



INTRODUCTION TO HPC IN COMPUTATIONAL MODELLING

PATC: Short course on HPC-based Computational Bio-Medicine

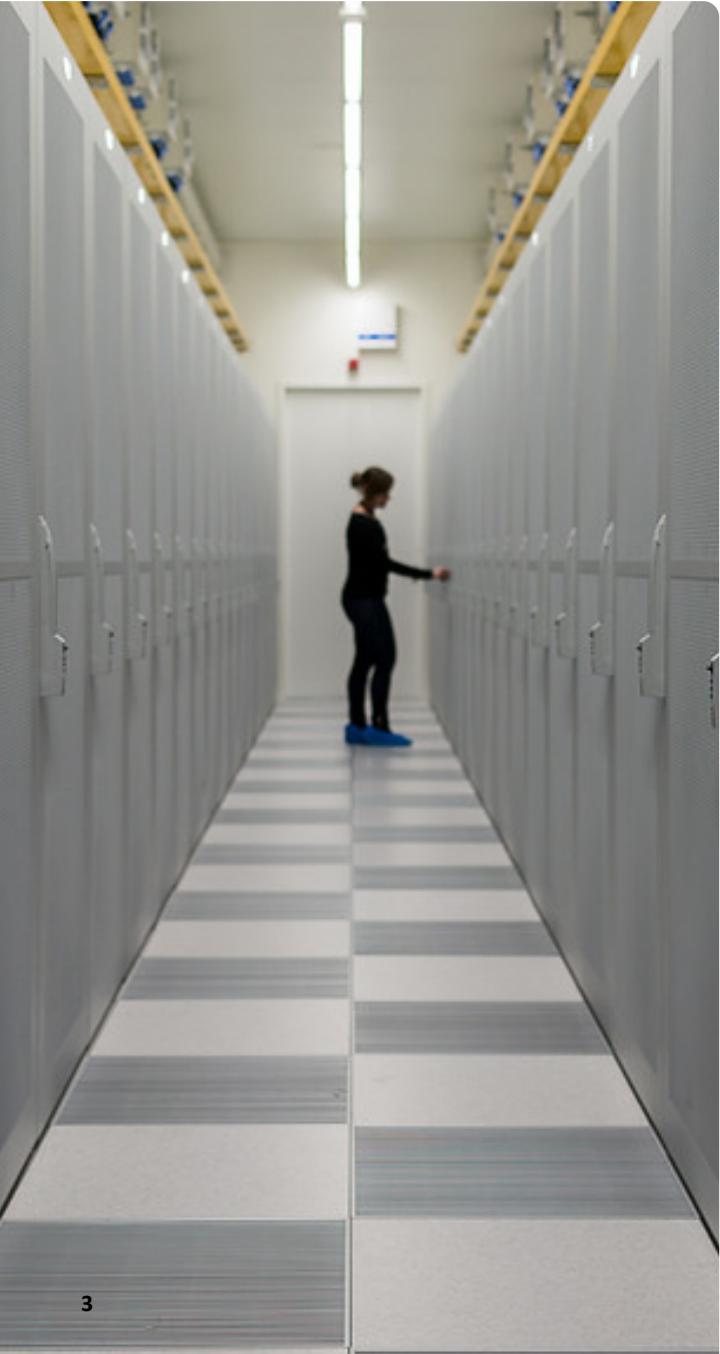
Marco Verdicchio - SURFsara



High Performance Computing at SURFsara

- HPC Consultant
- Science Park, Amsterdam
- About 70 op. people
 - 50% Consultants
 - 50% System programmers

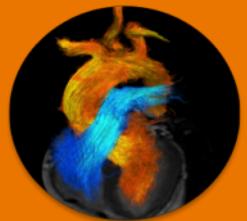




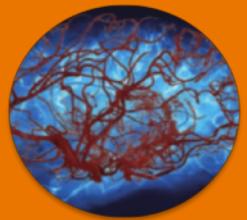
High Performance Computing at SURFsara

- Maintain Cartesius and Lisa
- User support
- Training
- Development and Innovation
- Involvement in EU projects

