Cluster-user meeting

Tom de Geus
Jim Schormans
Leo Wouters

L.H.G.Wouters@tue.nl
MaTeCluster@tue.nl

Before we start

Updates

- dr. Jeroen van Beeck and Bart Vossen are leaving the university
- Jim Schormans joins the cluster team

Getting help

www.mate.tue.nl/~cluster

- Cluster manual
- This presentation
- …

Feel free to interrupt at any time

Outline

increase knowledge
and
stimulate discussion/collaboration

1. New cluster: rng
2. Common mis-practices
3. Computing cluster, the basics…
4. Monitoring jobs
5. Etiquette
6. Getting help

History

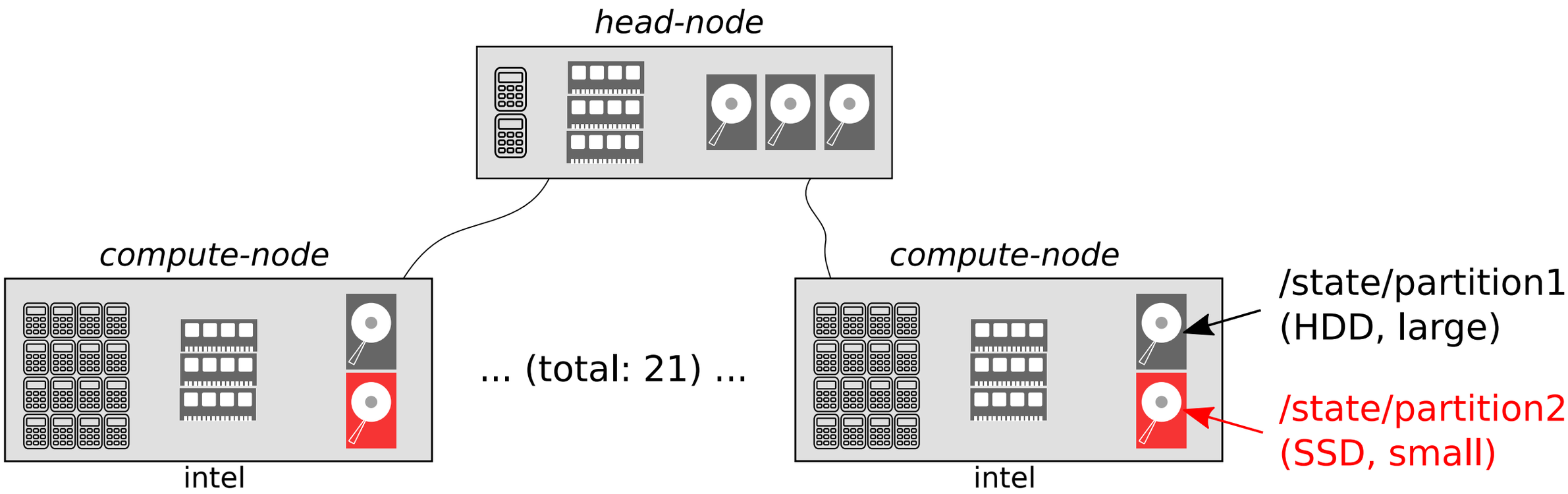
blower

noise

furnace

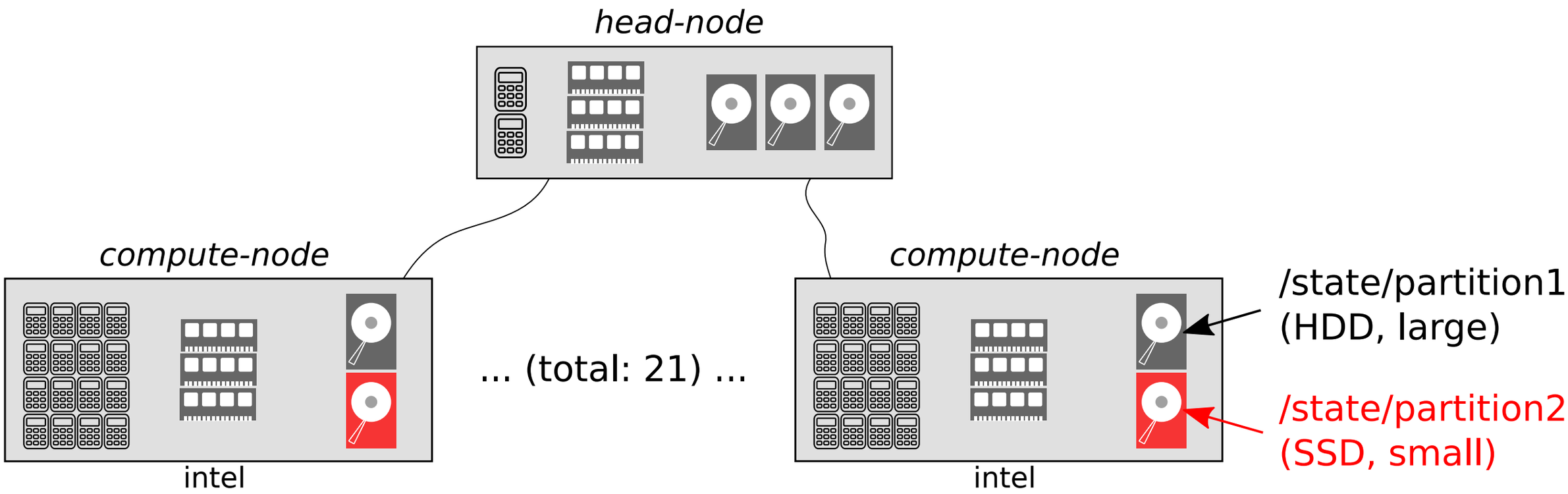
rng

New cluster: rng




```
#!/bin/bash
#PBS -S /bin/bash
#PBS -j oe
#PBS -o pbs.out
#PBS -l nodes=1:ppn=1
#PBS -l pmem=3gb
#PBS -l pvmem=3gb

# print the working directory
pwd

# print a personal string
echo "Hello world"
```

New cluster: rng



- Experienced PhD students use **rng**, newbies, and other students use **furnace**
- Use /state/partition2 for: MSC.Marc, Abaqus, …
- Some things have changed or are missing: consult Leo in that case

Common mis-practices

Shared resources require:

★ **communication**:
- consult each other

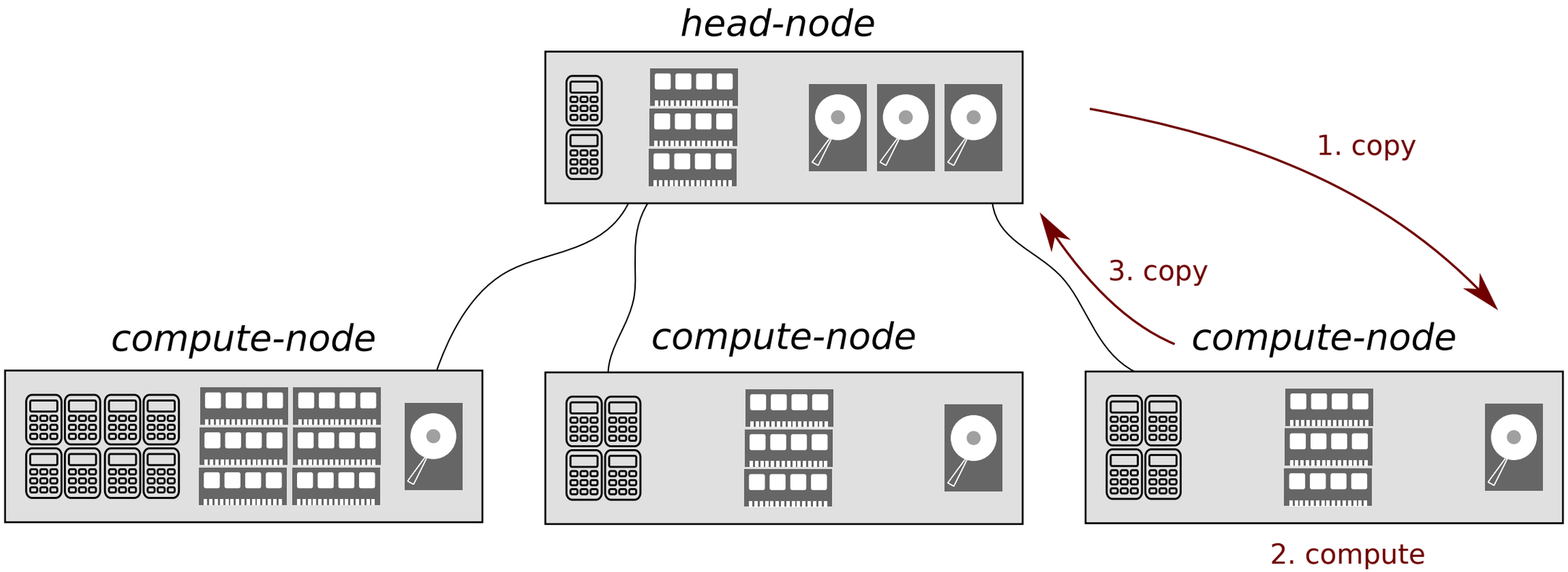
★ **knowledge**:
- study www.mate.tue.nl/~cluster until you understand
- ask questions

