

Introduction to HPC in Computational Modelling

PATC: HPC-based simulations, Engineering and Environment with applications in Bioengineering

Marco Verdicchio
SURFsara

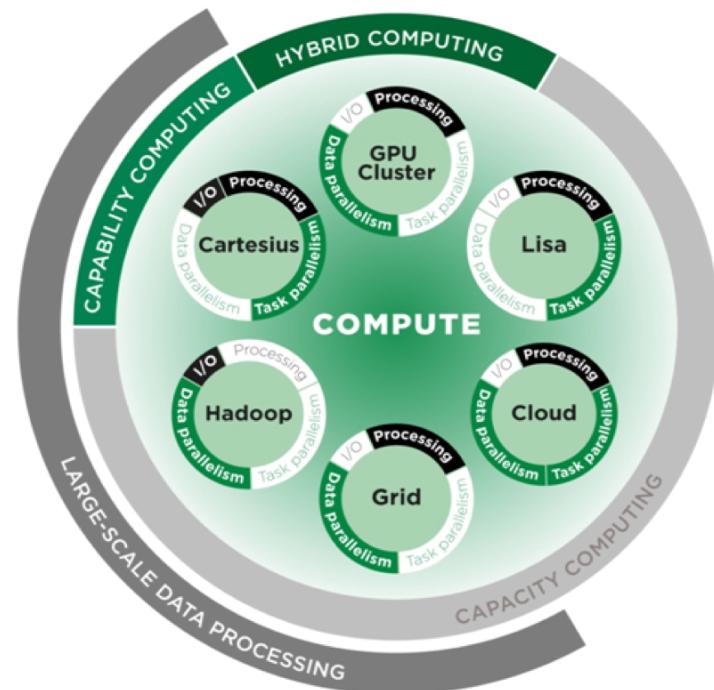


HPC at SURFsara



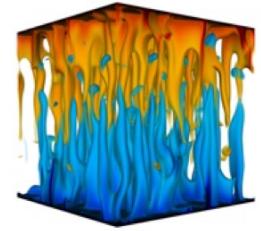
- 📍 HPC Consultant in the Supercomputing Team
- 🌐 Science Park, Amsterdam
- 👤 About 70 op. people
 - 50% Consultants
 - 50% System programmers

HPC at SURFsara



HPC at SURFsara

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



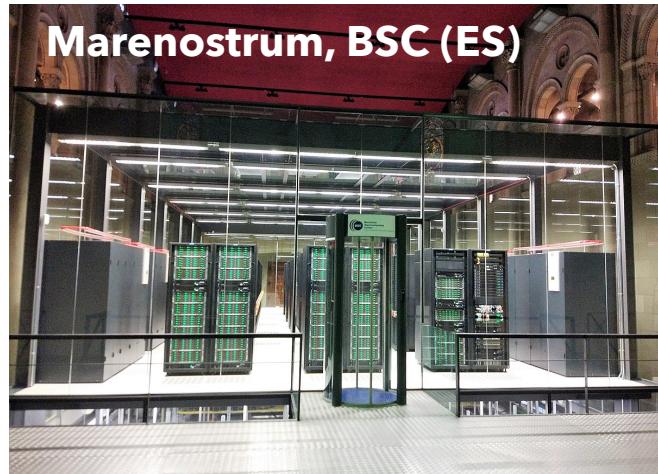
Intel Parallel Computing Center



Introduction to HPC - Outline

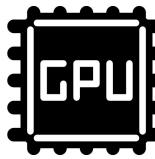
- What is a Supercomputer?
 - Working on a Supercomputer
 - Supercomputer access and usage
- Getting started with HPC
 - Linux basic command
 - Bash scripting
- Running jobs
 - Use the batch system
 - Execute parallel programs

What is a Supercomputer?



User Experience

- Multiuser system
- Unix OS
- Optimized software



Compute power

- Many CPUs system
- Specialized Hardware
- Low-latency/High bandwidth Connections



Storage

- Efficient I/O
- Large Memories

What is a Supercomputer?

TOP 10 Sites for November 2017

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	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
2	Tianhe-2 [MilkyWay-2] - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P , NUDT National Super Computer Center in Guangzhou China	3,120,000	33,862.7	54,902.4	17,808
3	Piz Daint - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 , Cray Inc. Swiss National Supercomputing Centre (CSCS) Switzerland	361,760	19,590.0	25,326.3	2,272
4	Gyoukou - ZettaScaler-2.2 HPC system, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 700Mhz , ExaScaler Japan Agency for Marine-Earth Science and Technology Japan	19,860,000	19,135.8	28,192.0	1,350
5	Titan - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x , Cray Inc. DOE/SC/Oak Ridge National Laboratory United States	560,640	17,590.0	27,112.5	8,209

www.top500.org

What is a Supercomputer?

