Introduction to Cluster Computing

Zheng Meyer-Zhao - zheng.meyer-zhao@surfsara.nl
Consultant Clustercomputing

SURF SARA

Outline

Cartesius and Lisa

- Architectures and Specifications
- File systems
- Funding

Hands-on

- Logging in
- Module environment
- Batch system

Supercomputers / Cartesius / Lisa

- **What is a Supercomputer?**
  - A fast computer
  - A large computer (memory/storage)
  - An expensive computer (millions of € for hardware, electricity and man power)
- **Why/when do you need a Super?**
  - If your task would take months/years on a normal PC
  - If your task requires more space (memory/storage) than available in PC
- **Why do you, SURFsara, own two Supercomputers?**
  - Historic reasons
    - Cartesius – via NWO
    - Lisa – via UvA, VU, FOM, CWI and NWO
- **What is the difference?**
  - Cartesius – larger "blocks" (**capability** computing – fewer large scale jobs)
  - Lisa – smaller "blocks" (**capacity** computing – more small(er) scale jobs)
  - Cartesius – expensive expensive
  - Lisa – cheaper, but still expensive

Lisa / Cartesius – Nodes

Lisa:

• Total cores	7856
• Total memory	26 TB
• Total peak pf	149 TFlop/sec
• Disk space	100 TB for the home file systems
• OS	Debian Linux AMD64 OS
• Network	Ethernet / Infiniband

Cartesius:

• Total cores	47776 CPU + 132 GPU (incl. KNL, broadwell)
• Total memory	130 TB
• Total peak pf	1.843 PFlop/sec
• Disk space	180 TB home, 7.7PB project + scratch
• OS	BullX
• Network	Infiniband 56 Gbps, 3μs latency