High Performance Computing in CompBioMed



Cardiovascular
medicine



Neuro
Musculoskeletal
medicine

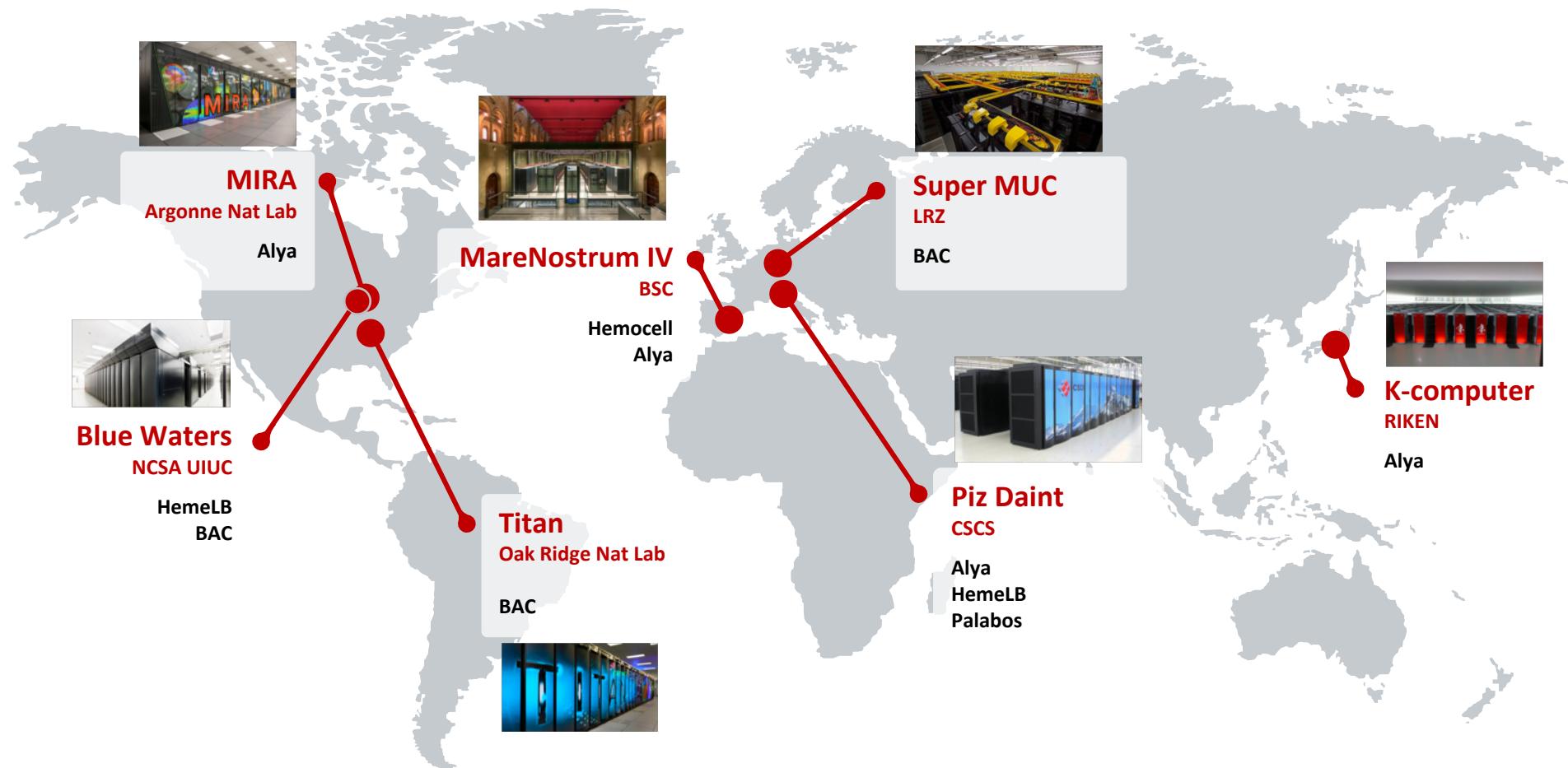


Molecularly
based
medicine



- Support and facilitate modeling and simulation activities within biomedical community.
- Development and sustainability of software tools and services.
- Enhance industries in the healthcare sector (pharmaceuticals & medical device manufacture).

High Performance Computing in CompBioMed





Outline

What is a Supercomputer?

- Working with an HPC system
- HPC access and usage

Getting started with HPC

- Linux basic command
- HPC tools

Running jobs on a Supercomputer

- Use the batch system
- Running jobs

What is a Supercomputer?

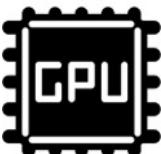
User Experience

- Multiuser system
- Unix OS
- Optimized software



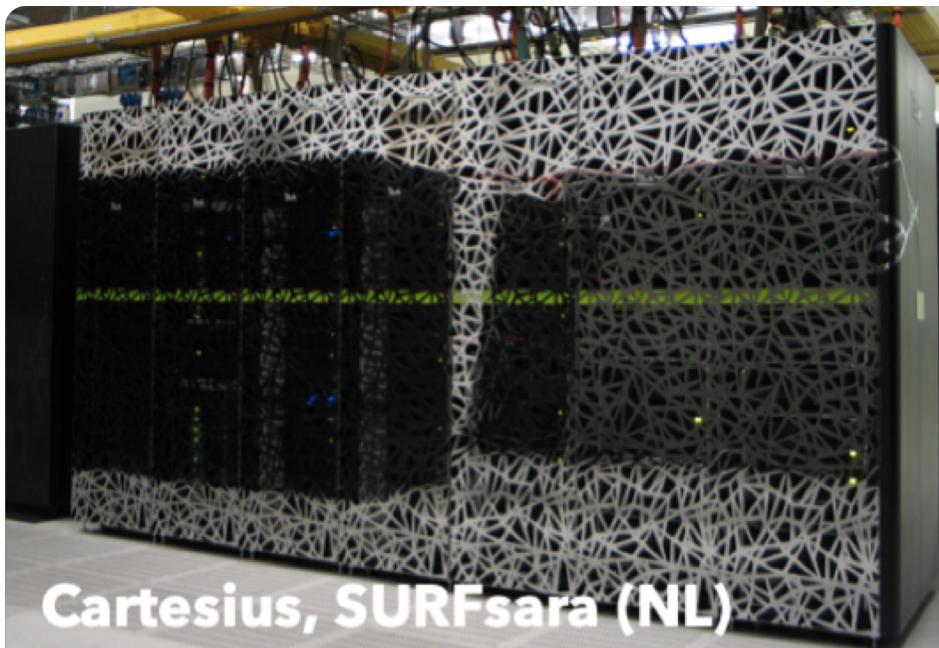
Compute power

- Many CPUs system
- Specialized Hardware
- Low-lat/High bw connections



Storage

- Efficient I/O
- Large Memories



What is a Supercomputer?

TOP 10 Sites for November 2018

For more information about the sites and systems in the list, click on the links or view the complete list.

[1-100](#) [101-200](#) [201-300](#) [301-400](#) [401-500](#)

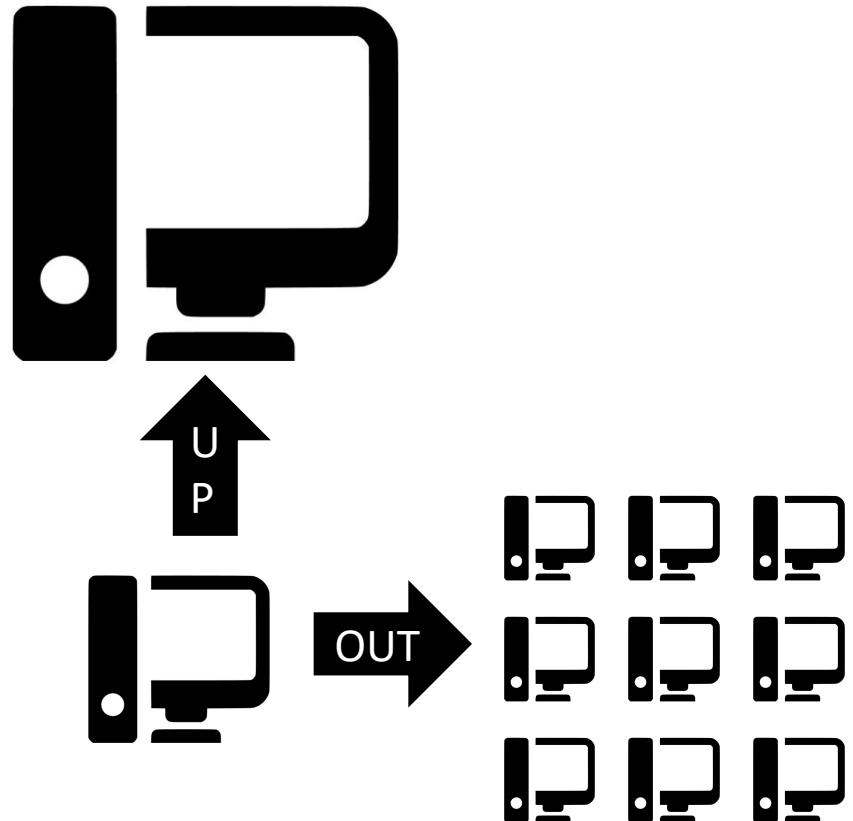
Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/SC/Oak Ridge National Laboratory United States	2,397,824	143,500.0	200,794.9	9,783
2	Sierra - IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
3	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway , NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
4	Tianhe-2A - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000 , NUDT National Super Computer Center in Guangzhou China	4,981,760	61,444.5	100,678.7	18,482

What is a Supercomputer?