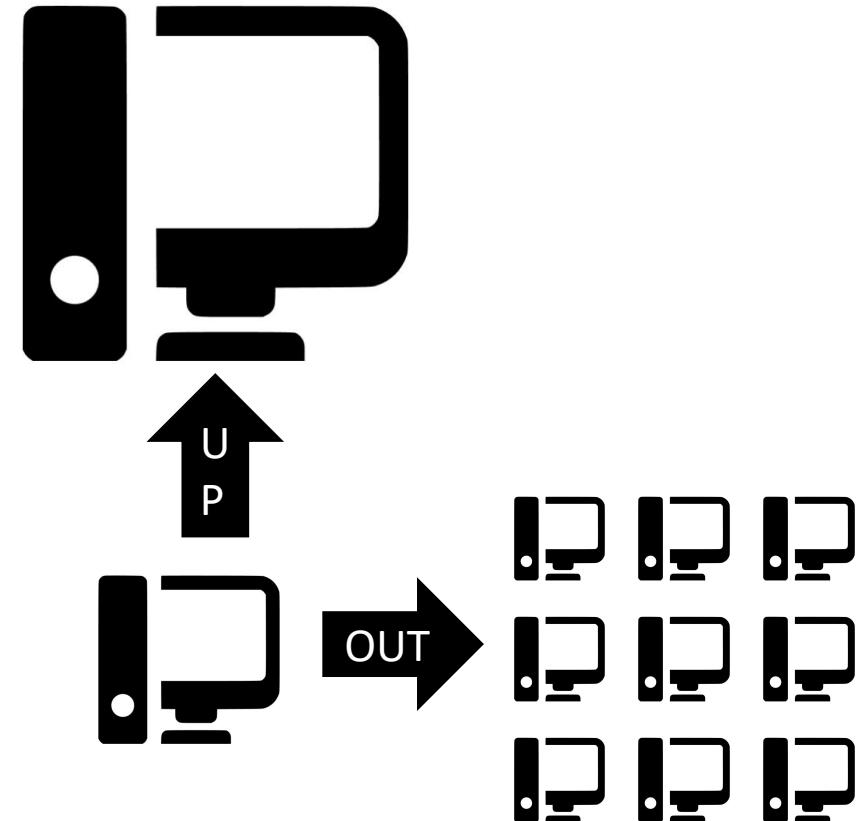
Why, or more, when you need a Supercomputer?

