High Performance Computing at ITU

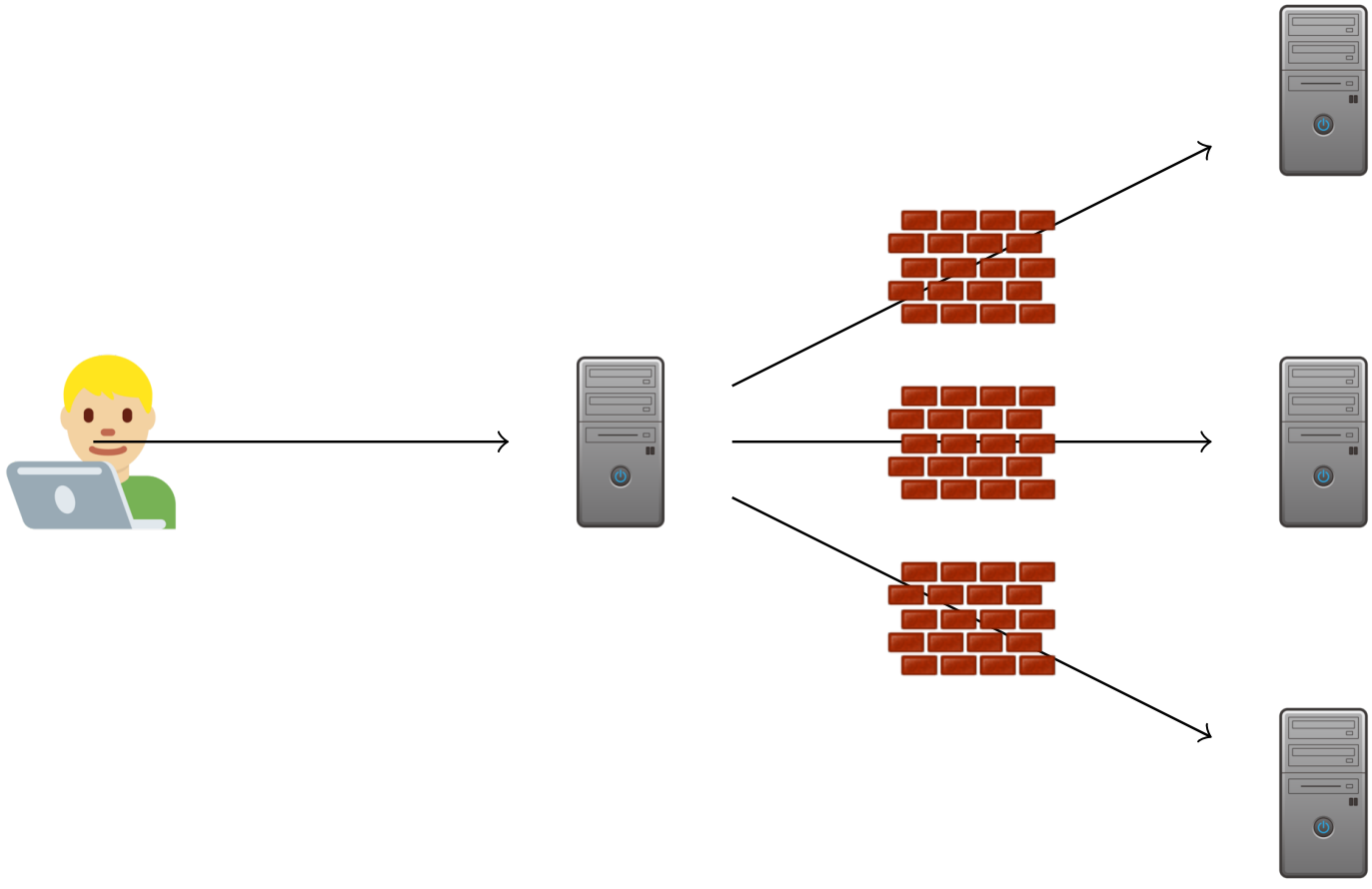
08-03-2023

Rob van der Goot

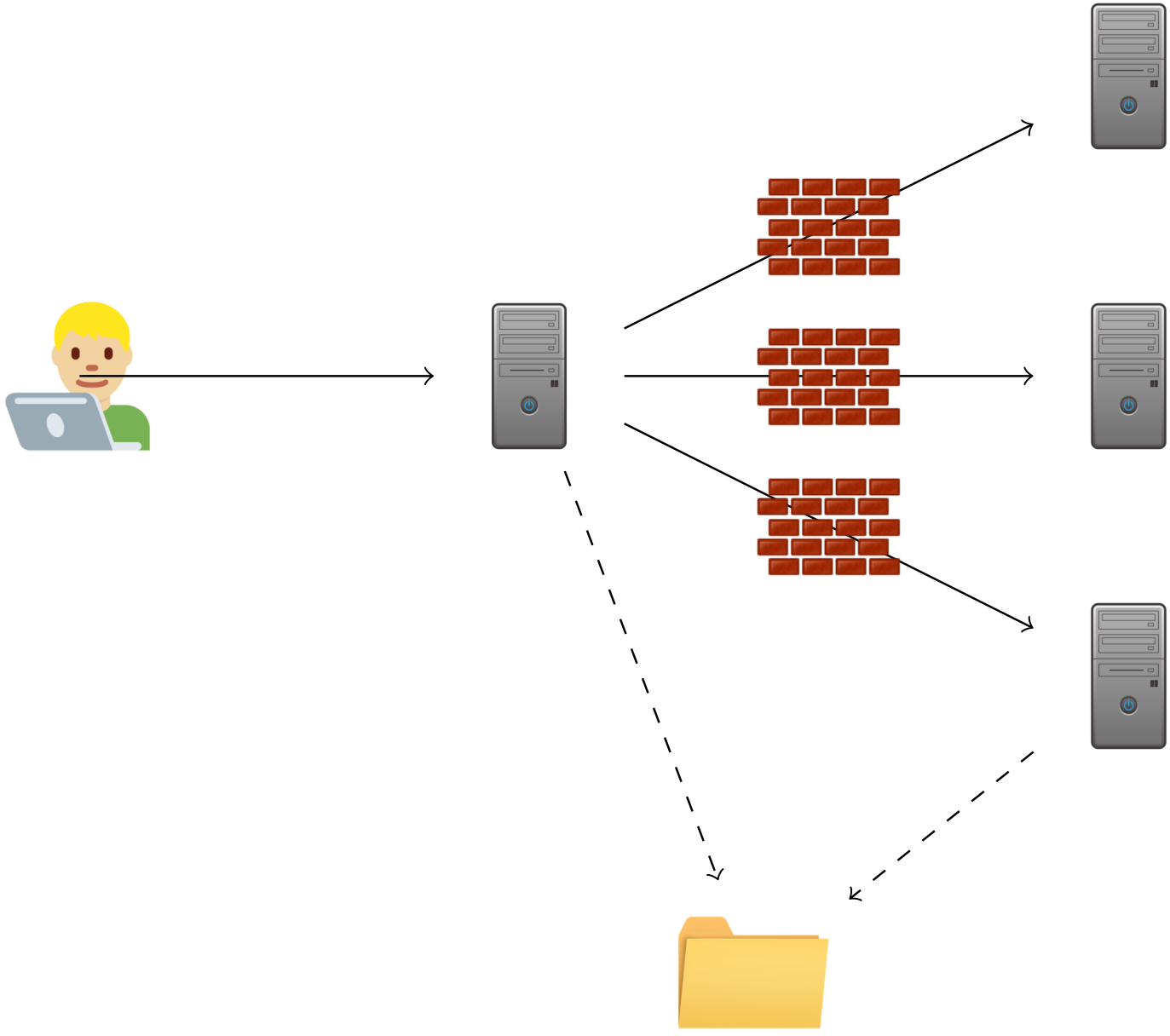
Machines on brown queue:

```
- desktop1-10:  CPU: Intel(R) Core(TM) i7-4790 CPU @ 3.60GHz Cores: 8
                MEM: 32 GiB / 30000 MiB schedulable
                GPU: 1x GeForce RTX 2070
- desktop11-16: CPU: Intel(R) Core(TM) i7-4790 CPU @ 3.60GHz Cores: 8
                MEM: 32 GiB / 30000 MiB schedulable
                GPU: None
- desktop17:    2x CPU: Intel(R) Xeon(R) Gold 5218R CPU @ 2.10GHz Cores: 80
                MEM: 394 GiB / 385414 MiB schedulable
                GPU: 2x Quadro RTX 8000 48GiB
- desktop18:    2x CPU: AMD EPYC 7352 24-Core Processor Cores: 96
                MEM: 256 GiB / 250000 MiB schedulable
                GPU: 4x NVIDIA A30 24GiB
- desktop19:    CPU: AMD EPYC 7402P 24-Core Processor @ 2.8GHz Cores: 48
                MEM: 120GiB / 120000MiB schedulable
                GPU: None
- desktop20:    CPU: AMD EPYC 7402P 24-Core Processor @ 2.8GHz Cores: 48
                MEM: 120GiB / 120000MiB schedulable
                GPU: None
- desktop21:    CPU: Intel(R) Xeon(R) CPU E5-2660 v3 @ 2.60GHz Cores: 40
                MEM: 250GiB / 257560MiB schedulable
                GPU: 2x GeForce RTX 1080
- desktop22:    CPU: AMD EPYC 7252 8-Core Processor Cores: 32
                MEM: 120GiB / 120000MiB schedulable
                GPU: 4x NVIDIA A100 40GiB
```