★ **moderation:**
- clean up the head-node
- check if others are queued
- decide if jobs are (still) relevant

Common mis-practices: network

- Limit network usage as much as possible
  - only at the beginning and end (“heavy-IO job”)
  - limit output to what you need

- Copy only the current simulation
  (not the `/home/user/` folder)



Common mis-practices: memory

If a node runs out of memory it fails, including **all** jobs

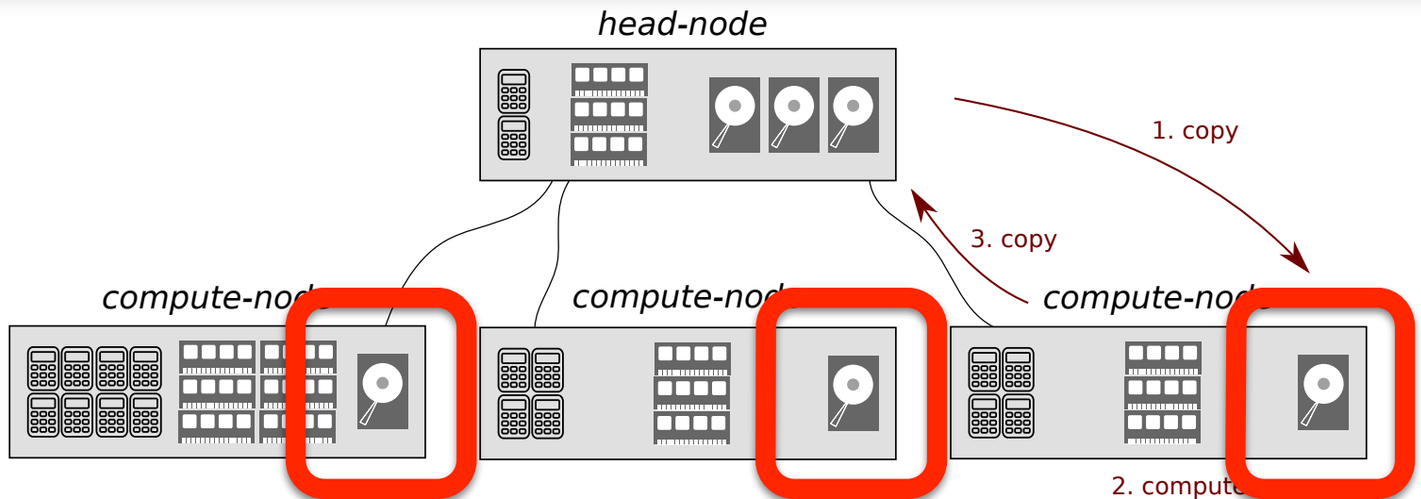
```
#!/bin/bash
#PBS -S /bin/bash
#PBS -j oe
#PBS -o pbs.out
#PBS -l nodes=1:ppn=1
#PBS -l pmem=3gb
#PBS -l pvmem=3gb

# print the working directory
pwd

# print a personal string
echo "Hello world"
```

Help the scheduler

Kills the job

Common mis-practices: clean-up after yourself

```
$ rocks run host “ls /state/partition1/`whoami`”
compute-0-30:
compute-0-19:
compute-0-31:
compute-0-15:
compute-0-27:
compute-0-17:
compute-0-32:
compute-0-26:
compute-0-16:
compute-0-13:
compute-0-21:
compute-0-18:
compute-0-20:
compute-0-28:
compute-0-29:
compute-0-3:
compute-0-5:
compute-0-24:
compute-0-25:
compute-0-6:
compute-0-10:
compute-0-1:
compute-0-11:
compute-0-0:
compute-0-14:
compute-0-22:
compute-0-8:
compute-0-9:
compute-0-7:
compute-0-2:
compute-0-12:
compute-0-23: down
```



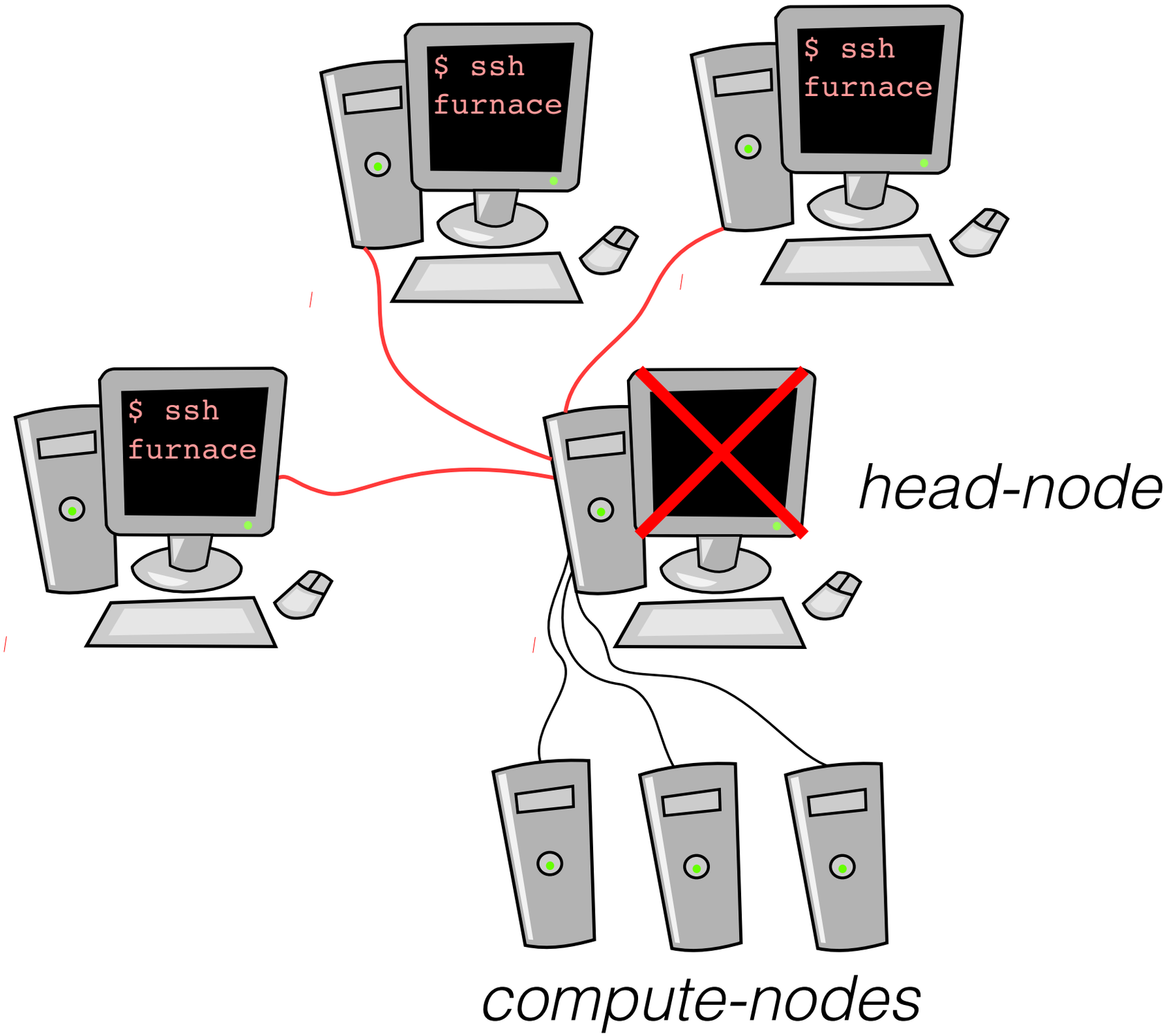
Questions?