- **Scale up**

- Faster CPUs
- Large memories
- Specialized Hardware/Software

- **Scale out**

- Large parallel applications
- Many small- to medium- size jobs

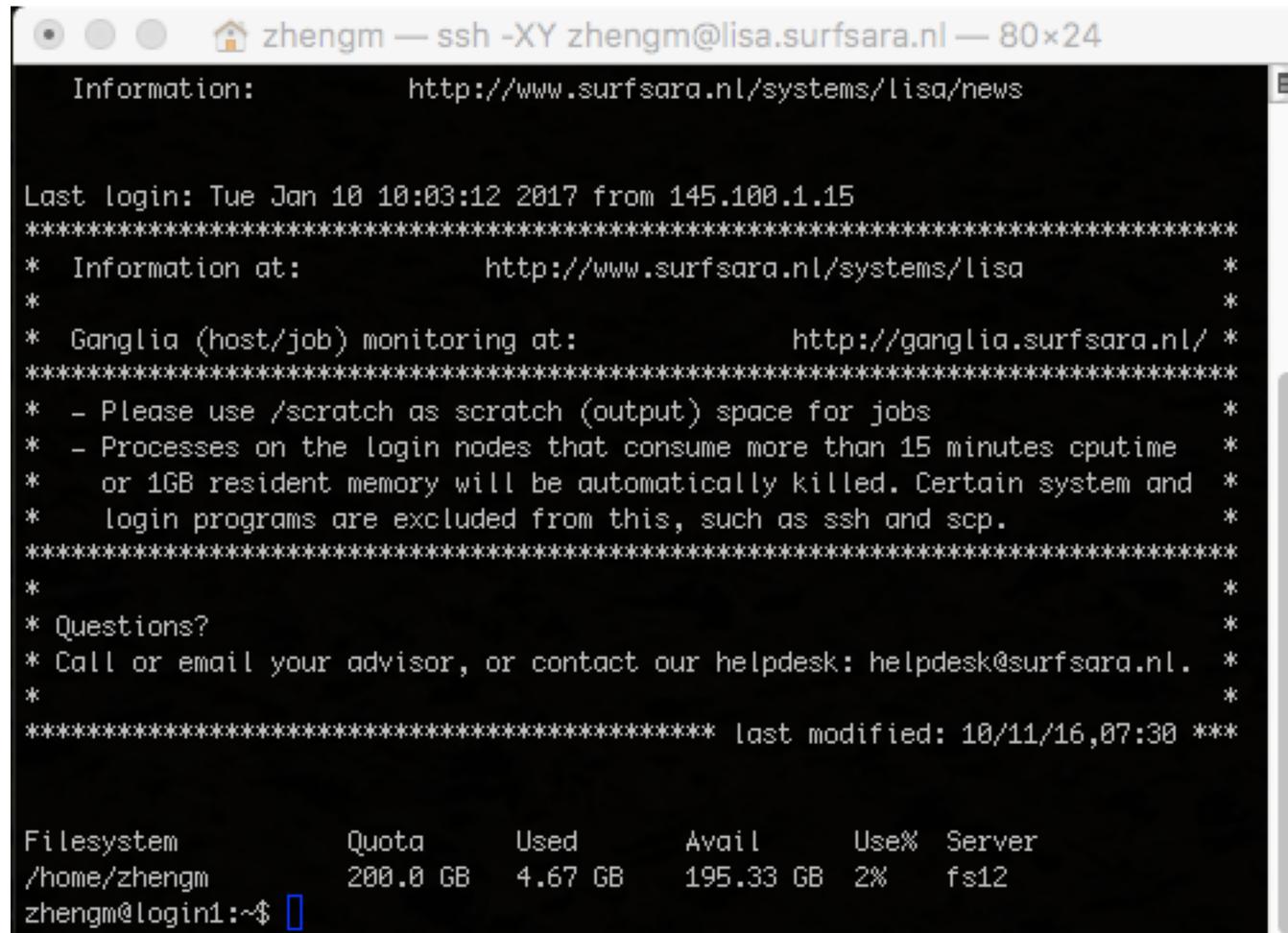


Working with a Supercomputer

Is NOT like this...



