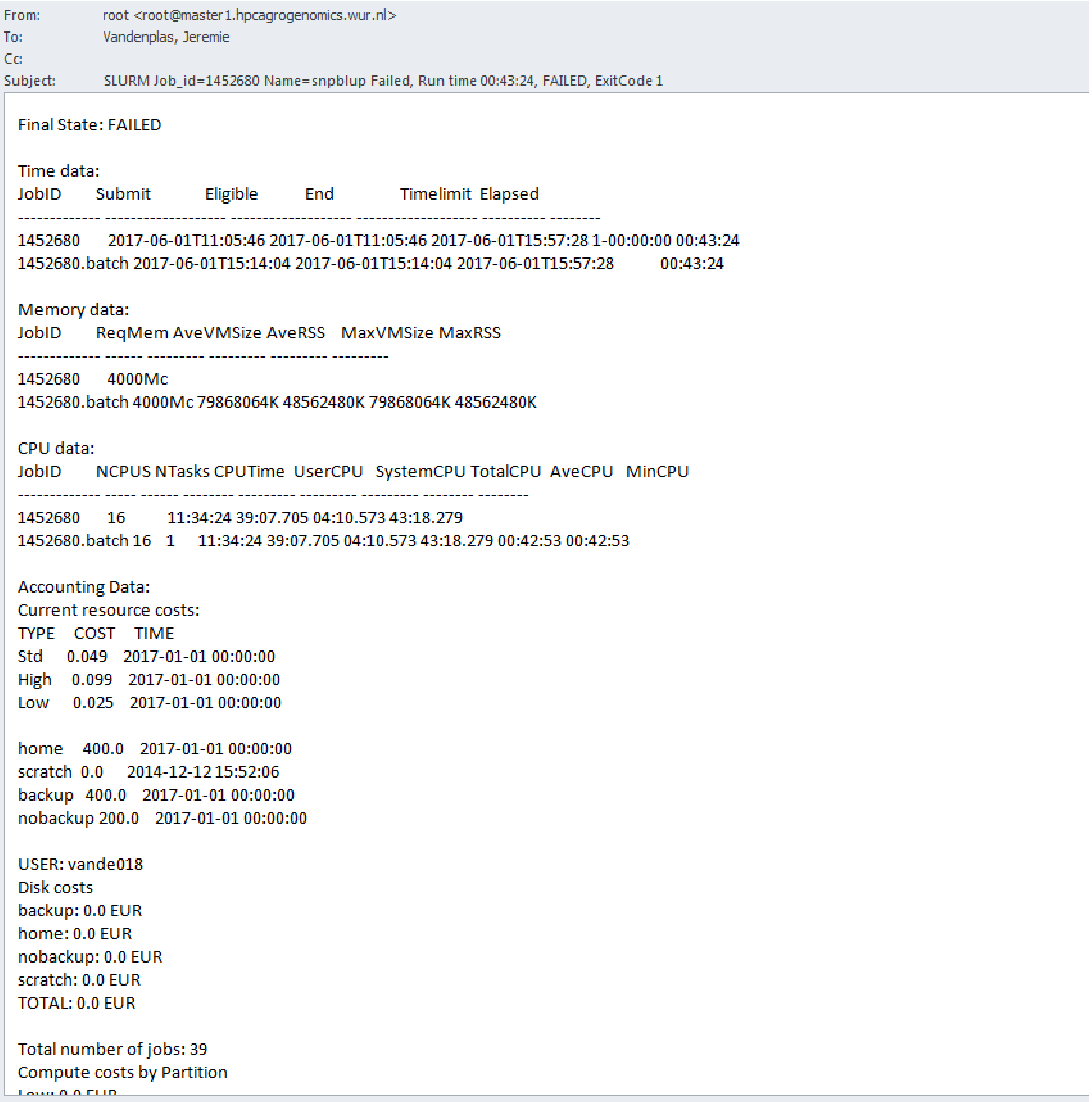
5. Getting an overview of jobs
emails

- Displays time, memory and CPU data

5. Ge

emai

- Displ

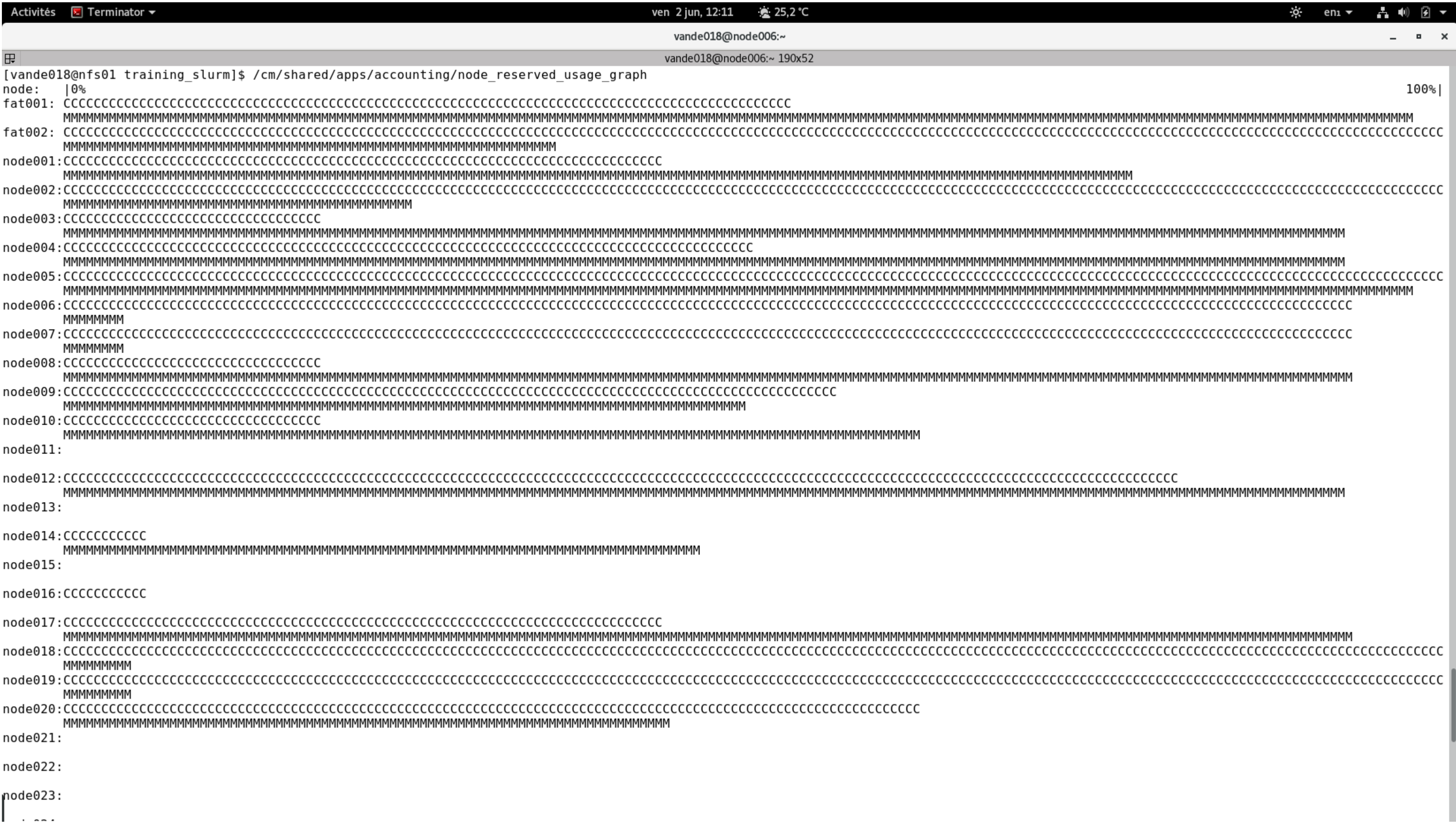


From: root <root@master1.hpcagrogenomics.wur.nl>
To: Vandenplas, Jeremie
Cc:
Subject: SLURM Job_id=1452680 Name=snpblup Failed, Run time 00:43:24, FAILED, ExitCode 1

```
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