Outline

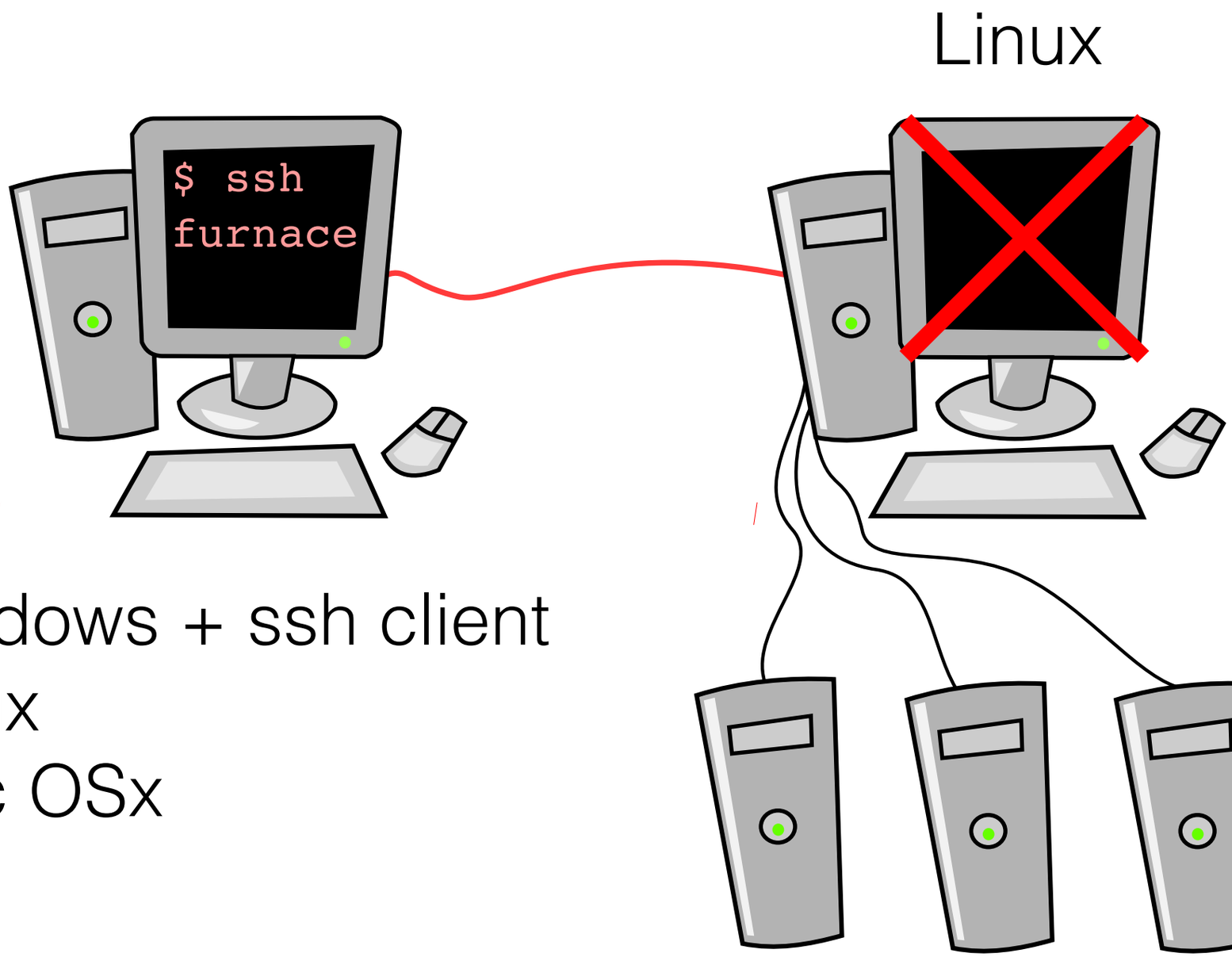
increase knowledge
and
stimulate discussion/collaboration