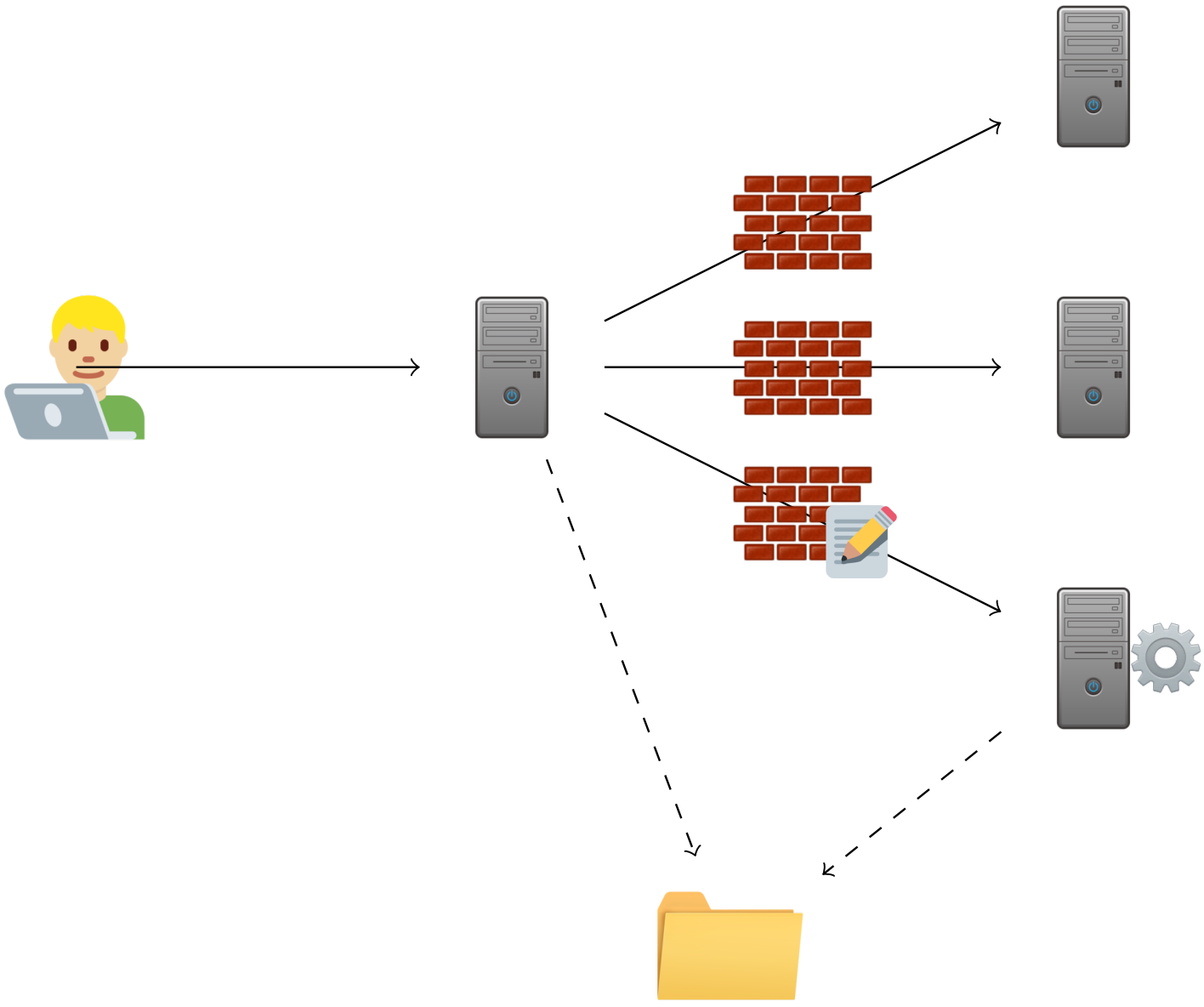
You can not directly access the compute nodes