```
[vande018@nfs01 training_slurm]$ /cm/shared/apps/accounting/node_reserved_usage_graph
node:    |0%                                                                                                                                                                          100%|
fat001: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
fat002: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node001:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node002:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node003:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node004:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node005:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node006:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMM
node007:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMM
node008:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node009:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node010:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node011:

node012:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node013:

node014:CCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node015:

node016:CCCCCCCCCCC

node017:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node018:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMM
node019:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMM
node020:CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
        MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
node021:

node022:

node023:
```

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**

Gwen ‘s presentation

- Scontrol
- Sbatch
- Dependencies
- …

Parallel jobs on the HPC Anunna

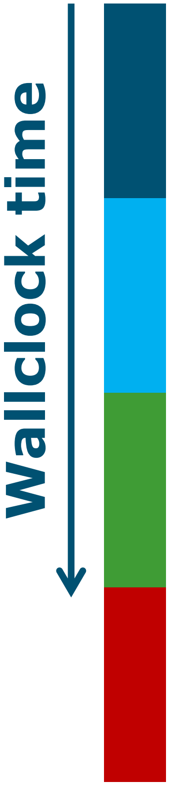
Jeremie Vandenplas, Gwen Dawes

WAGENINGEN UR
For quality of life

Some jobs and their option requirements

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

A serial example

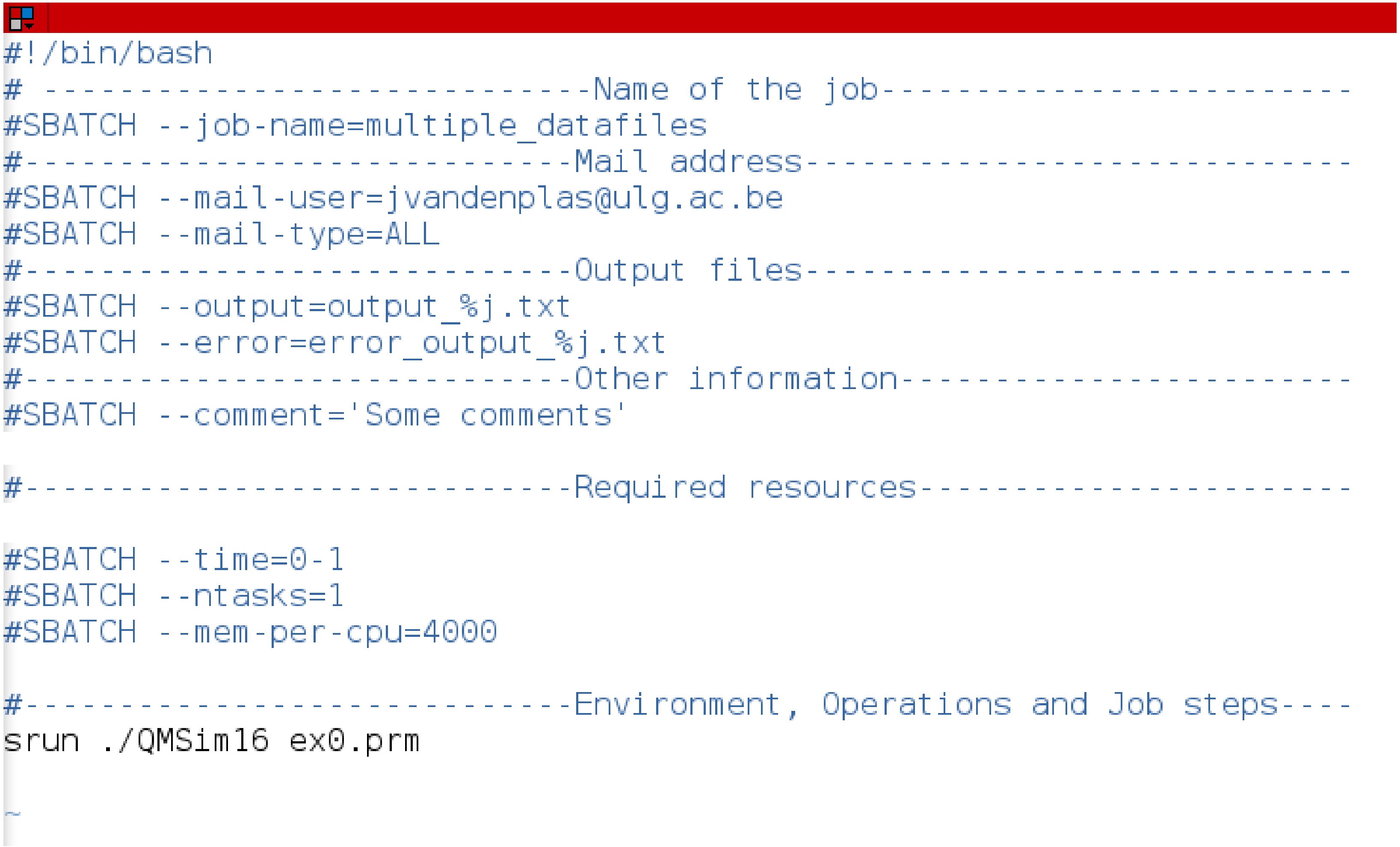


- You run one (several) program(s) serially
- There is no parallelism

A serial example: resource

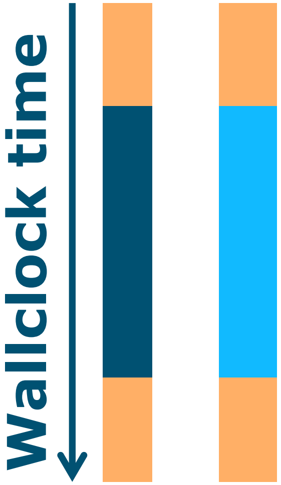
You want	SLURM options
8 hours	--time=00-08:00:00
1 independent process	--ntasks=1
4000MB per CPU	--mem-per-cpu=4000
You use	(srun) ./myprog

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'

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

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

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

~
```