1. Computing cluster, the basics…
2. Monitoring jobs
3. Etiquette
4. Getting help
5. Future

The cluster


$ ssh furnace
$ ssh furnace
$ ssh furnace
head-node
compute-nodes

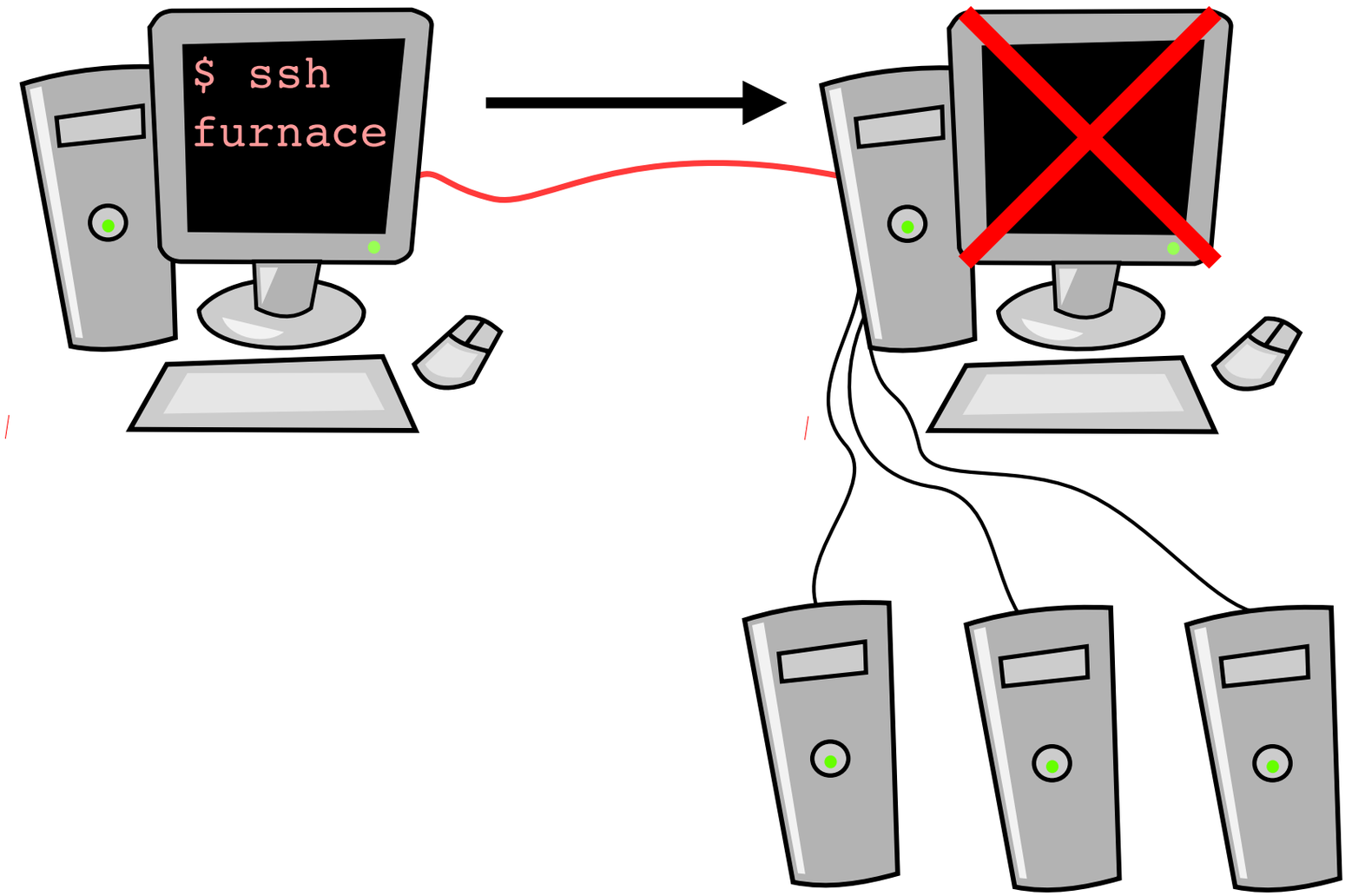
Interfacing with the cluster



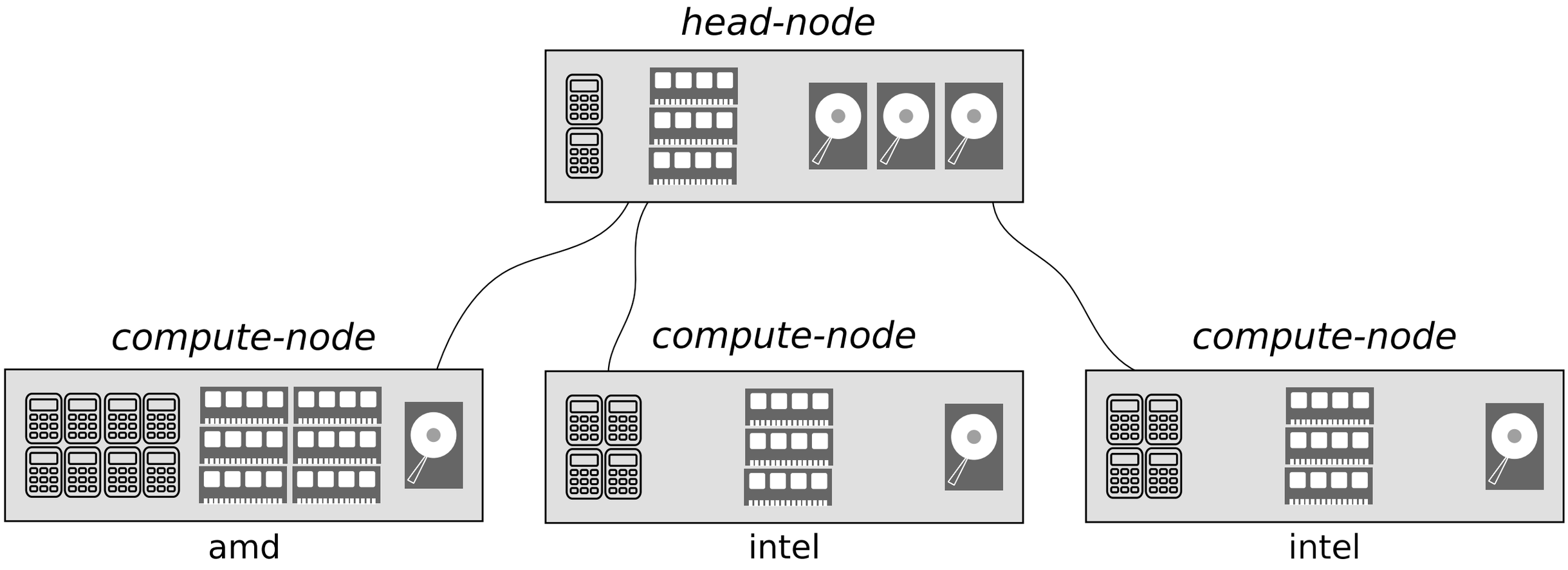
- Windows + ssh client
- Linux
- Mac OSx

Connecting

```
$ ssh tdegeus@furnace.wfw.wtb.tue.nl
```

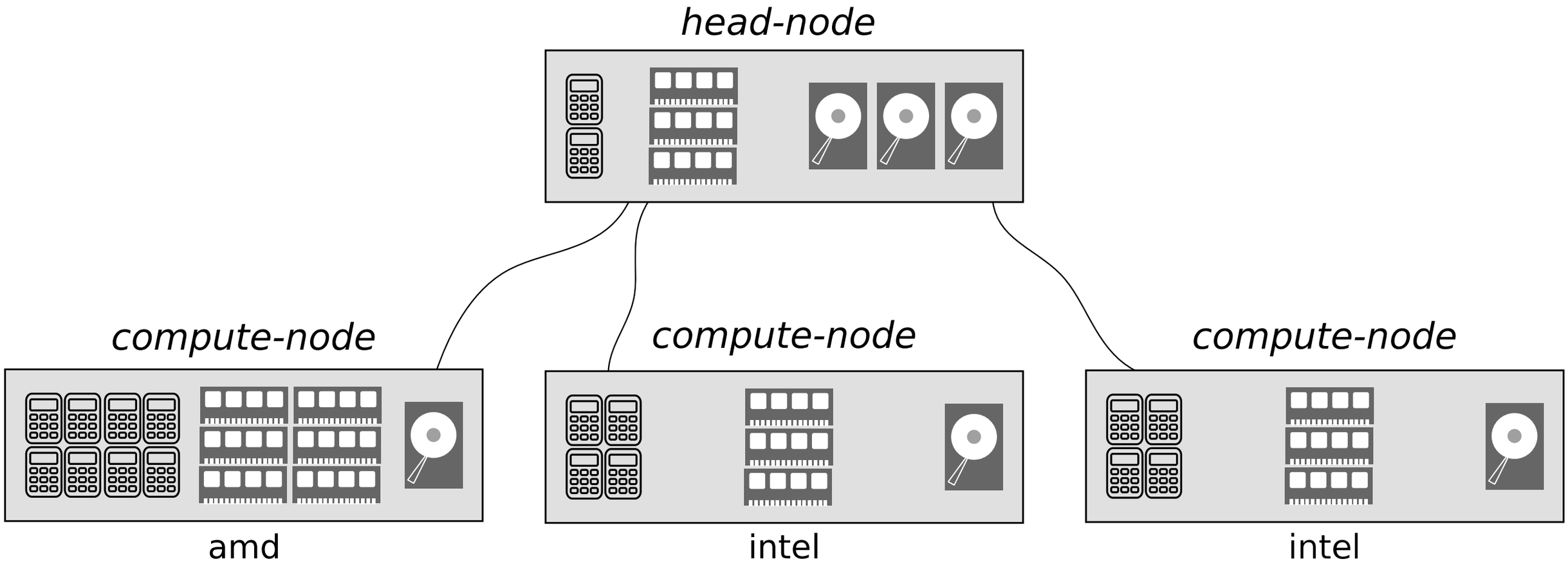


Connecting: details



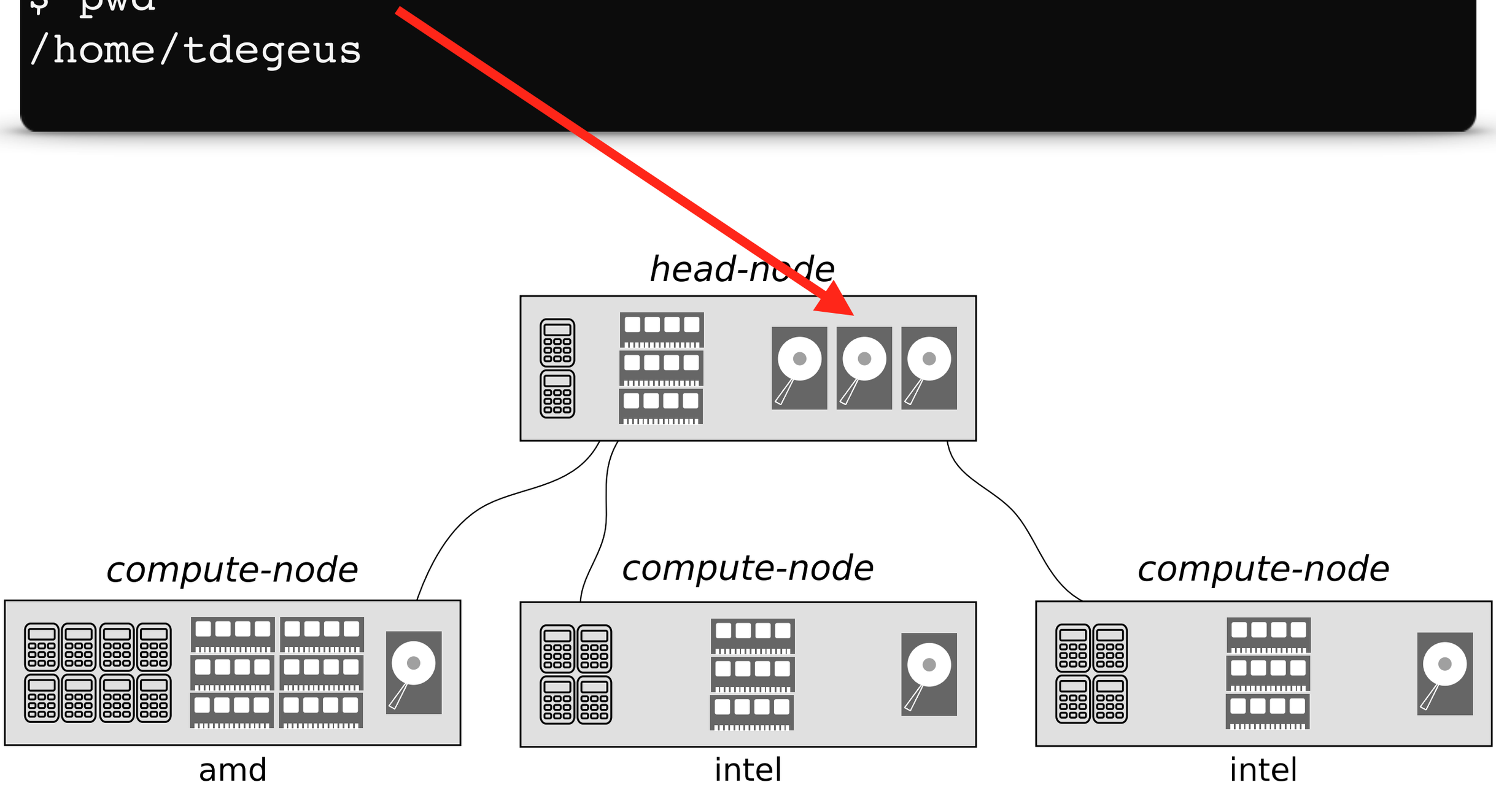
Connecting: details

```
$ ssh tdegeus@furnace.wfw.wtb.tue.nl

$ pwd
/home/tdegeus
```