Why you need a Supercomputer?

- **Scale up**
 - Faster CPUs
 - Large memories
 - Specialized Hardware/Software

- **Scale out**
 - Large parallel applications
 - Many small- to medium- size jobs



What is a Supercomputer?

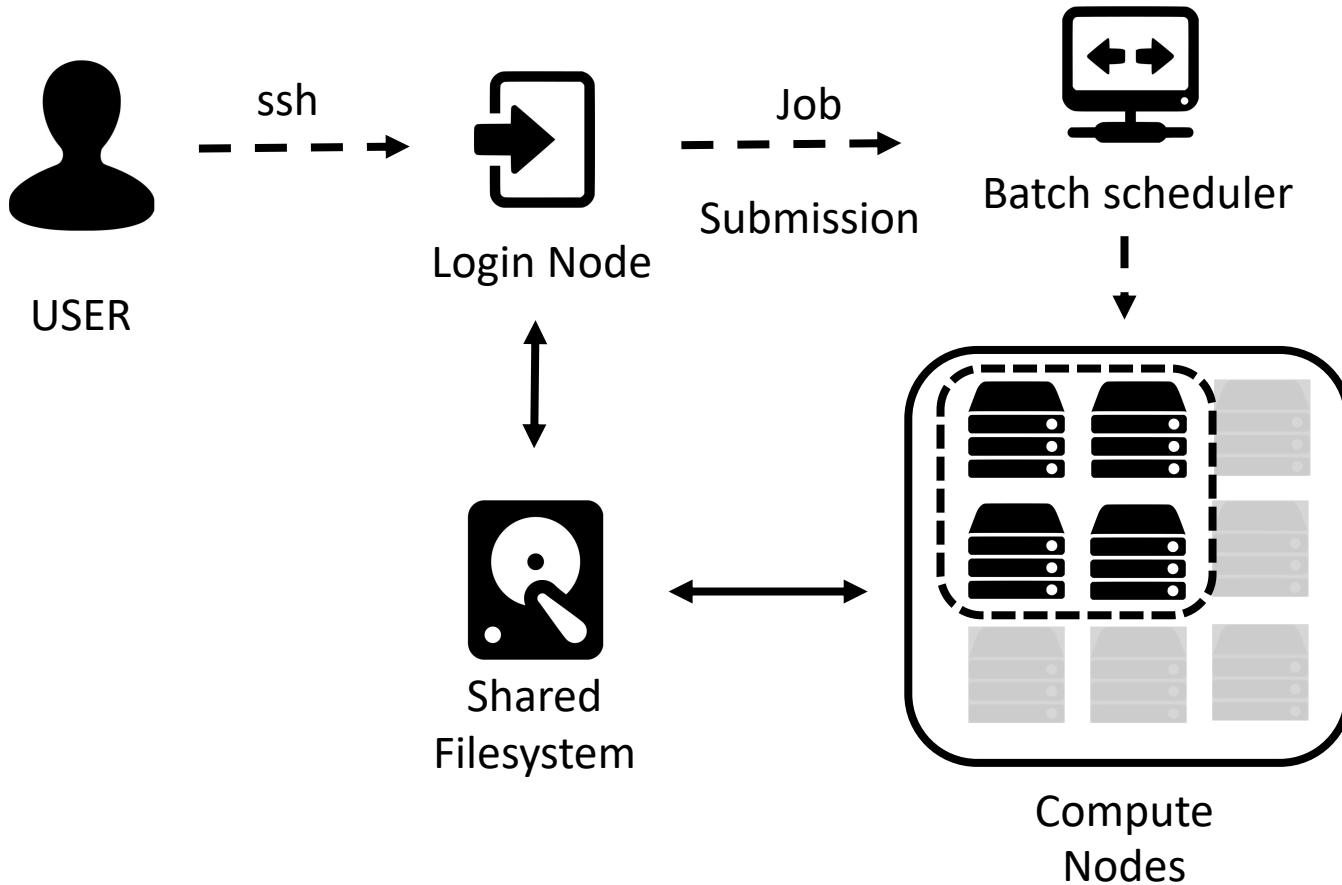
Is NOT like this...



What is a Supercomputer?

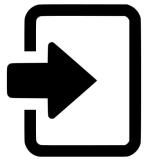
What is a Supercomputer?

Working with a Supercomputer



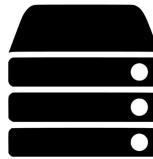
What is a Supercomputer?

Working with a Supercomputer



Login node(s)

- Editing and transferring files
- Compile programs
- Prepare simulations



Compute nodes

- Multicore nodes
- Large memories
- High-speed interconnections



Batch scheduler

- Resource allocation
- Job queueing
- Accounts and budget



File system

- Parallel FS
- Efficient I/O
- Node local disks

Getting started with HPC

Working with a Supercomputer

Login and transfer files to remote machine

1

- ssh, scp/ftp
- Command line, GUI

Prepare your jobs

2

- Input + Software
- Job submission script

Submit your job and retrieve output

3

- Submit job to the batch system
- Monitor job, retrieve output (remote visualization)