Working with a Supercomputer

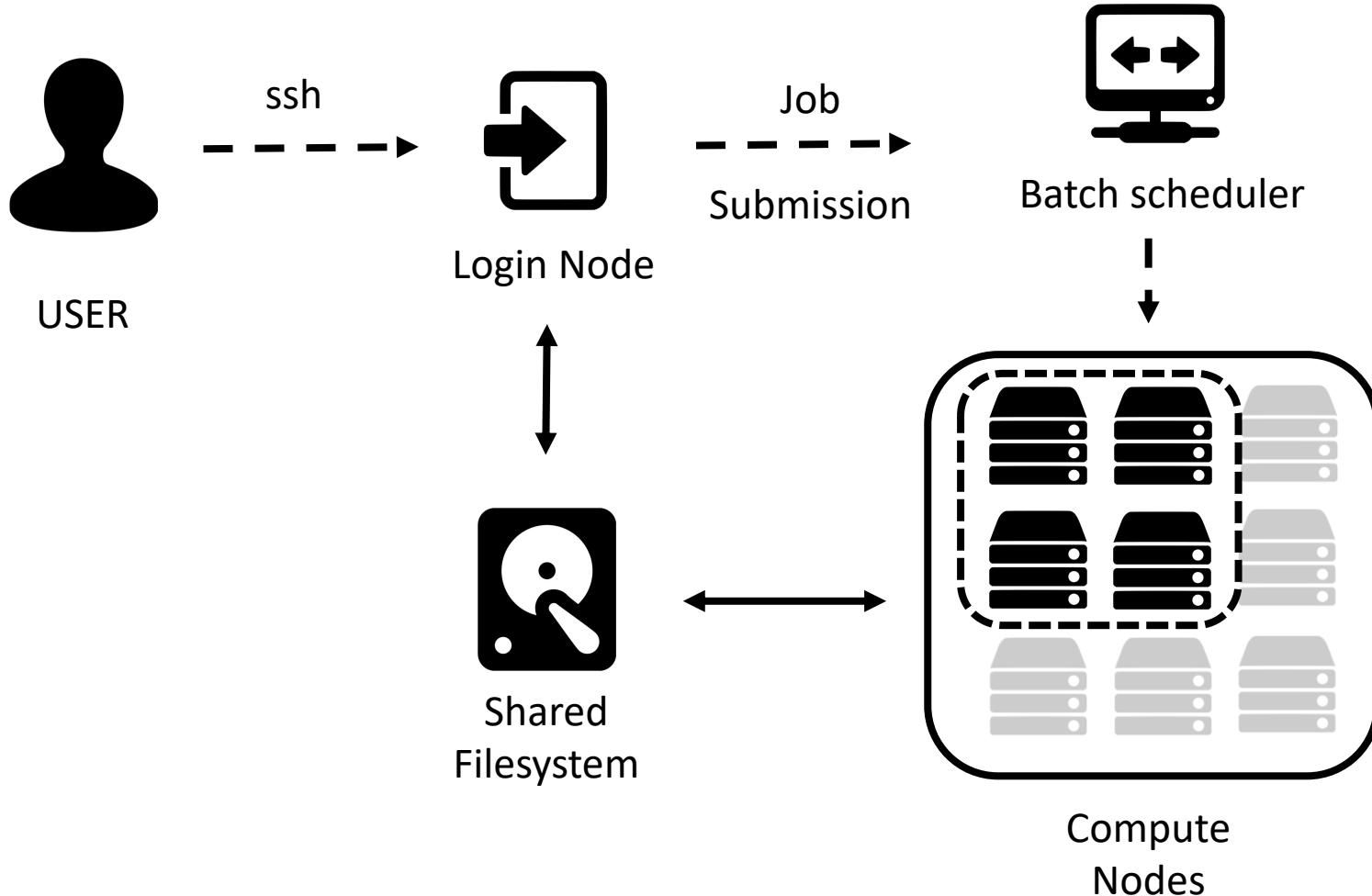


A screenshot of a terminal window titled "zhengm — ssh -XY zhengm@lisa.surfsara.nl — 80x24". The window displays a welcome message from the LISA supercomputer, including links for information, Ganglia monitoring, and scratch space usage guidelines. It also includes sections for questions and last modified information. At the bottom, it shows a table of file system usage statistics.

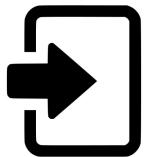
```
Last login: Tue Jan 10 10:03:12 2017 from 145.100.1.15
*****
* Information at:          http://www.surfsara.nl/systems/lisa      *
*                         *
* Ganglia (host/job) monitoring at:      http://ganglia.surfsara.nl/  *
***** 
* - Please use /scratch as scratch (output) space for jobs      *
* - 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:~$
```

Working with a Supercomputer

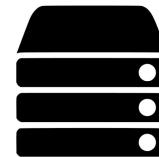


Working with a Supercomputer



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
- Accounting and



File system

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

Working with a Supercomputer

1. Login and transfer files to the remote machine

- ssh, scp/ftp
- Command line, GUI

2. Prepare your job(s)

- Input preparation
- Job submission script
- Software preparation

3. Submit your job and retrieve output

- Submit job to the batch system
- Monitor job
- Retrieve outputs / Remote visualization

Login to an HPC system

Introduction to HPC in Computational Modelling

GETTING STARTED WITH HPC

Login to an HPC system

Getting an account on the system

- EU funded projects (PRACE, CompBioMed, etc.)
- National initiatives (NWO, RES)
- Special agreements with Universities or research centers
- Contact the HPC center
 - helpdesk@surfsara.nl
 - support@bsc.es

Login to an HPC system

Install UNIX tools on your local machine

Windows

Putty

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

Mac OSX

Terminal (pre-installed)