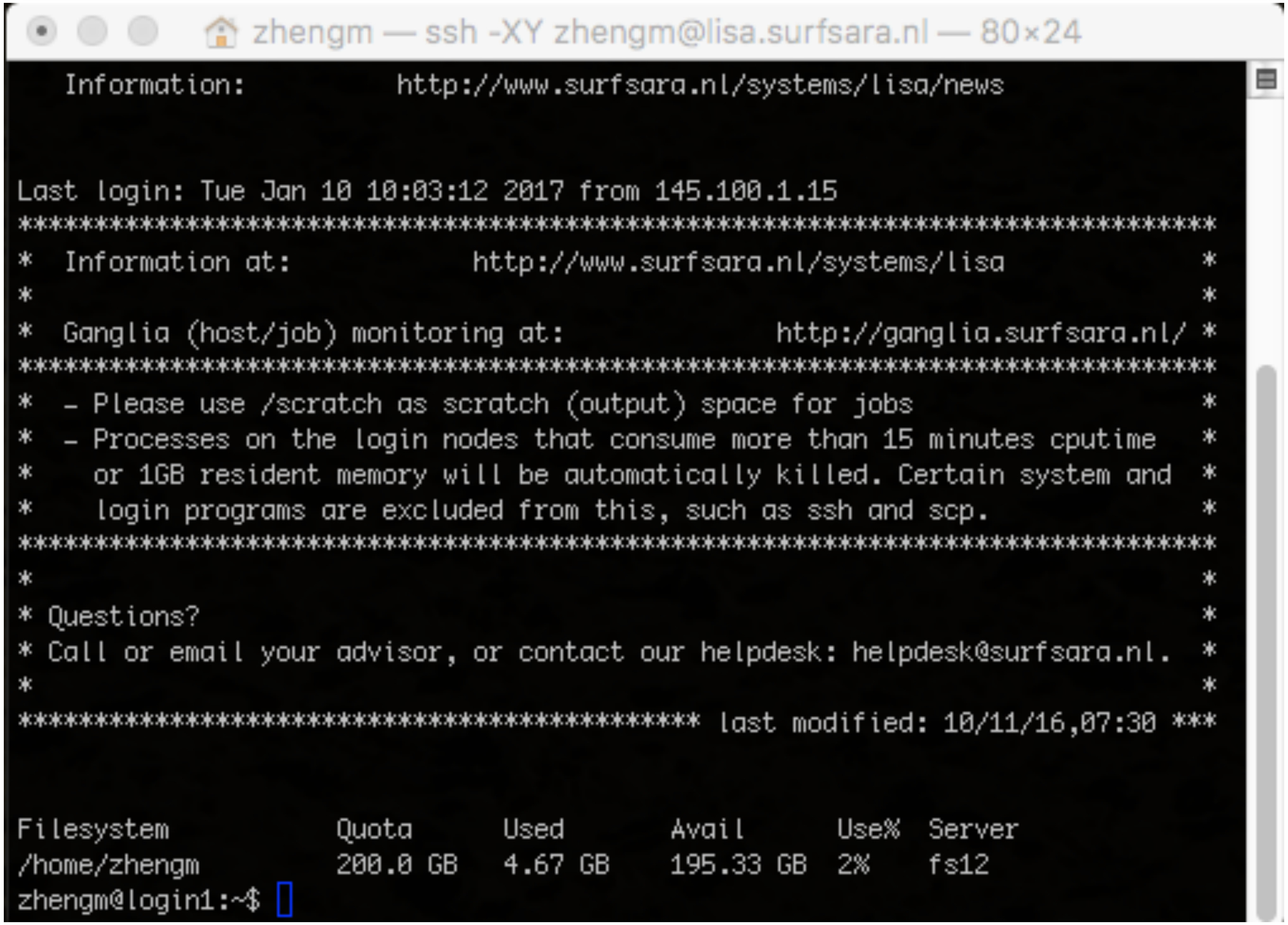
Working on Supercomputers nowadays

So, how does working on a supercomputer look like nowadays?

Is NOT like:

Also NOT like:

Typically it is like:

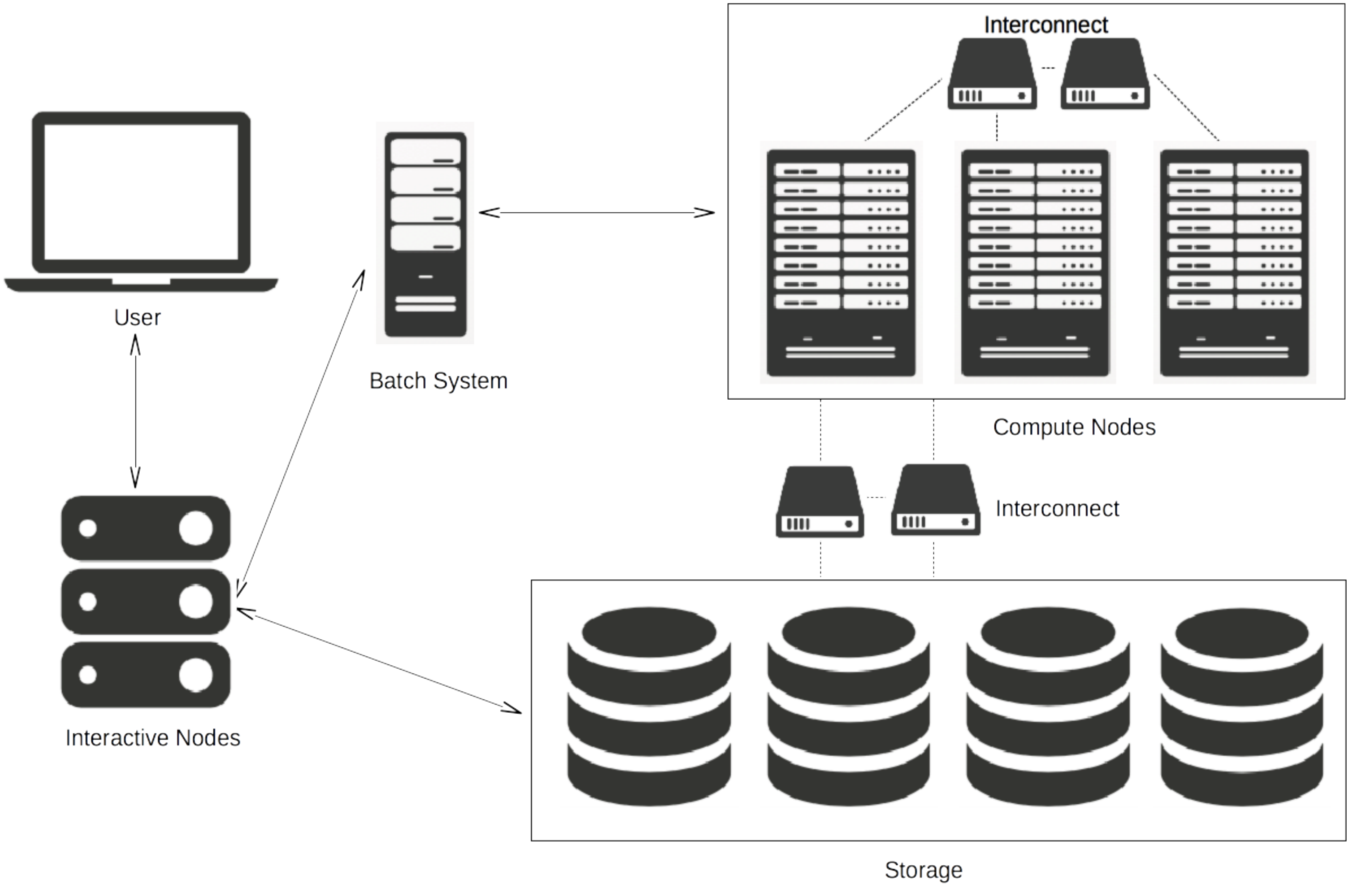


```
   Information:          http://www.surfsara.nl/systems/lisa/news


Last login: Tue Jan 10 10:03:12 2017 from 145.100.1.15
********************************************************************************
*  Information at:            http://www.surfsara.nl/systems/lisa              *
*                                                                              *
*  Ganglia (host/job) monitoring at:               http://ganglia.surfsara.nl/ *
********************************************************************************
*  - Please use /scratch as scratch (output) space for jobs                   *
*  - Processes on the login nodes that consume more than 15 minutes cputime   *
*    or 1GB resident memory will be automatically killed. Certain system and *
*    login programs are excluded from this, such as ssh and scp.               *
********************************************************************************
*                                                                              *
* Questions?                                                                   *
* Call or email your advisor, or contact our helpdesk: helpdesk@surfsara.nl.   *
*                                                                              *
********************************************** last modified: 10/11/16,07:30 ***


Filesystem           Quota      Used       Avail      Use%  Server
/home/zhengm         200.0 GB   4.67 GB    195.33 GB  2%    fs12
zhengm@login1:~$
```