GETTING STARTED WITH HPC

Introduction to HPC in Computational
Modelling



Getting started with HPC

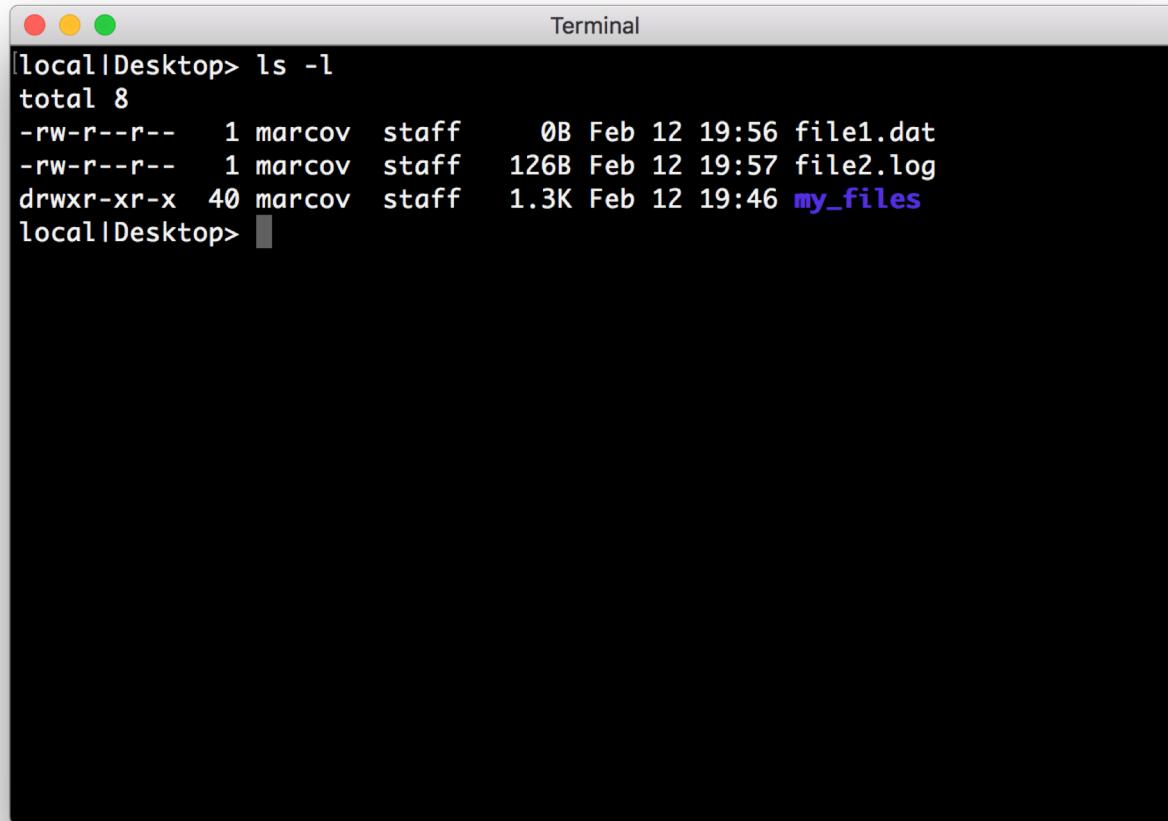


What is UNIX?

- Operating System
 - Program that controls all other parts of a computer system
 - Allocates computer's resources and schedules tasks
 - Allows the user to use the facilities provided by the system
 - Essential to all computer systems
- Multi-User and Multi-Tasking
 - Multiple users have multiple tasks running simultaneously
- Designed to be machine independent
- Setup as a software development environment
- Suitable for scientific applications

Getting started with HPC

Terminal – Working with a Unix system



The image shows a terminal window with a dark background and light-colored text. At the top, there are three colored window control buttons (red, yellow, green) followed by the word "Terminal". The main area of the window displays the following command and its output:

```
[local|Desktop> ls -l
total 8
-rw-r--r--  1 marcov  staff      0B Feb 12 19:56 file1.dat
-rw-r--r--  1 marcov  staff   126B Feb 12 19:57 file2.log
drwxr-xr-x  40 marcov  staff   1.3K Feb 12 19:46 my_files
local|Desktop>
```

Getting started with HPC

Install UNIX tools on your local machine

- **Windows**

- Putty
- MobaXterm (<http://mobaxterm.mobatek.net>)

- **Mac OSX**

- Terminal (pre-installed)
- XQuartz (<http://www.xquartz.org>)

- **Linux**

- You are already well equipped!

Getting started with HPC

SSH, or Secure SHell

- establishing a cryptographically secured connection
- authenticating each side to the other
- passing commands and output back and forth

\$ ssh **nct0004@mn1.bsc.es**
Password:

username
Marenostrum login node

Structure of a Unix command

```
nct0004@login1:~> mkdir -p dir1/subdir
```

Command
The UNIX shell (bash) tries to find a program called 'mkdir' and takes care that the system executes it.

Options
Passed to the command as a parameter(s) to change its default behavior.

Arguments
Taken as input by the program.

Getting started with HPC

- Download the material:

http://bit.ly/HPC_CBM

- Transfer the zip file to MarenostrumIV:

```
~> scp IntroHPC_CBM-master.zip nct00013@mn1.bsc.es:
```

- Extract the zip in your home:

```
nct00013@login1:~> unzip IntroHPC_CBM-master.zip
```

- GUI for file transfer available for MobaXterm

Getting started with HPC

```
| 11:49:34 |marcov|~> cd Downloads/  
| 11:49:37 |marcov|Downloads> scp IntroHPC_CBM-master.zip nct00013@mn1.bsc.es:  
Password:  
IntroHPC_CBM-master.zip                                         100% 26KB 152.0KB/s 00:00  
| 11:50:06 |marcov|Downloads>
```

Getting started with HPC

Basic Unix commands

- Explore the file system
 - ls, cd, pwd
- Create files and directories
 - mkdir, touch, cp, mv
- File editing
 - less, cat, head/tail
- System tools
 - history, find, zip, tar

```
nct00013@login1:~> pwd  
/home/nct00/nct00013
```

```
nct00013@login1:~> ls  
bin file1.txt file2.log
```

```
nct00013@login1:~> cp file.in file.copy
```

```
nct00013@login1:~> mkdir -v data  
mkdir: created directory 'data'
```

```
nct00013@login1:~> man scp
```



Getting started with HPC

Basic scripting

- A Bash script is a plain text file which contains a series of commands.
- Any command you can run on the command line can be put into a script (v.v.)
- It will be executed like a normal program:

./script.sh

```
nct00013@login1:~> cat unix/simple.sh  
#!/bin/bash  
  
echo "Hi, I'm your first script."  
echo  
  
lscpu --help > cpu.log  
lscpu >> cpu.log  
  
echo "I've left something for you."  
echo "Ciao"
```



Getting started with HPC

Basic scripting

- A script need execution permissions

```
chmod +x script.sh
```

- A script (command) produce output and error messages

- Stdin: your keyboard
 - Stdout: your screen
 - Stderr: your screen

- Out/Err can be redirected to files or commands

```
echo "3/0" | bc > calc.log
```

```
nct00013@login1:~> cat unix/simple.sh
```

```
#!/bin/bash
```

```
echo "Hi, I'm your first script."  
echo
```