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

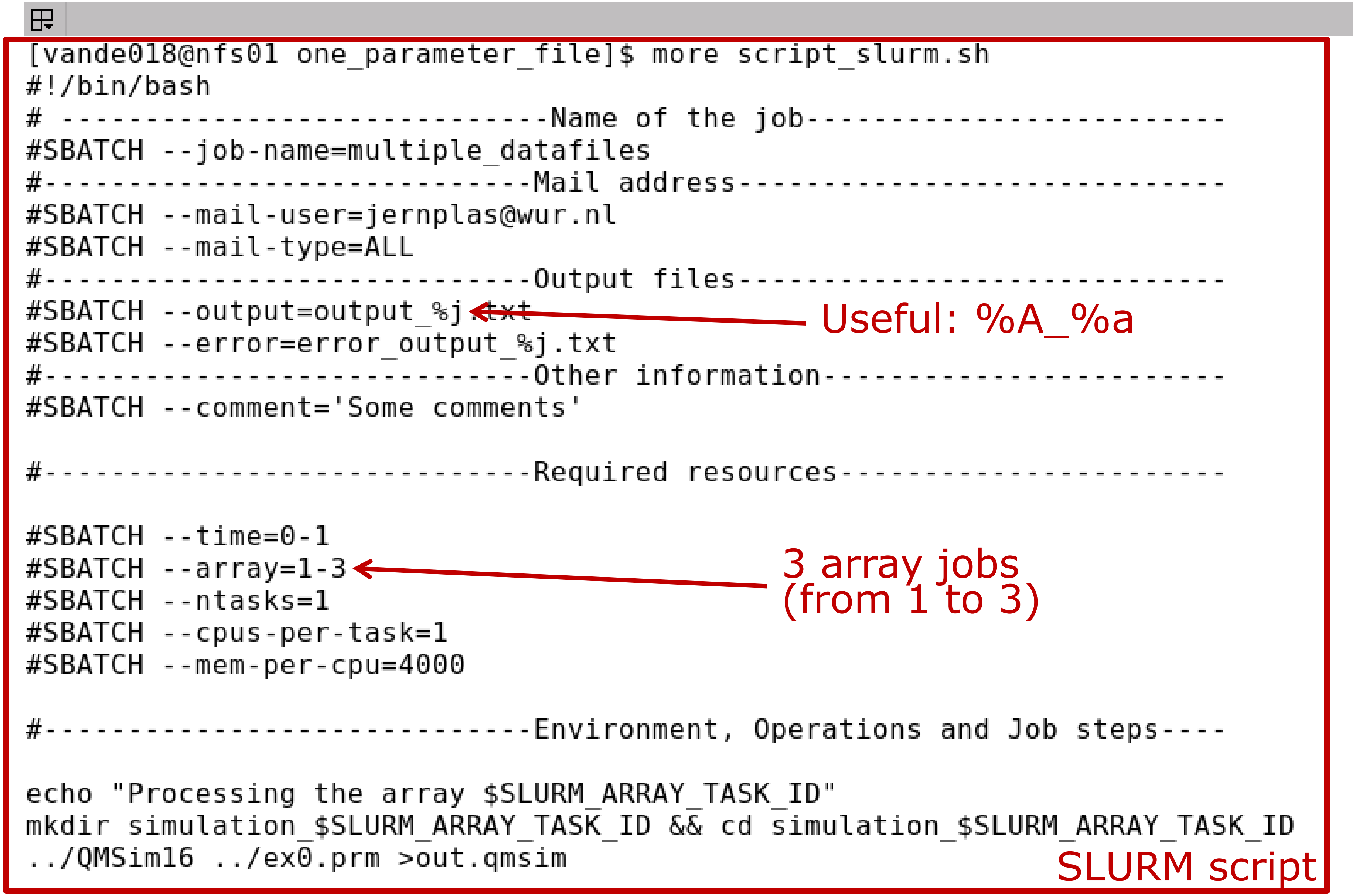
    ➔Launch the same program multiple times on distinct input/data files