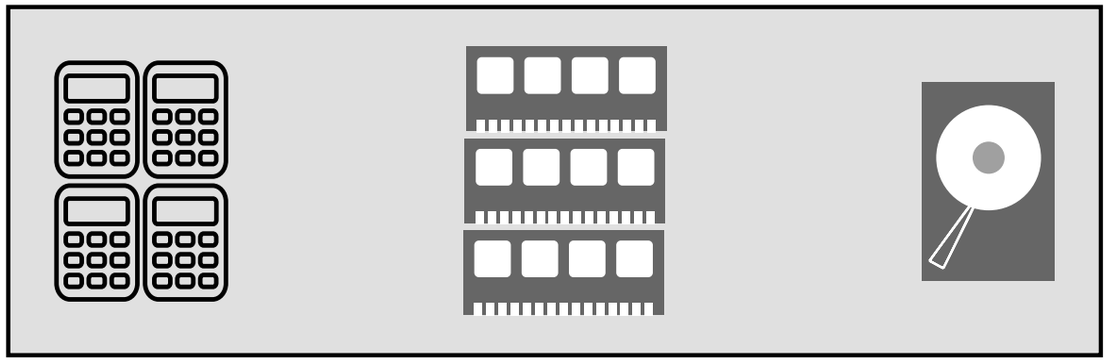


Connecting: details

```
$ ssh tdegeus@furnace.wfw.wtb.tue.nl

$ pwd
/home/tdegeus
```

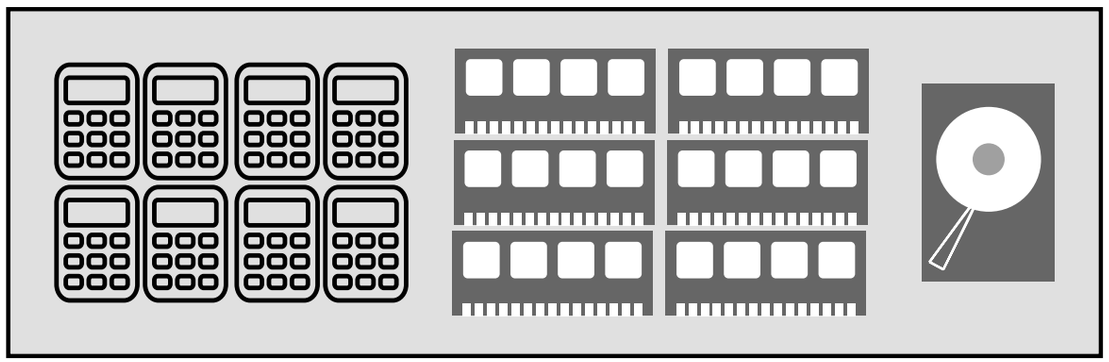


Two types of nodes



intel

- Fast
- 8 cpus per node
- Limited amount of memory
  - 48 GB

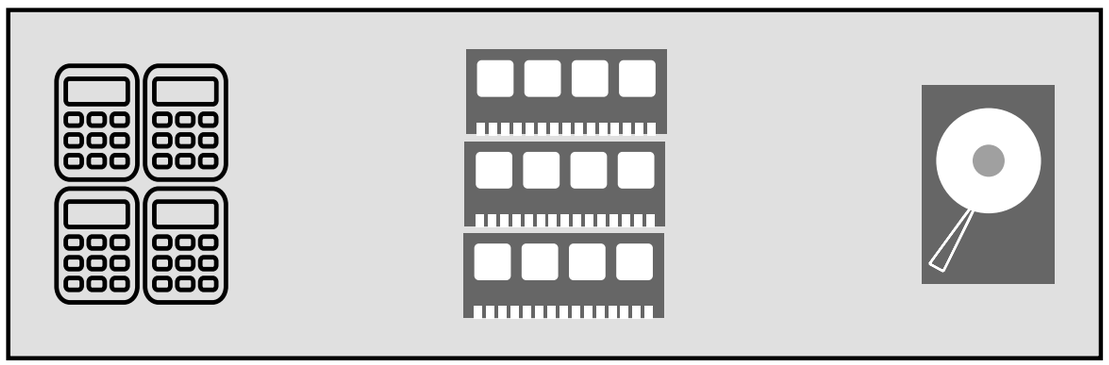


amd

- Slow
- 24 cpus per node
- Large amount of memory
  - 132 GB

The scheduler assigns jobs, once running:
everything is shared

Limited resources



everything is shared

CPUs:

- use > claim: every job slows down
- claim > use: blocking part of the cluster

Out of memory / out of disk space:
node is killed, all jobs fail!

Claiming resources

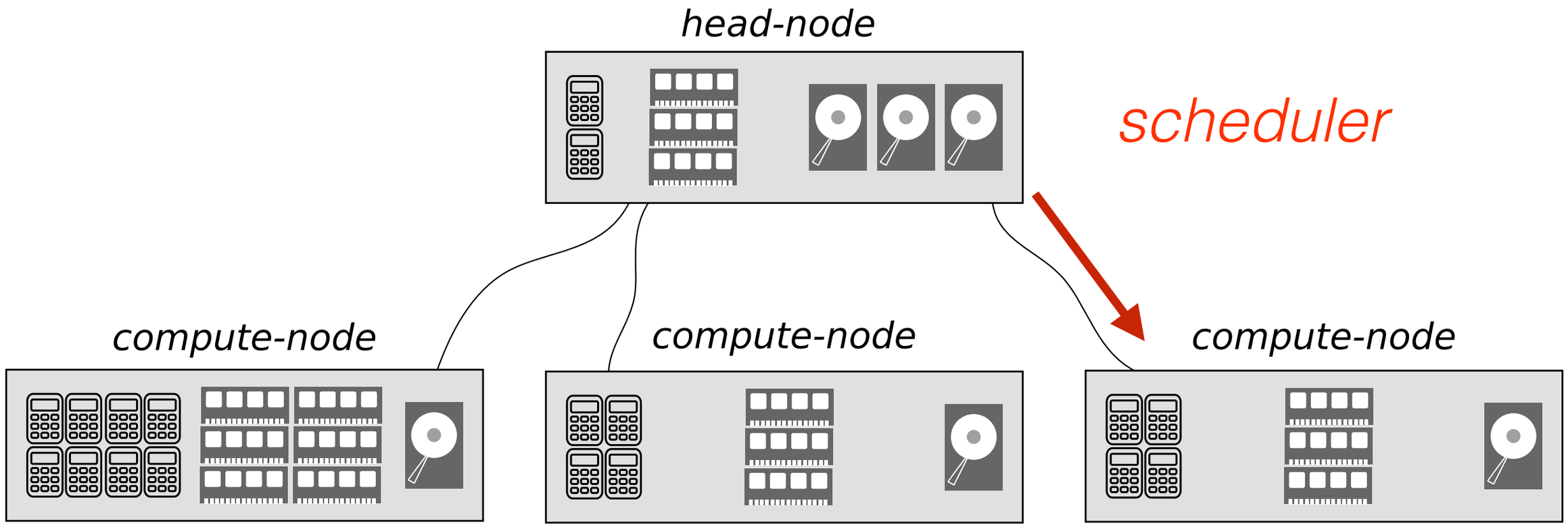
- Claim (a number) of cpus
  - `#PBS -l nodes=1:ppn=1:intel` *most jobs*
  - `#PBS -l nodes=1:ppn=2:amd` *heavy memory*

- Heavy memory jobs, claim memory
  - `#PBS -l pmem=20gb`
  - `#PBS -l pvmem=20gb`