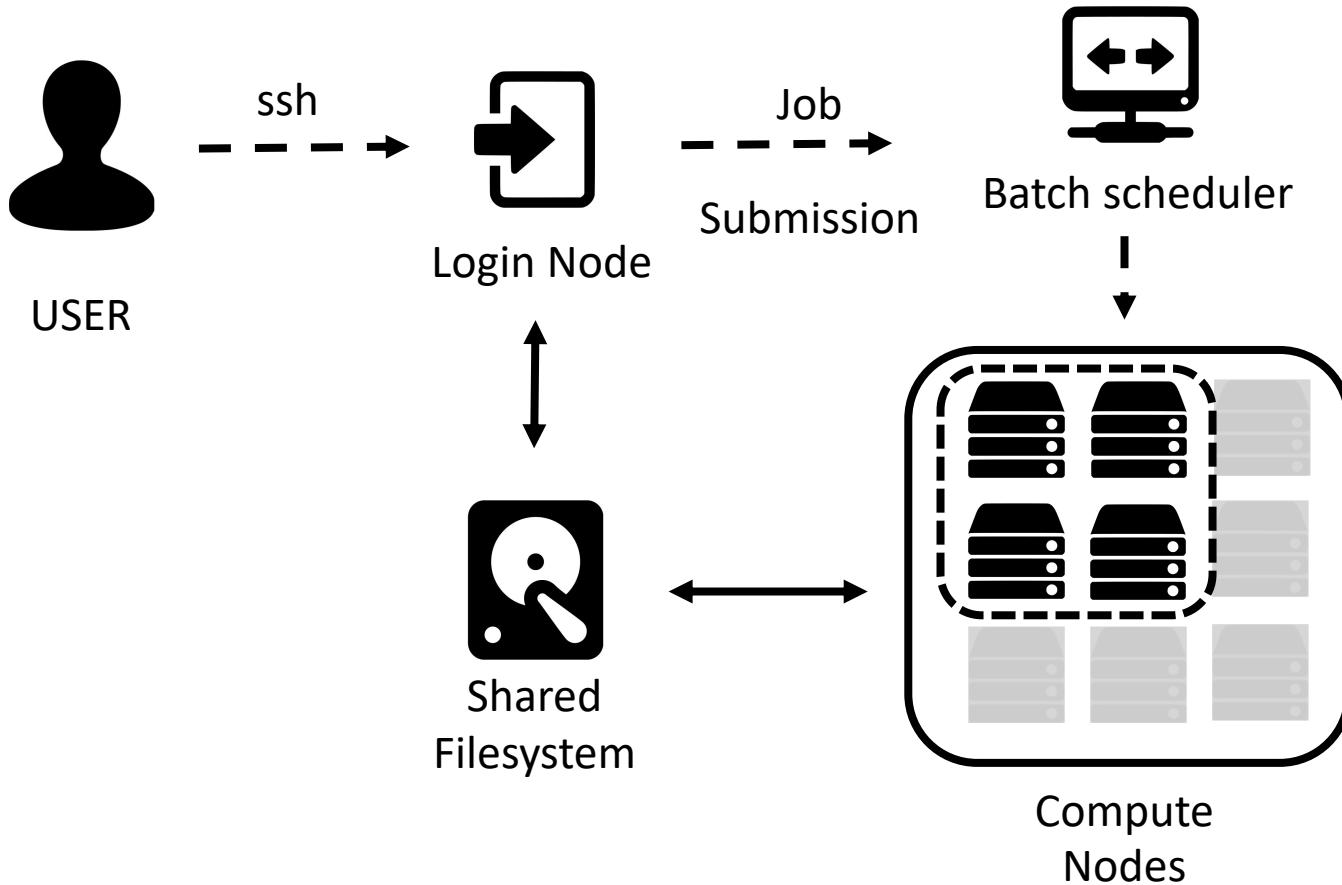
```
lscpu --help > cpu.log  
lscpu >> cpu.log
```

```
echo "I've left something for you."  
echo "Ciao"
```



Getting started with HPC

Submitting jobs in an HPC system



Getting started with HPC

- Supercomputers use batch systems to distribute computational tasks over the available nodes.
- Instead of executing commands interactively, you prepare a job script
 - Script containing the commands to execute
 - Resource characteristics (specific)
- The batch system is responsible for allocating cores, processors or nodes to a job.



Getting started with HPC

Advantages of a batch system are:

- It allows to run MANY jobs at the same time
 - The system takes care that they are run efficiently on the available resources.
- Multiusers, queue system
 - A batch system allows users to always submit jobs, even if a lot of people are using the system at the same time. In addition take care of budgeting and fair resource usage.
- System load balance
 - The system takes care of balancing the load across nodes and during time. In a batch system, most jobs may be submitted during office hours, but the scheduler will continue to start jobs at night as nodes become available.



RUNNING ON A SUPERCOMPUTER

Introduction to HPC in Computational Modelling



Running on a Supercomputer

Job submission script

■ SLURM Job directives

A job script must contain directives to inform the batch system about the characteristics of the job. This directives appear as comments (#SBATCH) in the job script and have to conform with the sbatch syntax.

- number of compute nodes
- number of processes to start
- total wall clock time of the job
- requesting a specific queue
- name of the file where std out is printed

<https://slurm.schedmd.com/sbatch.html>

www.bsc.es/support/MareNostrum4-ug.pdf

```
nct00013@login1:~> head batch/slurm2.sub  
  
#!/bin/bash  
#SBATCH --job-name="test_multinode"  
#SBATCH --nodes=2  
#SBATCH --tasks-per-node=3  
#SBATCH --time=00:02:00  
#SBATCH --qos=training  
#SBATCH --workdir=.  
#SBATCH --output=multinode_%j.out  
#SBATCH --error=multinode_%j.err
```



Running on a Supercomputer

Submitting and monitoring jobs

Jobs are submitted and controlled using SLURM commands

- submits a “job script” to the queue system:

```
nct00013@login1:~> sbatch <job script>
```

- shows all the submitted jobs and their status:

```
nct00013@login1:~> squeue
```

- remove the job from the queue system:

```
nct00013@login1:~> scancel <jobid>
```