- It could be submit several times
    - manually
    - with some tricks (loops, srun environment variables,...)
- Or use job arrays!

An embarrassingly parallel example

Resource

You want	SLURM options
8 hours	--time=00-08:00:00
6 processes to launch 6 completely independent jobs	--array=1,3-5,8
3 processes to launch 3 completely independent jobs (2 at a time)	--array=1-3%2
1 process per array	--ntasks=1
4000MB per CPU	--mem-per-cpu=4000
You use	$SLURM_ARRAY_TASK_ID (srun) ./myprog



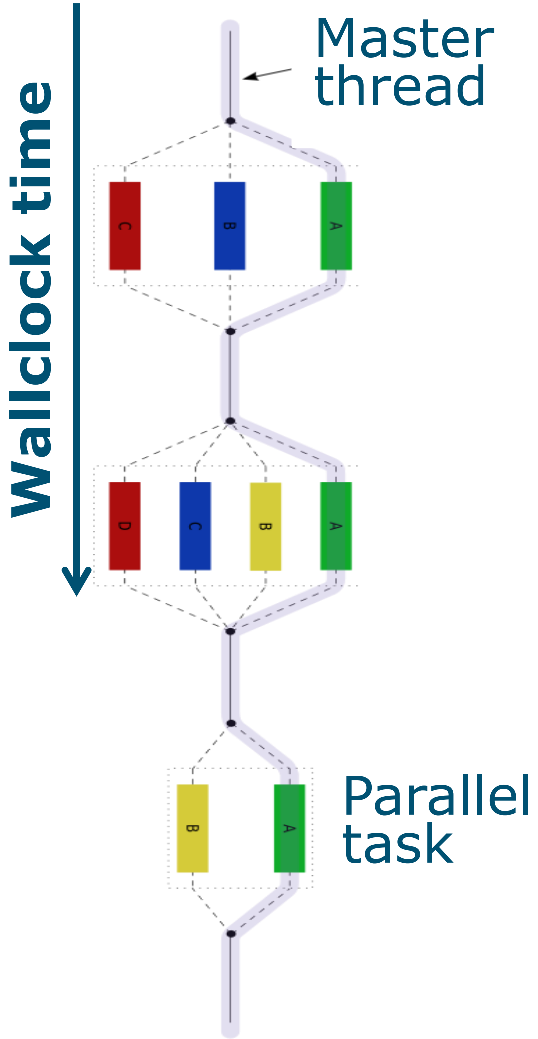
```
[vande018@nfs01 one_parameter_file]$ more script_slurm.sh
#!/bin/bash
# -----------------------------Name of the job-------------------------
#SBATCH --job-name=multiple_datafiles
#-----------------------------Mail address-----------------------------
#SBATCH --mail-user=jernplas@wur.nl
#SBATCH --mail-type=ALL
#-----------------------------Output files-----------------------------
#SBATCH --output=output_%j.txt
#SBATCH --error=error_output_%j.txt
#-----------------------------Other information------------------------
#SBATCH --comment='Some comments'

#-----------------------------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
```

Useful: %A_%a

3 array jobs
(from 1 to 3)

SLURM script

A shared memory example



- Parallelism is obtained by launching a multithreaded program
  - E.g., using OpenMP or TBB
- The program spawns itself on the node
- Generally run job on a single node
  - The threads cannot be split across several nodes
- Communication by shared memory