General Architecture



Supercomputer Architecture

Cartesius & Lisa – File systems (1)

- **/home/user**
- User home directory (quota - currently 200GB)
- Backed up
- Meant for storage of important files (sources, scripts, input and output data)
- Not the fastest file system

- **/scratch**
- Cartesius: /scratch-local & /scratch-shared (quota – currently 8 TB)
- Lisa: /scratch (quota – depends on disk size)
- Not backed up
- Meant for temporary storage (during running of a job and shortly thereafter)
- The fastest file systems on Cartesius & Lisa

Cartesius & Lisa – File systems (2)

- **/archive**
- Connected to the tape robot (quota – virtually unlimited)
- Backed up
- Meant for long term storage of files, zipped, tarred, combined into small number of files
- Slow – especially when retrieving “old” data
- Not available to worker nodes

- **/project**
- Only available on Cartesius !
- For special projects requiring lots of space (quota – as much as needed/possible)
- Not backed up
- Meant for special projects
- Comparable in speed with /scratch

Cartesius & Lisa – Funding model

Compute time and storage is paid for by:

- **NWO – Fully subsidized**
  - application through ISAAC
  - peer reviewed
  - administration and reporting involved
  - free
- **Your university or institute (RCCS)**
  - application through local owner or chair

Take a look at the SURFsara website:
https://userinfo.surfsara.nl/systems/cartesius/account

Questions?

Hands-on: Let’s play!

Contents

- Install Terminal software
- Login to Cartesius
- Look at some scripts
- Submit a few jobs

… wait for the result …

- Analyze the results
- (Copy back output/results locally)

Hands-on : Preparation

- **Install Terminal software**

For Windows users only:

- Install MobaXterm (installer edition) from http://mobaxterm.mobatek.net/
- ... and, run it

Linux users:

- Run a terminal

Max OS-X users:

- Find “Terminal”, run it
- Install XQuartz (http://www.xquartz.org)

Logging in on Cartesius

Windows, MobaXterm:

- Start a new session
- Hostname is "**cartesius.surfsara.nl**" (all lowercase)
- Username is "**sdemoXXX**" – use the address received by mail

Linux and mac:

- Start a new terminal; do (replace XXX with your actual username)