Claim what you use and use what you claim

Submitting a job

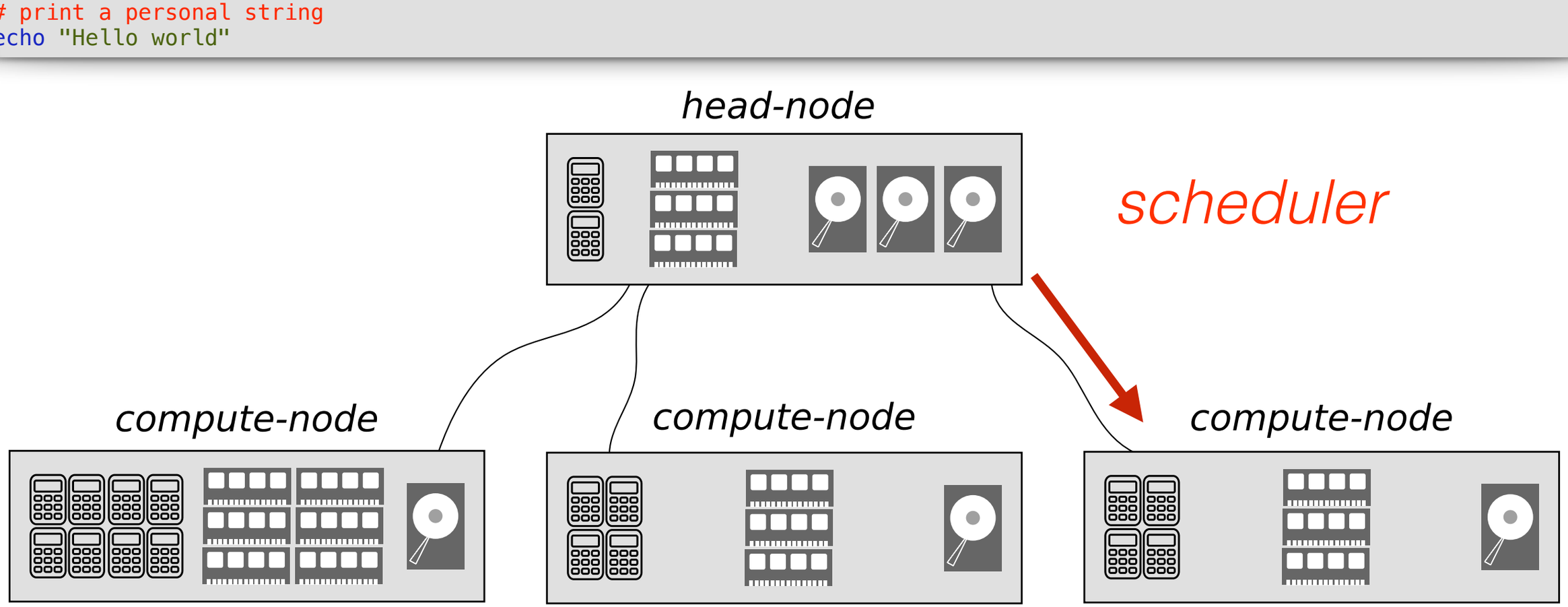
```
$ qsub myjob.pbs
```



Submitting a job

```
$ qsub myjob.pbs
```

```
#!/bin/bash
#PBS -S /bin/bash
#PBS -j oe
#PBS -o pbs.out
#PBS -l nodes=1:ppn=1:intel

# print the working directory
pwd

# print a personal string
echo "Hello world"
```



Submitting a job

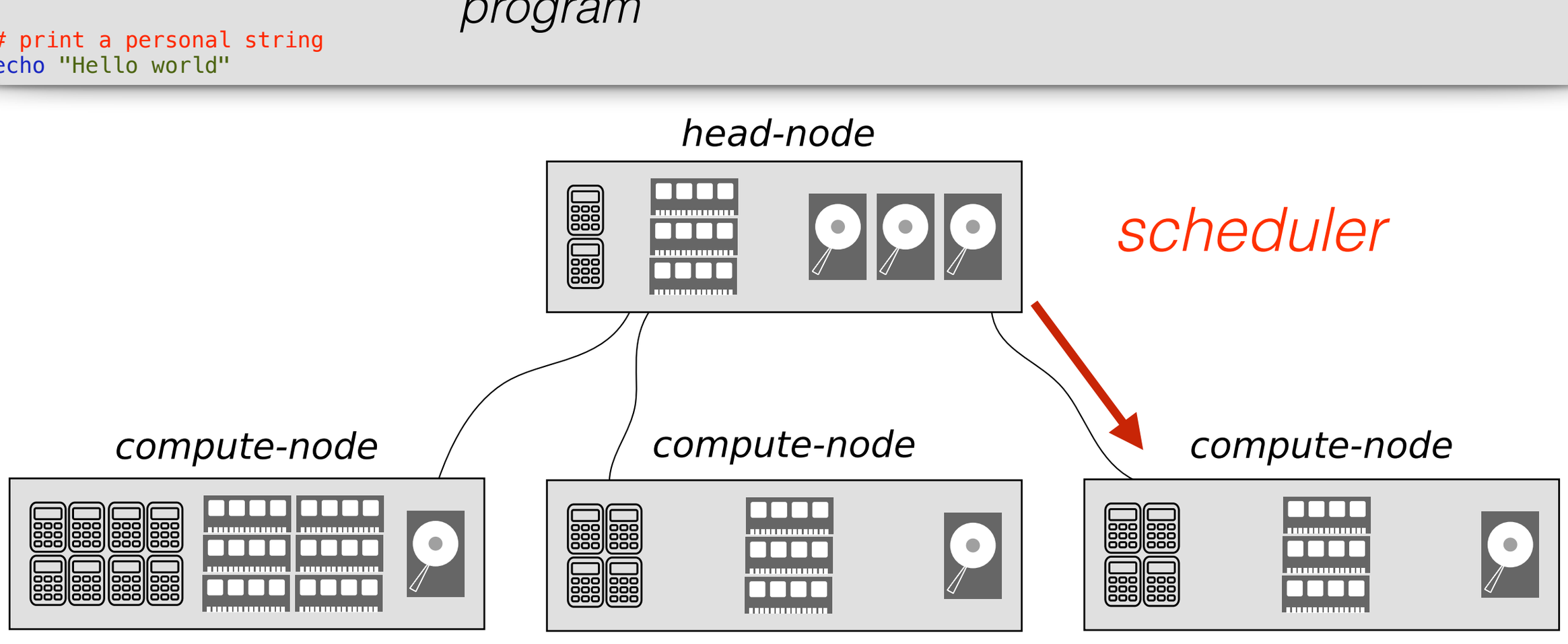
```
$ qsub myjob.pbs
```

```
#!/bin/bash
#PBS -S /bin/bash
#PBS -j oe
#PBS -o pbs.out
#PBS -l nodes=1:ppn=1:intel

# print the working directory
pwd

# print a personal string
echo "Hello world"
```

script interpreter

scheduler directives

program



Monitoring

```
$ myqstat

jid    , owner     , job name       , host , cpus   , mem  , S , time , score
------ , --------- , ------------ , ---- , ------ , ---- , - , ---- , -----
202169 , tdegeus   , myjob.pbs      ,   11 ,  1:1:i , 1mb  , R ,  10s ,  1.00
...
```

> 3 GB risky

<<1 waste

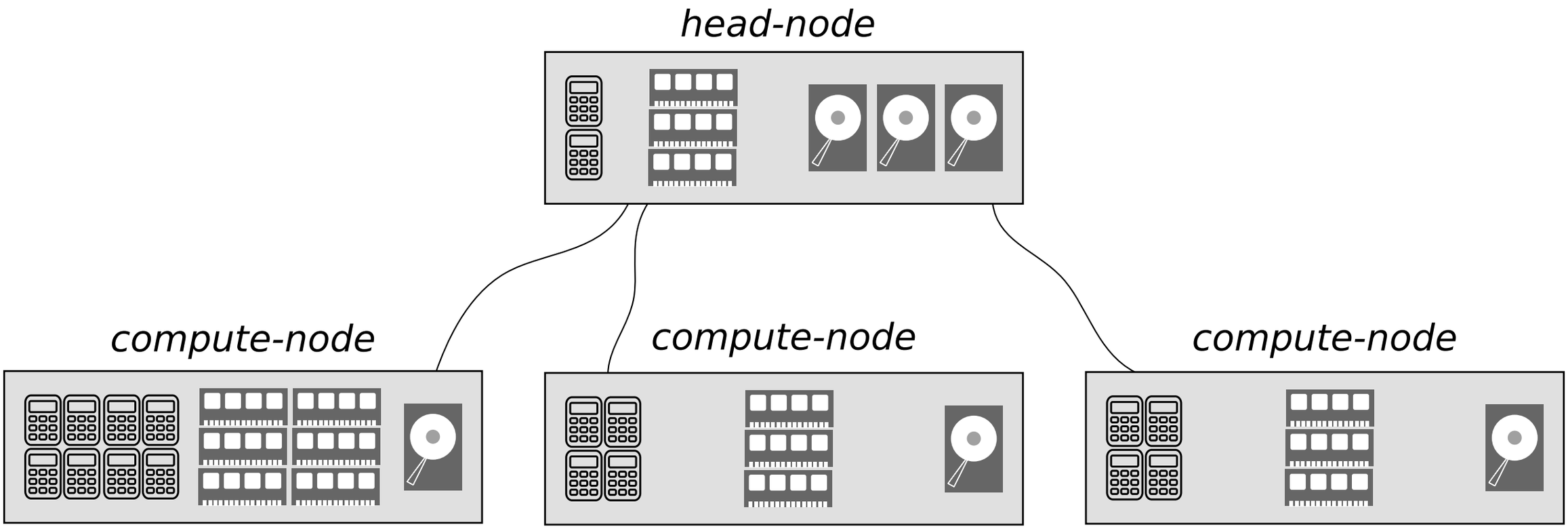
=1 good

>1 harming others

Etiquette: monitor resources

Monitor:

- memory usage
- CPU usage
- disk usage



Etiquette: monitor resources

```
$ myqstat -N --long
```

```
Node, State        , Type , Ctot, Cused, Cfree, Load , Mtot , Mused, Mem%, HDtot, HDfree, HD% , Btot, Bin  , Bout
----, -------------, -----, ----, -----, -----, -----, -----, -----, ----, -----, ------, ----, ----, -----, ----
   0, job-exclusive,   amd,   24,    24,     0,  1.24, 132gb,  18gb, 0.09, 177gb,  110gb, 0.38,  8kb,   8kb, 329b
   1, job-exclusive,   amd,   24,    24,     0,  1.54, 132gb,  19gb, 0.10, 177gb,  120gb, 0.32,  8kb,   8kb, 326b
   2, job-exclusive,   amd,   24,    24,     0, 24.00, 132gb,  11gb, 0.06, 419gb,  378gb, 0.10,  8kb,   8kb, 380b
   3, job-exclusive,   amd,   24,    24,     0,  1.51, 132gb,  20gb, 0.10, 177gb,  149gb, 0.16,  8kb,   8kb, 320b
   5, job-exclusive,   amd,   24,    24,     0,  1.33, 132gb,  23gb, 0.11, 177gb,  145gb, 0.18,  8kb,   8kb, 320b
   6, job-exclusive,   amd,   24,    24,     0, 24.00, 132gb,  15gb, 0.08, 177gb,  151gb, 0.15,  8kb,   8kb, 353b
   7, job-exclusive,   amd,   24,    24,     0, 24.00, 132gb,  16gb, 0.08, 177gb,  157gb, 0.12,  8kb,   8kb, 344b
   8, job-exclusive,   amd,   24,    24,     0, 24.00, 132gb,  12gb, 0.06, 177gb,  161gb, 0.09,  8kb,   8kb, 339b
   9, job-exclusive,   amd,   24,    24,     0, 24.00, 132gb,  10gb, 0.05, 177gb,  161gb, 0.09,  8kb,   8kb, 332b
  10,          free,   amd,   24,     6,    18,  1.18, 132gb,  19gb, 0.10, 419gb,  388gb, 0.07,  8kb,   8kb, 319b
  12,          free, intel,    8,     5,     3,  5.00,  49gb,  13gb, 0.12, 419gb,  368gb, 0.12,  8kb,   8kb, 296b
  11,          free, intel,    8,     2,     6,  2.00,  49gb,   1gb, 0.01, 419gb,  366gb, 0.13,  8kb,   8kb, 289b
  14, job-exclusive, intel,    8,     8,     0,  8.00,  49gb,   4gb, 0.03, 904gb,  850gb, 0.06,  8kb,   8kb, 280b
  13, job-exclusive, intel,    8,     8,     0,  8.00,  49gb,   4gb, 0.03, 177gb,  155gb, 0.12,  8kb,   8kb, 239b
  16, job-exclusive, intel,    8,     8,     0,  8.00,  49gb,   4gb, 0.04, 177gb,  147gb, 0.17,  8kb,   8kb, 242b
  15, job-exclusive, intel,    8,     8,     0,  8.00,  49gb,   5gb, 0.04, 177gb,  143gb, 0.19,  8kb,   8kb, 271b
  18, job-exclusive, intel,    8,     8,     0,  1.33,  49gb,   2gb, 0.02, 177gb,   89gb, 0.50, 21mb, 587kb, 20mb
  17, job-exclusive, intel,    8,     8,     0,  6.34,  49gb,  11gb, 0.10, 177gb,  137gb, 0.23,  8kb,   8kb, 270b
  20, job-exclusive, intel,    8,     8,     0,  1.53,  49gb,  19gb, 0.16, 177gb,  130gb, 0.27,  8kb,   8kb, 239b
  21, job-exclusive, intel,    8,     8,     0,  1.76,  41gb,  18gb, 0.17, 177gb,  142gb, 0.20,  8kb,   8kb, 253b
  22, job-exclusive, intel,    8,     8,     0,  8.00,  49gb,   4gb, 0.04, 177gb,  141gb, 0.20,  8kb,   8kb, 239b
  19,          free, intel,    8,     2,     6,  2.00,  49gb,   2gb, 0.02, 177gb,  109gb, 0.39,  8kb,   8kb, 274b
  23,          down, intel,    8,      ,      ,      ,      ,      ,      ,      ,       ,      ,      ,      ,
  24,          free, intel,    8,     2,     6,  2.00,  49gb,   2gb, 0.02, 177gb,  128gb, 0.28,  8kb,   8kb, 248b
  25, job-exclusive, intel,    8,     8,     0,  1.61,  49gb,  19gb, 0.17, 419gb,  319gb, 0.24,  8kb,   8kb, 237b
  26, job-exclusive, intel,    8,     8,     0,  3.19,  49gb,   6gb, 0.05, 177gb,  155gb, 0.12,  8kb,   8kb, 256b
  27, job-exclusive, intel,    8,     8,     0,  8.00,  49gb,   5gb, 0.04, 419gb,  346gb, 0.17,  8kb,   8kb, 243b
  28, job-exclusive, intel,    8,     8,     0,  8.03,  49gb,   4gb, 0.04, 177gb,  121gb, 0.32,  8kb,   8kb, 241b
  29, job-exclusive, intel,    8,     8,     0,  8.00,  49gb,   4gb, 0.03, 177gb,  134gb, 0.24,  8kb,   8kb, 244b
  30, job-exclusive, intel,    8,     8,     0,  8.00,  41gb,   4gb, 0.04, 177gb,  133gb, 0.25,  8kb,   8kb, 244b
  31, job-exclusive, intel,    8,     8,     0,  8.00,  49gb,   5gb, 0.04, 419gb,  377gb, 0.10,  8kb,   8kb, 248b
  32,          free, intel,    8,     1,     7,  1.00,  49gb,   2gb, 0.01, 177gb,  135gb, 0.24,  8kb,   8kb, 253b
-------------------------------------------------
number of CPUs total    : 416 ( 240 amd / 176 intel )
number of CPUs offline  :   8 (   0 amd /   8 intel )
number of CPUs online   : 408 ( 240 amd / 168 intel )
number of CPUs working  : 362 ( 222 amd / 140 intel )
number of CPUs free     :  46 (  18 amd /  28 intel )
```

Etiquette: monitor resources

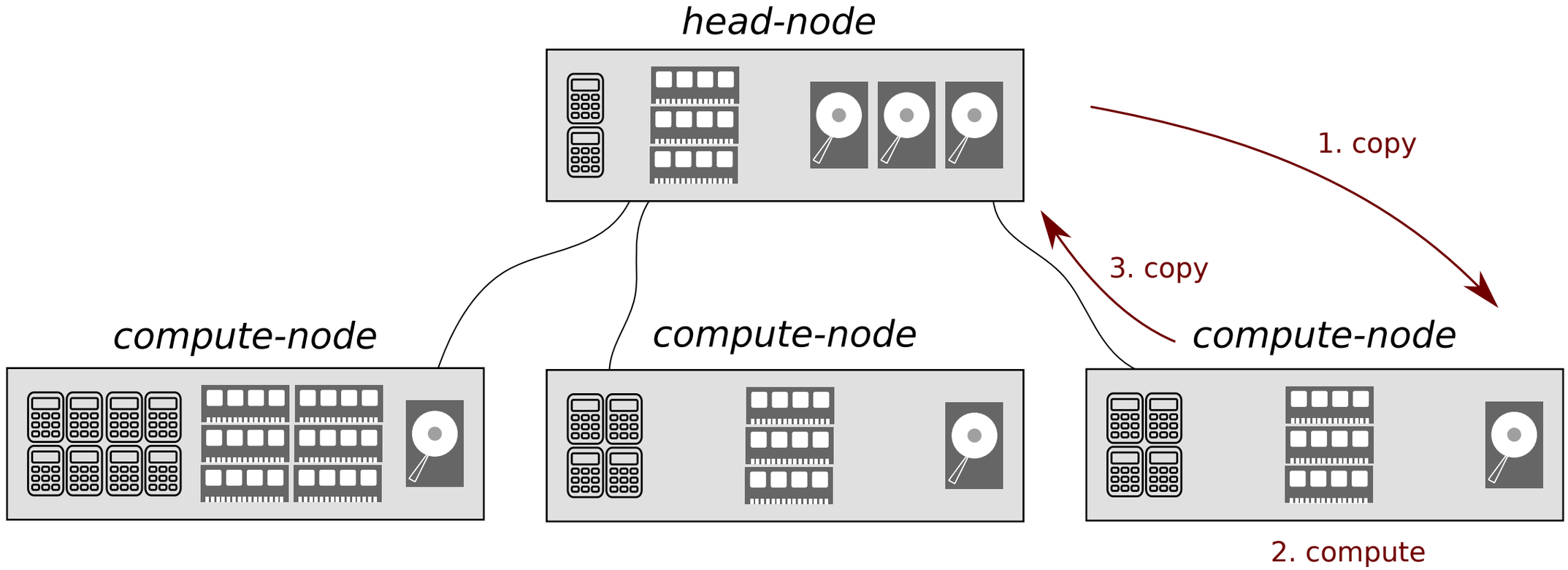
Monitor:

- memory usage
- CPU usage
- disk usage

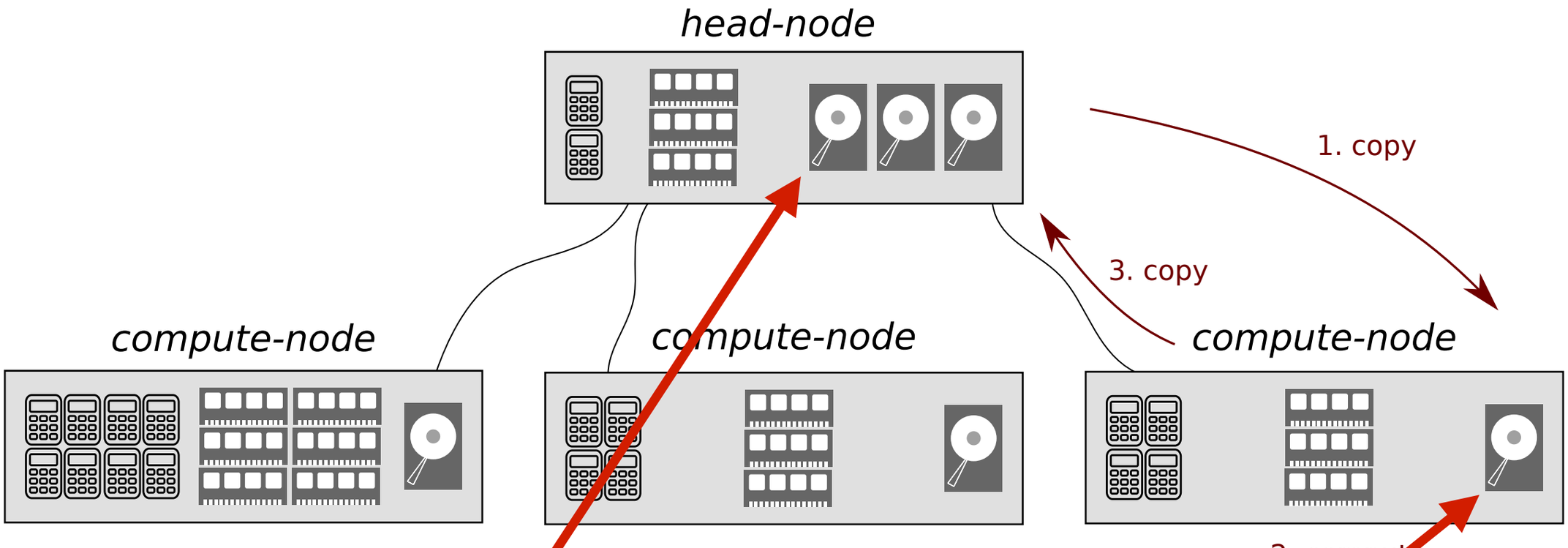
```
$ ssh compute-0-11

$ top
$ df -h
```

www.furnace.wfw.wtb.tue.nl/ganglia

Etiquette: minimize network usage



Etiquette: minimize network usage



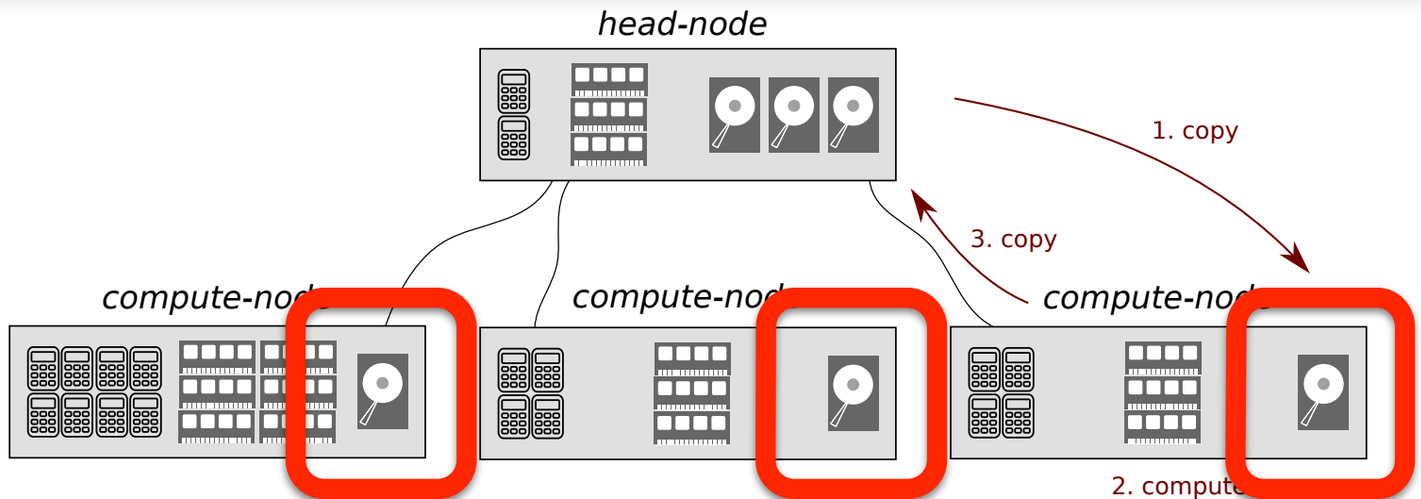

```
$ ssh compute-0-11

$ pwd
/home/tdegeus

$ cd /state/partition1/tdegeus
$ du -hs *
$ ls -lh
```

Stop a job

```
$ myqstat

jid    , owner     , job name       , host , cpus   , mem  , S , time , score
------ , --------- , ------------- , ---- , ------ , ---- , - , ---- , -----
202169 , tdegeus   , myjob.pbs      ,   11 ,  1:1:i , 1mb  , R ,  10s ,  1.00
...

$ qdel 202169
```

Monitor files

```
$ rocks run host “ls /state/partition1/`whoami`”
compute-0-30:
compute-0-19:
compute-0-31:
compute-0-15:
compute-0-27:
compute-0-17:
compute-0-32:
compute-0-26:
compute-0-16:
compute-0-13:
compute-0-21:
compute-0-18:
compute-0-20:
compute-0-28:
compute-0-29:
compute-0-3:
compute-0-5:
compute-0-24:
compute-0-25:
compute-0-6:
compute-0-10:
compute-0-1:
compute-0-11:
compute-0-0:
compute-0-14:
compute-0-22:
compute-0-8:
compute-0-9:
compute-0-7:
compute-0-2:
compute-0-12:
compute-0-23: down
```



Etiquette

- **Monitor your jobs and resources**:
  - CPU usage (“score”)
  - Memory usage
  - Disk usage
  - Network usage
- When in doubt: **ask for help**
- If you plan on running a large simulation: **discuss with Leo Wouters first**
- **Claim what you use and use what you claim**
- Don’t claim too much at once

  Help others, share your experience

Collaboration

Full Name
E-mail
username @furnace
Software

Jim Schormans
J.M.J.Schormans@tue.nl
Jim

- Abaqus
- Dawn

Tom de Geus
T.W.J.d.Geus@tue.nl
tdegeus

- Linux/Bash
- Python
- C/C++
- MSC.Marc

Getting help

www.mate.tue.nl/~cluster

```
$ myqstat –help
```

- Cluster manual
- This presentation
- …

MaTeCluster@tue.nl

- Jim Schormans (J.M.J.Schormans@tue.nl)
- Tom de Geus (T.W.J.d.Geus@tue.nl)

L.H.G.Wouters@tue.nl

- Leo Wouters
- Obtain account