WAGENINGEN UR
For quality of life

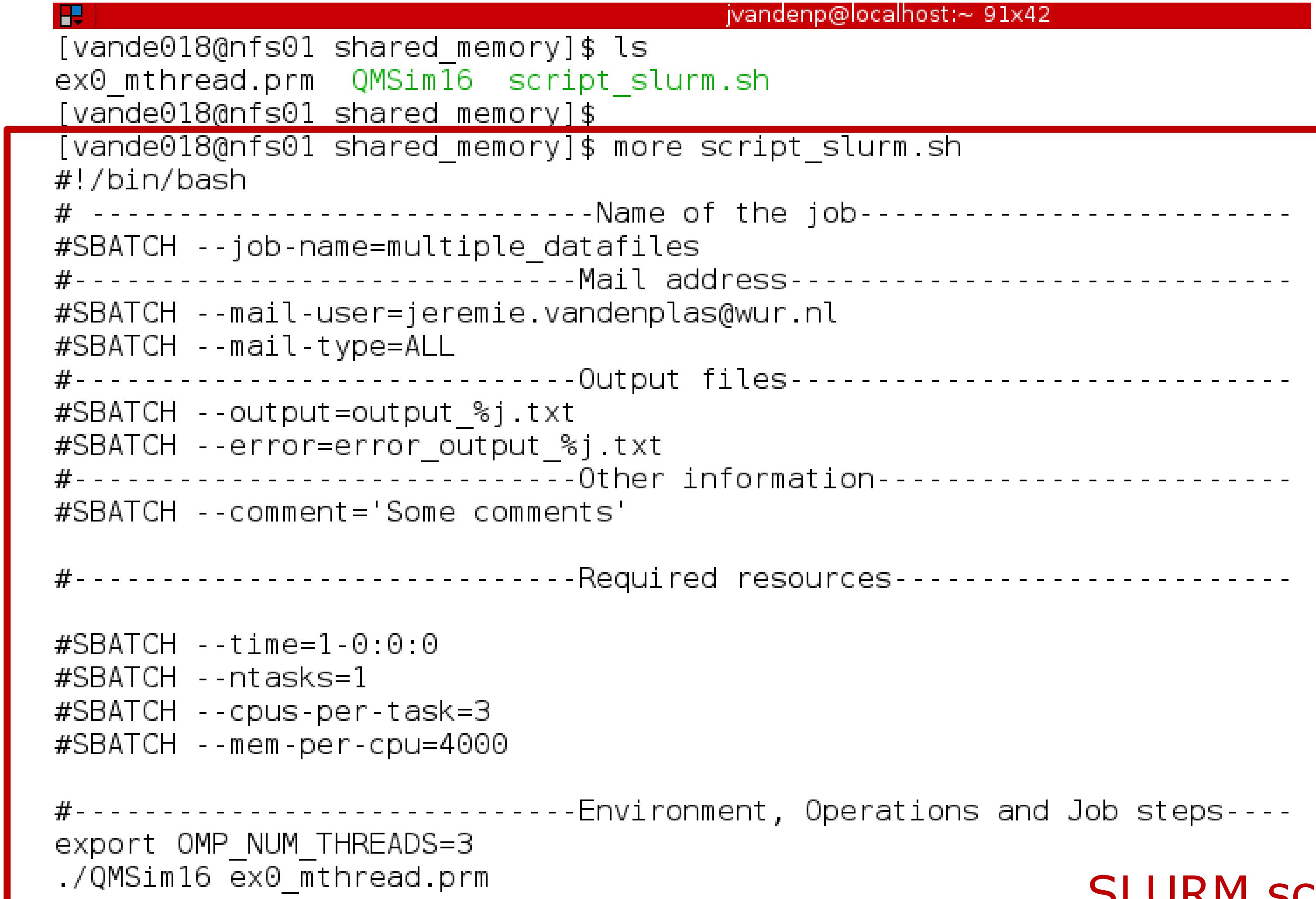
A shared memory example: resource

You want	SLURM options
8 hours	--time=00-08:00:00
1 process that can use 3 cores for multithreading	--ntasks=1 --cpus-per-task=3
4000MB per CPU	--mem-per-cpu=4000
You use	export OMP_NUM_THREADS=3 (export MKL_NUM_THREADS=3) (srun) ./myprog