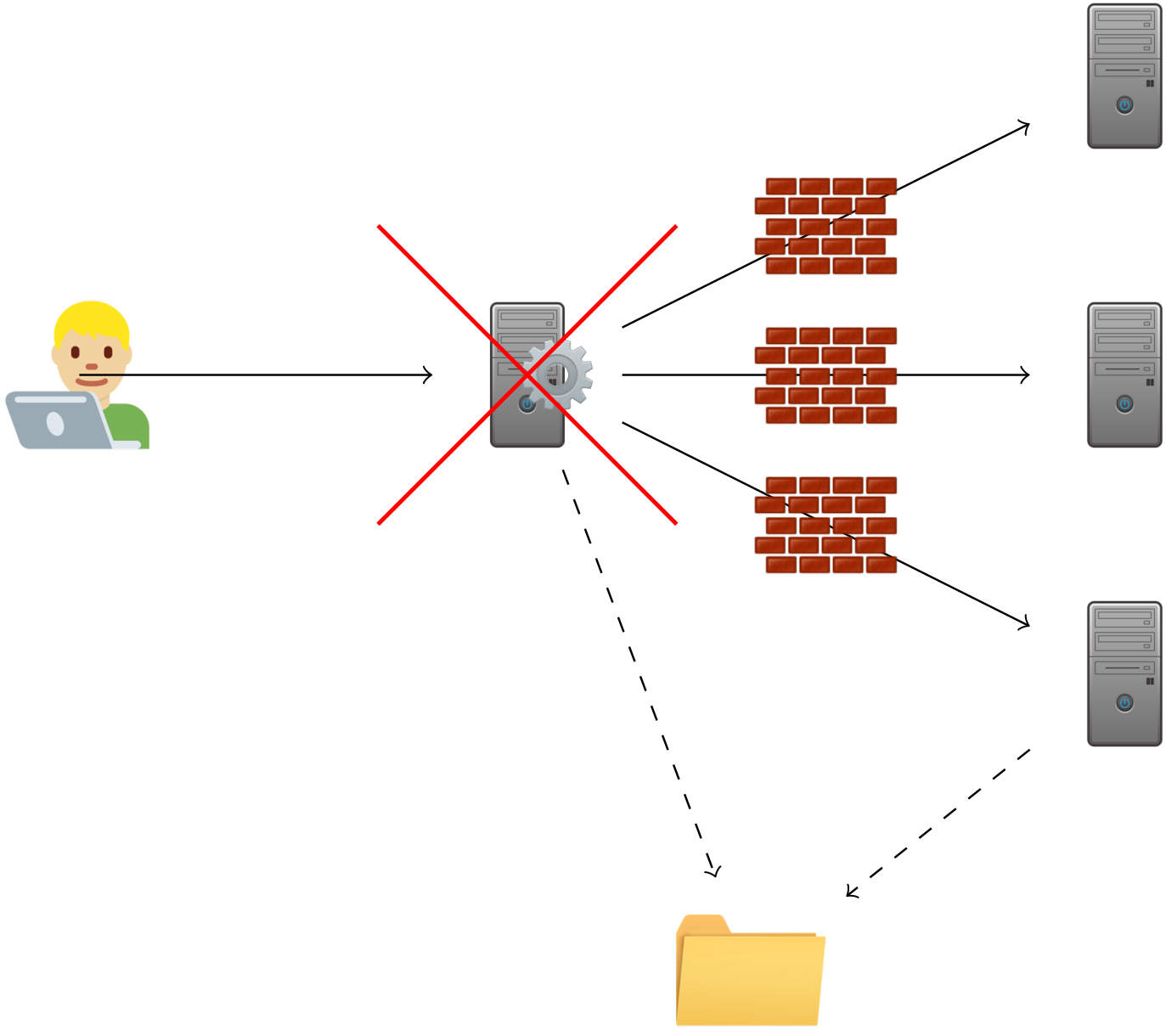
The login node has access to the same data storage as the compute nodes