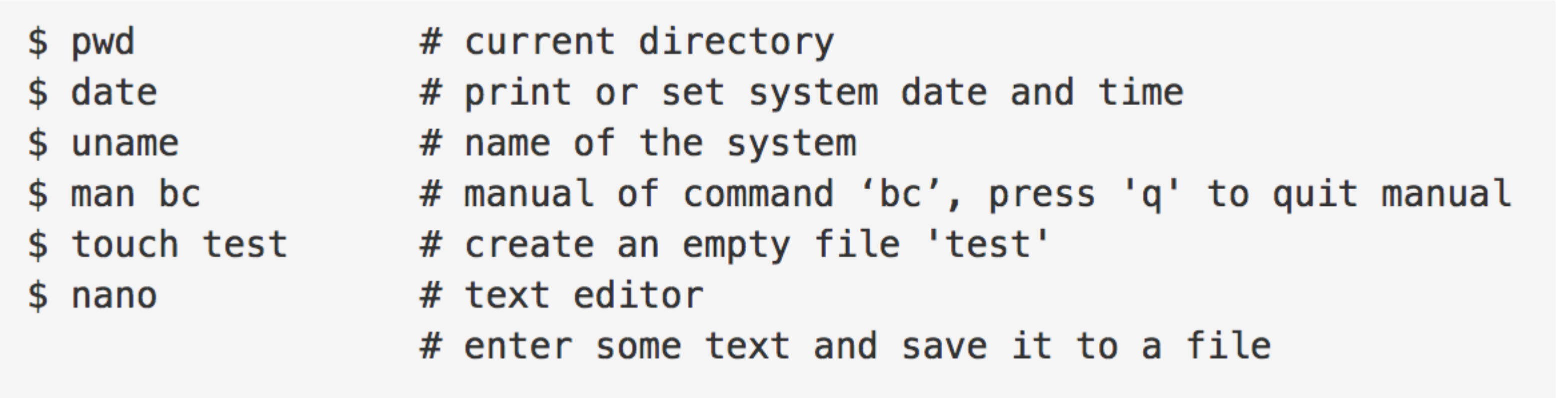
```
ssh sdemoXXX@cartesius.surfsara.nl
```

- Use the password received by e-mail

Exercise 1: warm up

Go to the Hands-on page at http://bit.ly/2iC6UbT

Are you familiar with the following commands?



```
$ pwd               # current directory
$ date              # print or set system date and time
$ uname             # name of the system
$ man bc            # manual of command ‘bc’, press 'q' to quit manual
$ touch test        # create an empty file 'test'
$ nano              # text editor
                    # enter some text and save it to a file
```

Exercise 2: software modules

We have a lot of software installed.

1. **in your browser, go to**

   http://userinfo.surfsara.nl

   then systems -> Cartesius -> software, and look for programs that you use. Is there anything you already use? or would like to use?

2. **on Lisa/Cartesius, use**

   ```
   module avail
   module avail modulename
   module load modulename
   module unload modulename
   ```

   to see what software we have installed, and to load/unload a module.

Modules – Why modules?

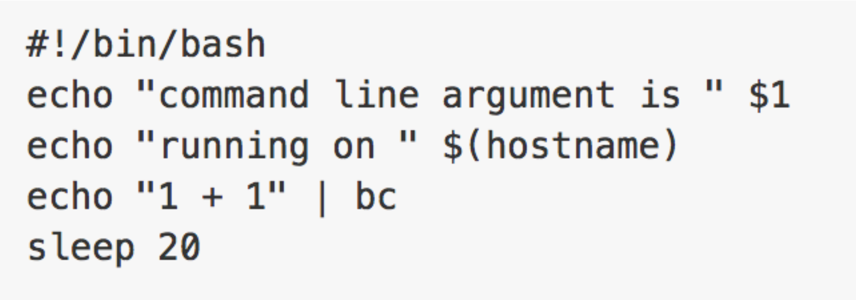
Why modules?

- Environment variables are set for you, like:
  - **$PATH**
  - **$LD_LIBRARY_PATH**

- Multiple versions of software
- **LOTS** of software already available and optimized, by us, for you!

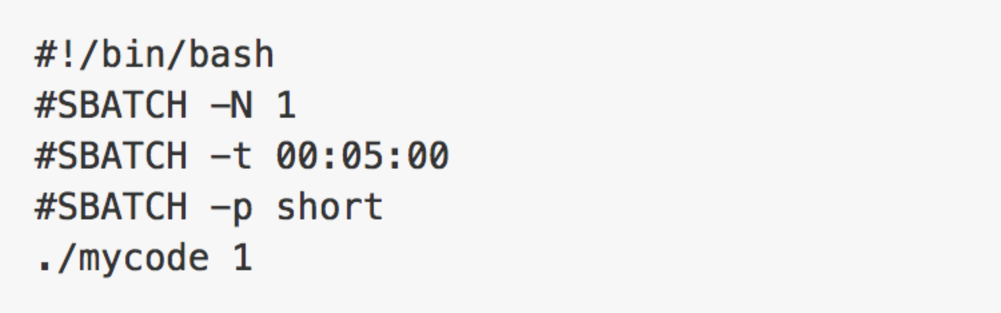
Exercise 3: running a job (1)

1. Use the *nano* text editor to create a file “mycode” with the following contents:



```
#!/bin/bash
echo "command line argument is " $1
echo "running on " $(hostname)
echo "1 + 1" | bc
sleep 20
```

2. Create another file “job.sh” with the contents below:



```
#!/bin/bash
#SBATCH -N 1
#SBATCH -t 00:05:00
#SBATCH -p short
./mycode 1
```

Exercise 3: running a job (2)

3. submit the job with

```
sbatch job.sh
```

4. use

```
squeue –u sdemoXXX
```

to find out what your job is doing.