→Run the job on a single node with

- max. 3 threads
- max. RAM = 3*4000=12000 MB

A shared memory example: script



```
[vande018@nfs01 shared_memory]$ ls
ex0_mthread.prm  QMSim16  script_slurm.sh
[vande018@nfs01 shared_memory]$
[vande018@nfs01 shared_memory]$ more script_slurm.sh
#!/bin/bash
# -----------------------------Name of the job-------------------------
#SBATCH --job-name=multiple_datafiles
#-----------------------------Mail address-----------------------------
#SBATCH --mail-user=jeremie.vandenplas@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=1-0:0:0
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=3
#SBATCH --mem-per-cpu=4000

#-----------------------------Environment, Operations and Job steps----
export OMP_NUM_THREADS=3
./QMSim16 ex0_mthread.prm
```

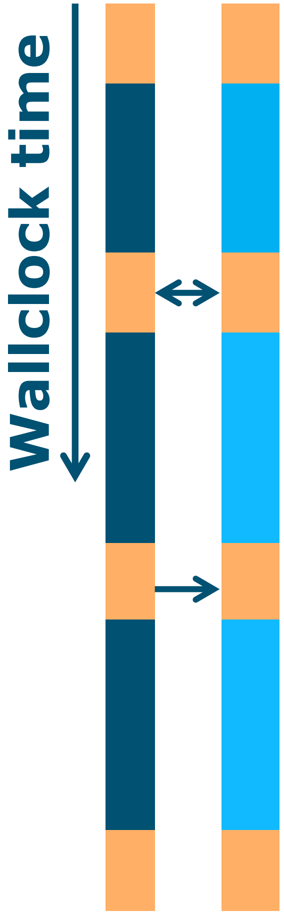
SLURM script

Pitfalls

- Using --ntasks=*n* for shared memory programs
  - Could work **or not**!
  - ➔Use --ntasks=1 --cpus-per-task=*n*

- Forgetting to mention the number of threads to the shared memory program (e.g., OpenMP programs)
  - ➔Add *export OMP_NUM_THREADS=1* to your *~/.bashrc*

A message passing example



- Parallelism is obtained by launching a multi-process program
  - E.g., MPI, PGAS (Coarray Fortran, UPC)
- One program spawns itself on several nodes
- Inter-process communication by the network