Submit your jobs to the scheduler, which will distribute it to the compute nodes



Please, do not run heavy jobs on `front` (the login node)



Access:

```
ssh <username>@hpc.itu.dk
```

To communicate to the scheduler job scripts are used. They contain:

- Information about what is required
- Command(s) to run
- (modules to load)

```
#!/bin/bash
#SBATCH --job-name=simple    # Job name
#SBATCH --output=simple.out  # Name of output file
#SBATCH --cpus-per-task=1    # Schedule one core
#SBATCH --time=00:01:00      # Run time (hh:mm:ss)
#SBATCH --partition=brown

# Print out the hostname of the node
hostname
```

To queue a job:

```
[robv@front ~]$ sbatch test.sh
Submitted batch job 3458
[robv@front ~]$
```

Other useful options:

```
#SBATCH --output=job.%j.out  # (%j expands to jobId)
#SBATCH --gres=gpu           # Request a GPU
#SBATCH --mail-type=BEGIN,END,FAIL
                             # E-mail when status changes
```

`--gres` should be before `--partition`!

To see all unfinished jobs on the cluster:

```
[robv@front ~]$ squeue
 JOBID PARTITION  NAME  USER ST     TIME  NODES NODELIST(REASON)
  3450     brown  ctrl  djgr  R 22:02:22      8 desktop1
  3441     brown  test  robv  R  0:00:10      2 desktop2
```

To see all unfinished jobs on the cluster:

```
[robv@front ~]$ squeue
 JOBID PARTITION  NAME  USER ST     TIME  NODES NODELIST(REASON)
  3450     brown  ctrl  djgr  R 22:02:22      8 desktop1
  3441     brown  test  robv  R  0:00:10      2 desktop2
```

To see all the jobs that I have queued:

```
[robv@front ~]$ squeue -u robv
 JOBID PARTITION  NAME  USER ST     TIME  NODES NODELIST(REASON)
  3441     brown  test  robv  R  0:00:10      2 desktop2
```

To cancel a job:

```
[robv@front ~]$ scancel 3441
[robv@front ~]$
```

To get more information about a job:

```
[robv@front ~]$ scontrol show jobid 3422
   UserId=robv(47396) GroupId=robv(78376) MCS_label=N/A
   Priority=16283 Nice=0 Account=researchers QOS=normal
   JobState=COMPLETED Reason=None Dependency=(null)
   Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
   RunTime=00:00:30 TimeLimit=00:01:00 TimeMin=N/A
   SubmitTime=2020-01-16T11:40:05 EligibleTime=2020-01-16T11:40:
   AccrueTime=2020-01-16T11:40:05
   StartTime=2020-01-16T11:40:05 EndTime=2020-01-16T11:40:35 Dea
   PreemptTime=None SuspendTime=None SecsPreSuspend=0
   LastSchedEval=2020-01-16T11:40:05
   Partition=brown AllocNode:Sid=front:3057
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=desktop2
```

```
NodeList=desktop2
BatchHost=desktop2
NumNodes=1 NumCPUs=2 NumTasks=0 CPUs/Task=1 ReqB:S:C:T=0:0:*:
TRES=cpu=2,mem=6G,node=1,billing=2
Socks/Node=* NtasksPerN:B:S:C=0:0:*:* CoreSpec=*
MinCPUsNode=1 MinMemoryCPU=3G MinTmpDiskNode=0
Features=(null) DelayBoot=00:00:00
OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)
Command=/home/robv/test.sh
WorkDir=/home/robv
StdErr=/home/robv/job.3459.out
StdIn=/dev/null
StdOut=/home/robv/job.3459.out
Power=
TresPerNode=gpu
```

To transfer files to the hpc storage:

```
rob@home: scp main.cc robv@hpc.itu.dk:
WARNING: Unauthorized access to this system is forbidden and wil
         prosecuted by law. By accessing this system, you agree
         actions may be monitored if unauthorized usage is suspe
robv@hpc.itu.dk's password:
main.cc                                   100% 3384   536.3KB/s   00:00
rob@home:
```

Robs .bashrc

```
alias sq='squeue -o "%.6i %.6P %.25j %.8u %.2t %.10M %.5c %
sq

module load Python/3.9.6-GCCcore-11.2.0
```

More info on:

- `hpc.itu.dk`
- see also the examples at `/opt/itu/templates/`