5. once your job is finished, use

```
cat slurm-NNNNN.out
```

to see the output. Discuss.

Lisa / Cartesius – batch commands

- **To submit a job**
  - Lisa: qsub <jobscript>
  - Cartesius: sbatch <jobscript>

Job submission returns a unique **jobid**.

- **To view submitted jobs (of yourself)**
  - Lisa: qstat –u <username>
  - Cartesius: squeue –u <username>
- **To cancel submitted jobs**
  - Lisa: qdel <jobid>
  - Cartesius: scancel <jobid>

Exercise 4: Run serial code on multiple cores

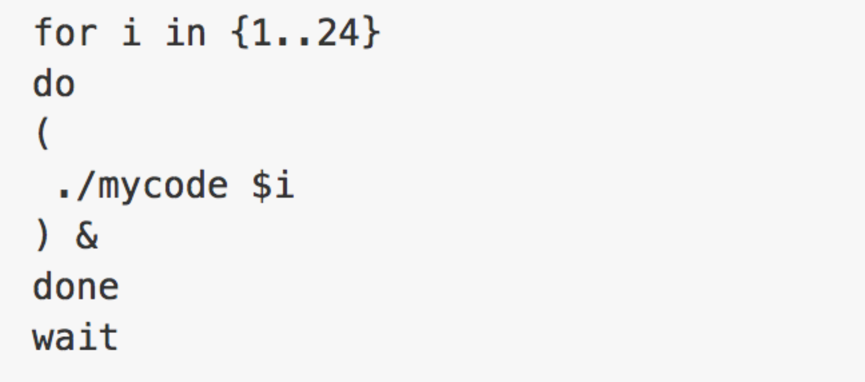
Why?

- One thin node on Cartesius has 24 cores
- It costs 24 SBUs per hour even if you only use one core

We want to use the computing resources efficiently.

How?

Batch for loop

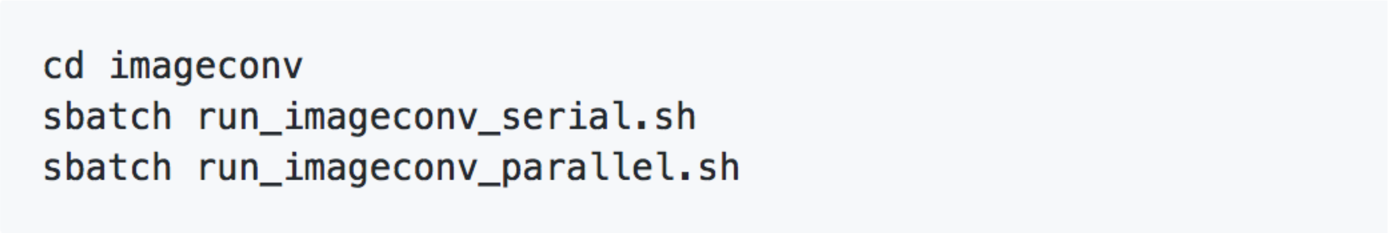


```
for i in {1..24}
do
(
 ./mycode $i
) &
done
wait
```

- \`$i\` is the value of \`i\` in the current loop
- \`&\` makes sure that each process runs at backgroud simultaneously
- \`wait\` tells the script to wait until all processes are finished

View matlab/matrixmul.sh and submit the job to Cartesius

Exercise 5: Use scratch space



```
cd imageconv
sbatch run_imageconv_serial.sh
sbatch run_imageconv_parallel.sh
```

- $TMPDIR is the temporary directory on the scratch space generated for your job.
- If data size is big, it is recommended to copy the data to the scratch space first, do the calculation, then copy the results back.

Exercise 6: running a wave equation

1. When logged in, go to the directory “wave”;
2. Type

```
module load openmpi
module load c/intel
module load hdf5
make
```

   to compile the program.

3. run the wave model with

```
sbatch run_wave
```

4. use

```
scp sdemoNNN@cartesius.surfsara.nl:usingcartesius/wave/wave.h5.gif  ./
```

   to copy the result animation to your own system

5. view the file in a web browser

That is all for today!

If you have any questions, please contact us at

helpdesk@surfsara.nl