- run a command on the cluster

```
nct00013@login1:~> srun <command>
```

Running on a Supercomputer

```
nct00013@login1:~/IntroHPC_CBH-master/batch> sbatch slurm2.sub
Submitted batch job 4596860
```

```
nct00013@login1:~/IntroHPC_CBH-master/batch> squeue
      JOBID PARTITION      NAME      USER ST      TIME  NODES NODELIST(REASON)
        4596860      main test_mul nct00013 R      0:05      2 s13r1b[34-35]
```

```
nct00013@login1:~/IntroHPC_CBH-master/batch> scancel 4596860
```

```
nct00013@login1:~/IntroHPC_CBH-master/batch> squeue
      JOBID PARTITION      NAME      USER ST      TIME  NODES NODELIST(REASON)
        4596860      main test_mul nct00013 CG     0:39      2 s13r1b[34-35]
```

```
nct00013@login1:~/IntroHPC_CBH-master/batch> squeue
      JOBID PARTITION      NAME      USER ST      TIME  NODES NODELIST(REASON)
```

```
nct00013@login1:~/IntroHPC_CBH-master/batch> ls -l
total 5
-rw-r--r-- 1 nct00013 nct00 298 Feb 12 01:31 interactive.txt
-rw-r--r-- 1 nct00013 nct00 84 Feb 12 13:41 multinode_4596860.err
-rw-r--r-- 1 nct00013 nct00 81 Feb 12 13:40 multinode_4596860.out
-rw-r--r-- 1 nct00013 nct00 274 Feb 12 13:33 slurm1.sub
-rw-r--r-- 1 nct00013 nct00 306 Feb 12 13:33 slurm2.sub
```

Running on a Supercomputer

Queues

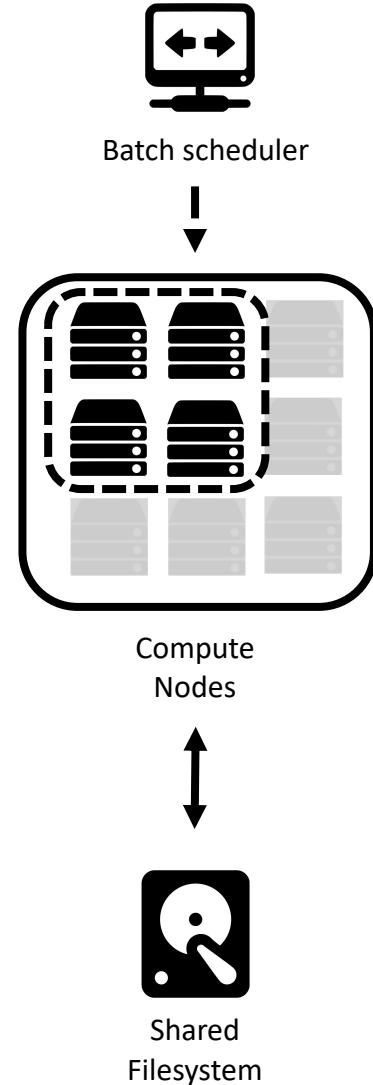
- There are several queues present in the machines and different users may access different queues.
- `bsc_queue` shows information of the available queues

Filesystems

- Each user has several areas of disk space for storing files.
- These areas may have size or time limits (`bsc_quota`).
- Choose carefully where to store your data!

Software stack

- HPC centers usually offer a set of software to their users
- `module` command show available software



Running on a Supercomputer

Module environment

- Provide lots of useful software packages
- In many different versions
- Maintained by experts
- Optimized for the architecture

- Available operations:
 - list all / specific software
 - load/unload a specific software
 - list loaded modules

```
nct00013@login1:~> module avail
```

```
nct00013@login1:~> module avail python
```

```
nct00013@login1:~> module load siesta
```

```
nct00013@login1:~> module load python/2.7.14
```

```
nct00013@login1:~> module unload siesta
```

```
nct00013@login1:~> module list
```



Running on a Supercomputer

```
nct00013@login1:~> module list
```

Currently Loaded Modules:

```
1) intel/2017.4  2) impi/2017.4  3) mkl/2017.4  4) bsc/1.0  5) lzo/2.10
```

```
nct00013@login1:~> gmx_mpi --version  
-bash: gmx_mpi: command not found
```

```
nct00013@login1:~> module load gromacs  
load gromacs/2016.4 (PATH, LD_LIBRARY_PATH)
```

```
nct00013@login1:~> which gmx_mpi  
/apps/GROMACS/2016.4/INTEL/IMPI/bin/gmx_mpi
```

```
nct00013@login1:~> gmx_mpi --version  
:-) GROMACS - gmx_mpi, 2016.4-dev-20170515-2eb5a6307-unknown (-:
```

```
nct00013@login1:~> which gmx_mpi  
/apps/GROMACS/2016.4/INTEL/IMPI/bin/gmx_mpi
```

Getting started with HPC

Working with a Supercomputer

Login and transfer files to remote machine

- ssh, scp/ftp
- Command line, GUI

Prepare your jobs

- Input + Software
- Job submission script

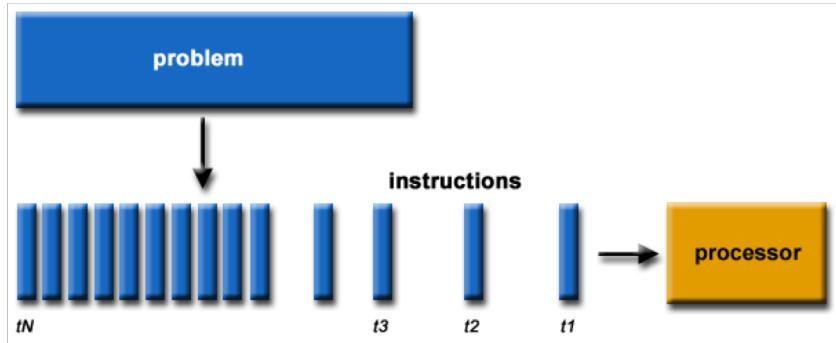
Submit your job and retrieve output

- Submit job to the batch system
- Monitor job, retrieve output (remote visualization)

Running on a Supercomputer

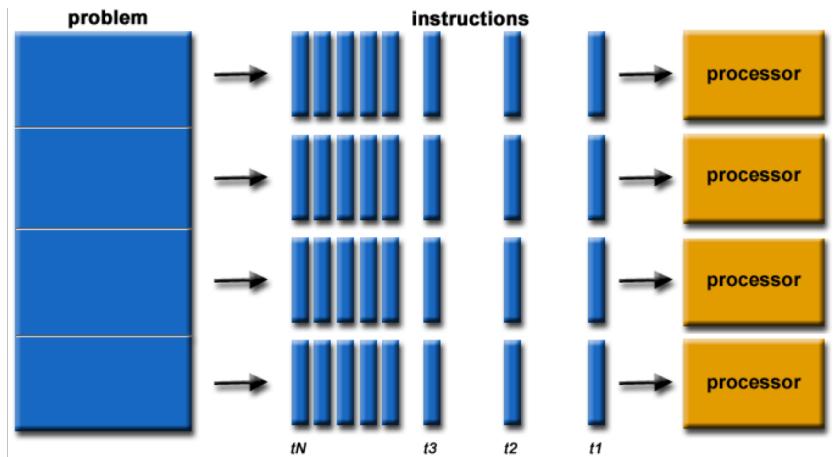
Serial computing

- A problem is broken into a discrete series of instructions, which are executed sequentially on a single processor.