A message passing example: resource

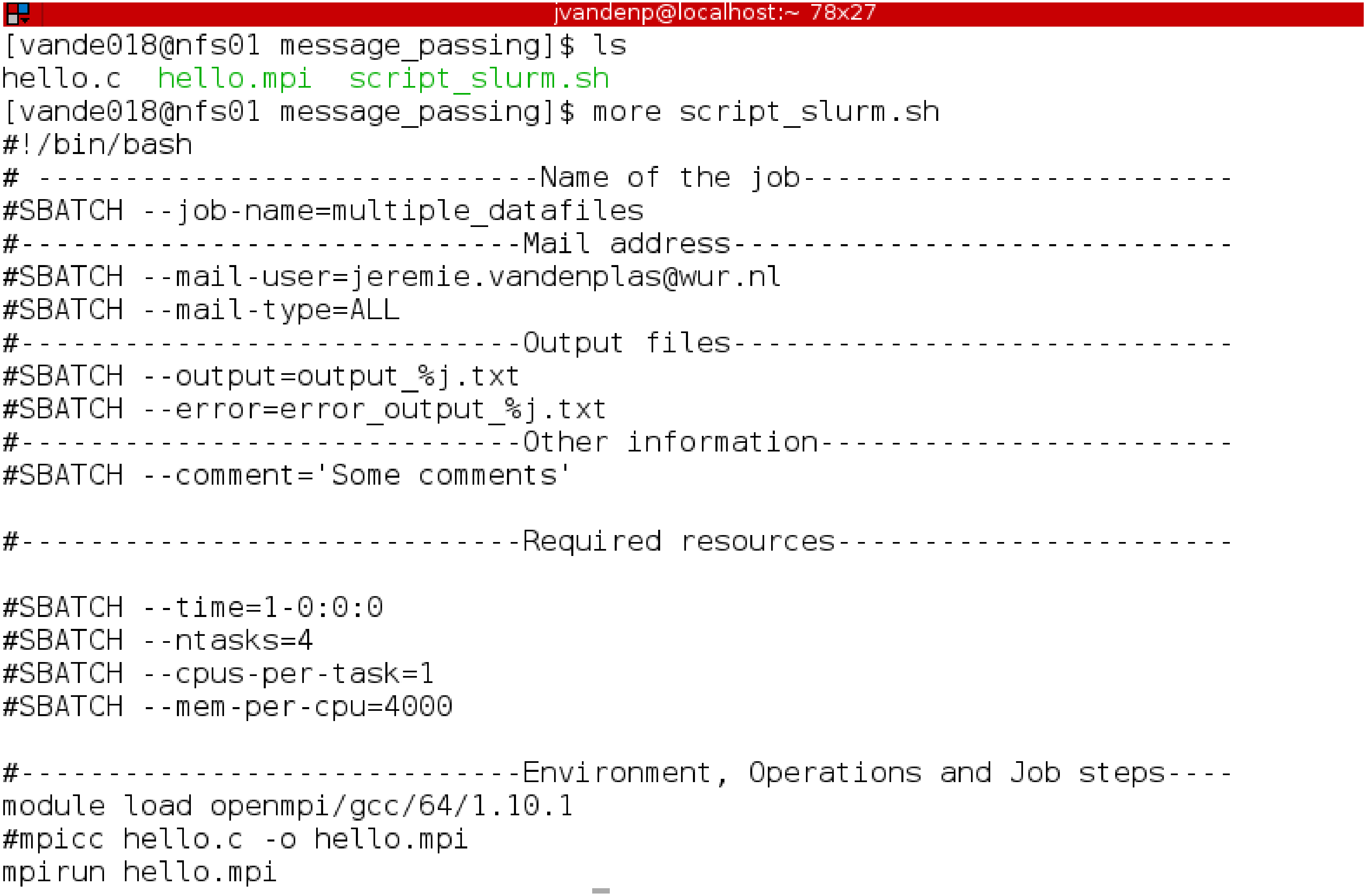
You want	SLURM options
8hours	--time=00-08:00:00
3 processes for use with MPI that can use 1 core for multithreading	--ntasks=3 --cpus-per-task=1
4000MB per CPU	--mem-per-cpu=4000
You use	Module load mpi_library mpirun myprog

➔Run the job on max. 3 nodes with

- max. RAM = 3*4000=12000 MB

WAGENINGEN UR
For quality of life

A message passing example: script



```
[vande018@nfs01 message_passing]$ ls
hello.c  hello.mpi  script_slurm.sh
[vande018@nfs01 message_passing]$ more script_slurm.sh
#!/bin/bash
# -----------------------------Name of the job-------------------------
#SBATCH --job-name=multiple_datafiles
#-----------------------------Mail address-----------------------------
#SBATCH --mail-user=jeremie.vandenplas@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=1-0:0:0
#SBATCH --ntasks=4
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=4000

#-----------------------------Environment, Operations and Job steps----
module load openmpi/gcc/64/1.10.1
#mpicc hello.c -o hello.mpi
mpirun hello.mpi
```

WAGENINGEN UR
For quality of life

Pitfalls

- Using --ntasks=*n* for shared memory programs
  - Could work or not!
  - ➔Use --ntasks=1 --cpus-per-task=*n*

- Forgetting to mention the number of threads to the shared memory program
  - ➔Add *export OMP_NUM_THREADS=1* to your *~/.bashrc*

- Shared memory program OR message passing program?
  - ➔RTFM!
  - ➔Check the output of ***top*** with a small example!

A mixed example

- A parallel job can included different parallelization paradigms!

You want	SLURM options
8 hours	--time=00-08:00:00
4 processes that can use 3 cores for multithreading	--ntasks=4 --cpus-per-task=3
4000MB per CPU	--mem-per-cpu=4000
You use	Module load mpi_library export OMP_NUM_THREADS=3 (export MKL_NUM_THREADS=3) mpirun myprog

Summary: resource requests

- Choose the number of processes (--ntasks)
- Choose the number of threads per process (--cpu-per-task)
- Set environment variables (OMP_NUM_THREADS, MKL_NUM_THREADS,...)
- Use SLURM environment variables if required
- Launch processes with srun or mpirun if required

Thank you!

Questions?