Parallel computing

- A problem is broken into discrete parts that can be solved concurrently using simultaneously multiple resources.

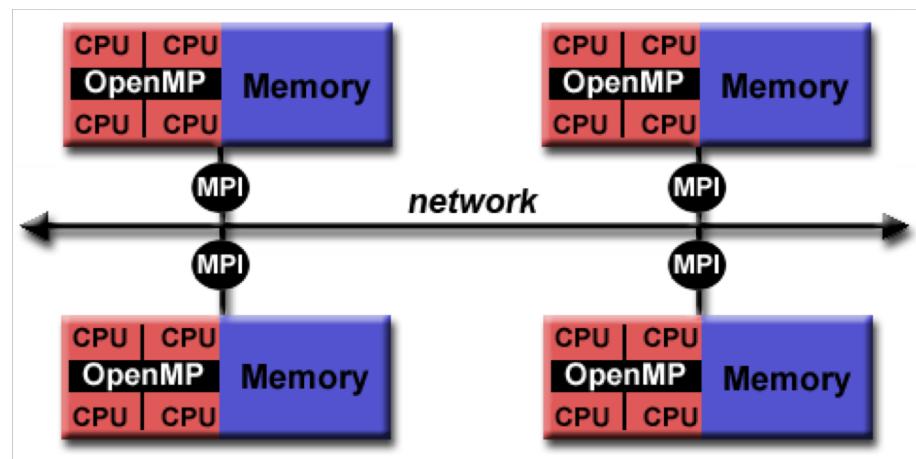
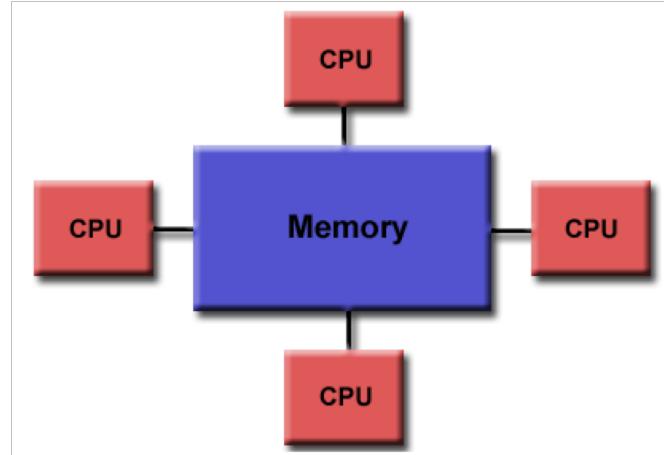


credits: https://computing.llnl.gov/tutorials/parallel_com

Running on a Supercomputer

Levels of parallelism

- Task parallel
 - many independent runs
 - needs orchestration
 - for monte-carlo, parameter sweeps
- Shared memory
 - always within one batch node
 - uses threads
 - often implicit
- Distributed memory
 - can use one or more batch nodes
 - uses separate processes
 - almost always using MPI
 - for PDE problems, time stepping



Acknowledgements

Caspar van Leeuwen

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Carlos Teijeiro Barjas

BSC support team



HANDS ON

Introduction to HPC in Computational
Modelling



Running on a Supercomputer

```

76
77     $_SESSION['_CAPTCHA']['code'];
78
79     return array(
80         'code' => $captcha_code,
81         'image_src' => $image_src
82     );
83
84 }
85
86
87
88 if( !function_exists('hex2rgb') )
89 {
90     function hex2rgb($hex_str, $s)
91     {
92         $hex_str = preg_replace(
93             '/^#([0-9a-f]{2})([0-9a-f]{2})([0-9a-f]{2})$/i',
94             '$1$2$3', $hex_str);
95
96         $hex_array = array();
97
98         if( strlen($hex_str) == 6 )
99         {
100             $color_val = hexdec($hex_str);
101             $hex_array['r'] = $color_val >> 16 & 0xFF;
102             $hex_array['g'] = ($color_val >> 8) & 0xFF;
103             $hex_array['b'] = $color_val & 0xFF;
104
105         } elseif( strlen($hex_str) == 3 )
106         {
107             $hex_array['r'] = hexdec(substr($hex_str, 0, 1).substr($hex_str, 0, 1));
108             $hex_array['g'] = hexdec(substr($hex_str, 1, 1).substr($hex_str, 1, 1));
109             $hex_array['b'] = hexdec(substr($hex_str, 2, 1).substr($hex_str, 2, 1));
110
111         } else {
112             return false;
113         }
114
115     }
116
117     // Draw the image
118     if( isset($_GET['
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- Download the material:

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- unix

- bash scripts and basic Unix commands

- batch

- simple submissions scripts to start using SLURM

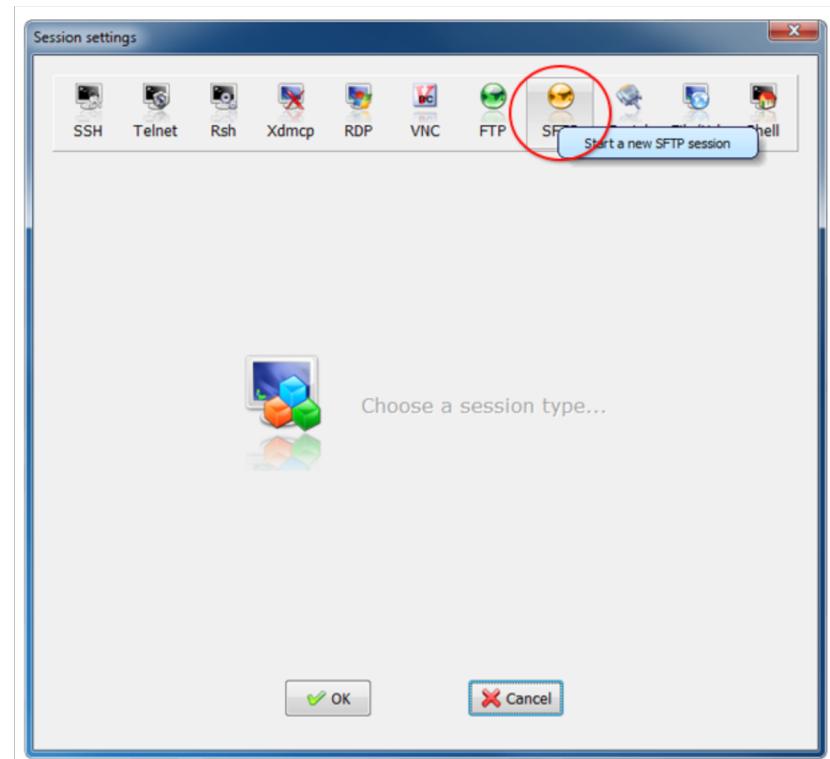
- parallel

- advanced submissions scripts to run parallel applications

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75      $_SESSION['_CAPTCHA']['c
76
77      return array(
78          'code' => $captcha_code,
79          'image_src' => $image_
80      );
81
82
83
84
85    )
86
87
88    if( !function_exists('hex2rgb')
89    function hex2rgb($hex_str, $s
90        $hex_str = preg_replace(
91            $rgb_array = array();
92            if( strlen($hex_str) >
93                $color_val = hexdec($
94                $rgb_array['r'] = 0xFF;
95                $rgb_array['g'] = 0xFF;
96                $rgb_array['b'] = 0xFF;
97            } elseif( strlen($hex_str)
98                $rgb_array['r'] = hexde
99                $rgb_array['g'] = hexde
100               $rgb_array['b'] = hexde
101
102           } else {
103               $return_string = implode(
104                   ) . ')';
105
106       }
107
108       // Draw the image
109       if( insert($_GET['
110
111
```

Running on a Supercomputer

■ MobaXterm



Hands on

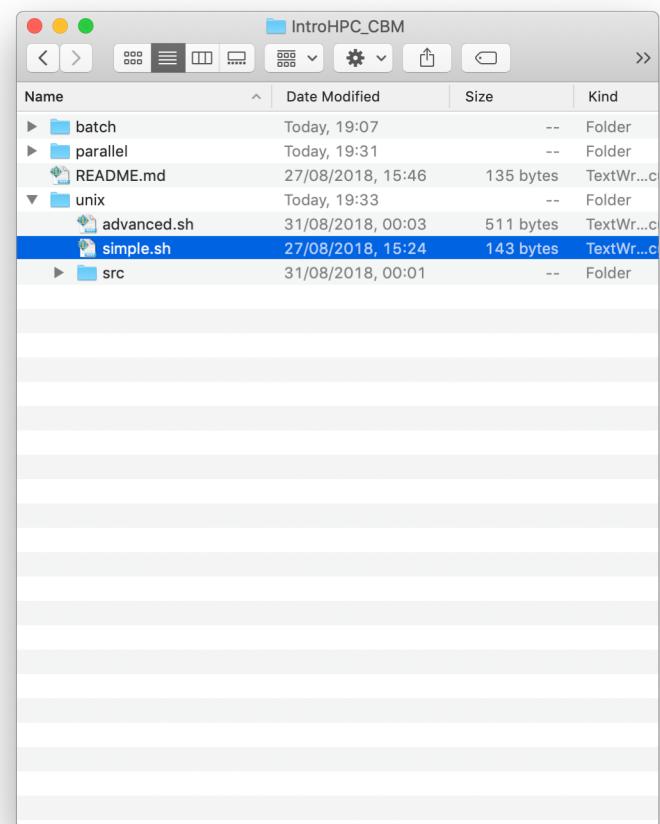
Getting ready

```
~> unzip IntroHPC_CBM-master.zip
```

```
~> ls -l IntroHPC_CBM/
total 8
-rw-r--r-- 1 marcov staff 135B Aug 27 15:46 README.md
drwxr-xr-x 5 marcov staff 160B Feb 12 14:44 batch
drwxr-xr-x 4 marcov staff 128B Feb 12 14:47 parallel
drwxr-xr-x 7 marcov staff 224B Aug 31 00:32 unix
```

```
~> cd IntroHPC_CBM/unix
```

```
~> ls -l
total 48
-rw-r--r-- 1 marcov staff 511B Aug 31 00:03 advanced.sh
-rw-r--r-- 1 marcov staff 143B Aug 27 15:24 simple.sh
drwxr-xr-x 5 marcov staff 160B Aug 31 00:01 src
```



Hands on

unix example

```
~> ls -l simple.sh
-rw-r--r-- 1 marcov staff 143B Aug 27 15:24 simple.sh

~> ./simple.sh
-bash: ./simple.sh: Permission denied

~> chmod +x simple.sh

~> ls -l simple.sh
-rwxr-xr-x 1 marcov staff 143B Aug 27 15:24 simple.sh

~> ./simple.sh

...
```

Hands on

batch example

```
~> cd ~/IntroHPC_CBM/batch  
  
~> ls -l  
total 24  
-rw-r--r-- 1 marcov staff 298B Aug 27 15:24 interactive.txt  
-rw-r--r-- 1 marcov staff 272B Feb 12 13:19 slurm1.sub  
-rw-r--r-- 1 marcov staff 308B Feb 12 13:22 slurm2.sub  
  
~> sbatch slurm2.sub  
  
~> squeue -u $USER  
  
...  
  
~> ls -l  
  
...  
  
~> cat interactive.txt
```

Hands on

parallel example (I)

```
~> cd ~/IntroHPC_CBM/parallel/python  
~> ls -l  
total 16  
-rw-r--r-- 1 marcov staff 115B Feb 12 14:45 linalg.py  
-rw-r--r-- 1 marcov staff 464B Feb 12 14:52 python.sub
```

```
~> sbatch python.sub
```

```
~> squeue -u $USER
```

```
...
```

```
~> ls -l
```

```
...
```

Hands on

parallel example (II)

```
~> cd ~/IntroHPC_CBM/parallel/mpi  
~> ls -l  
...  
~> module load intel impi hdf5  
~> make  
...  
~> sbatch run_wave  
...  
~> tail -f wave.out
```