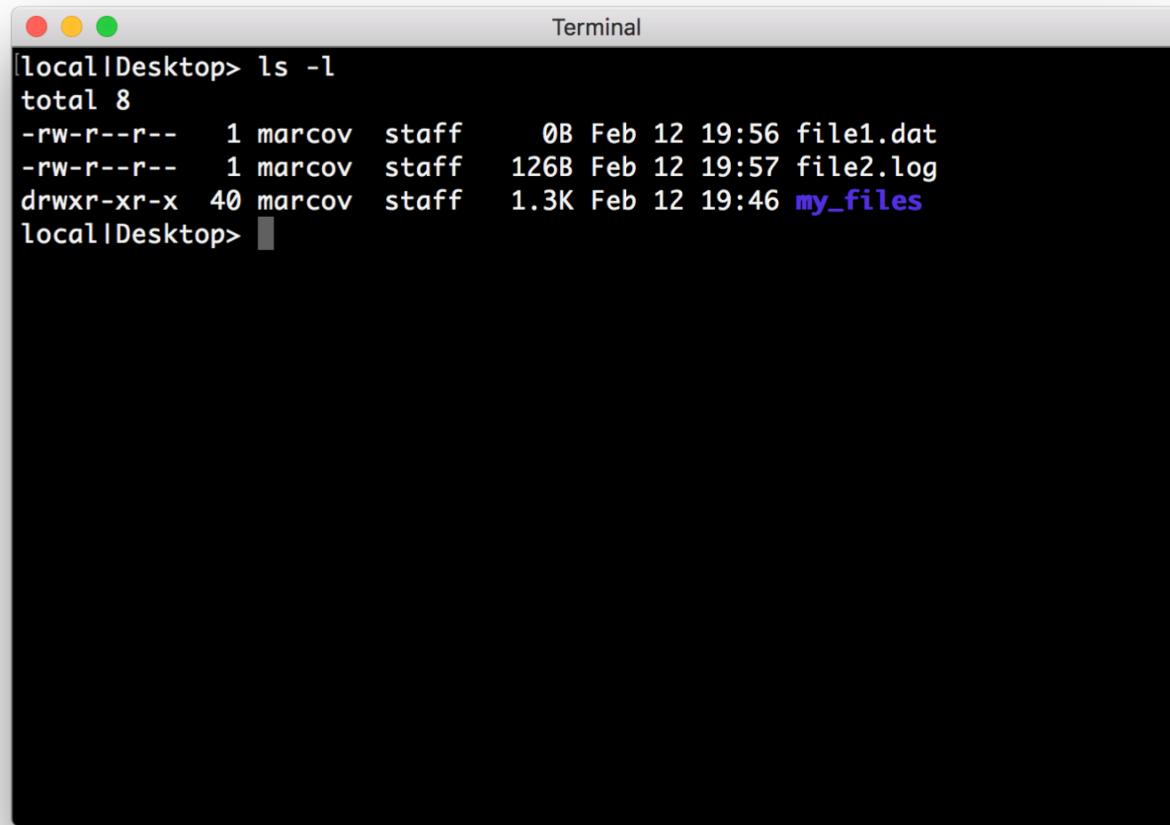
XQuartz (<http://www.xquartz.org>)

Linux

You are already well equipped!

Login to an HPC system

Terminal - Command line



```
[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>
```

Login to an HPC system

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:
```

Login to an HPC system

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

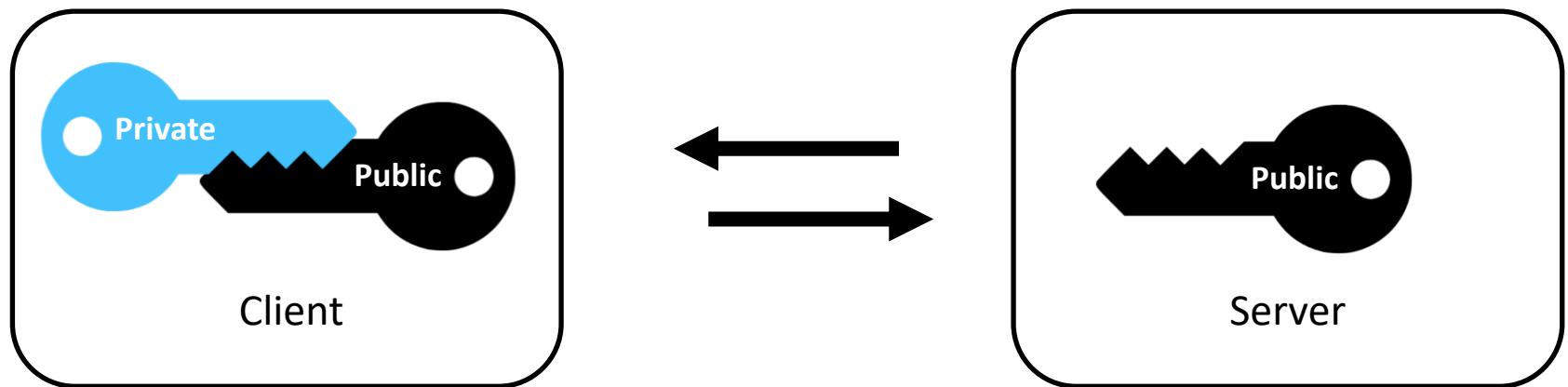
Marenostrum login node



Login to an HPC system

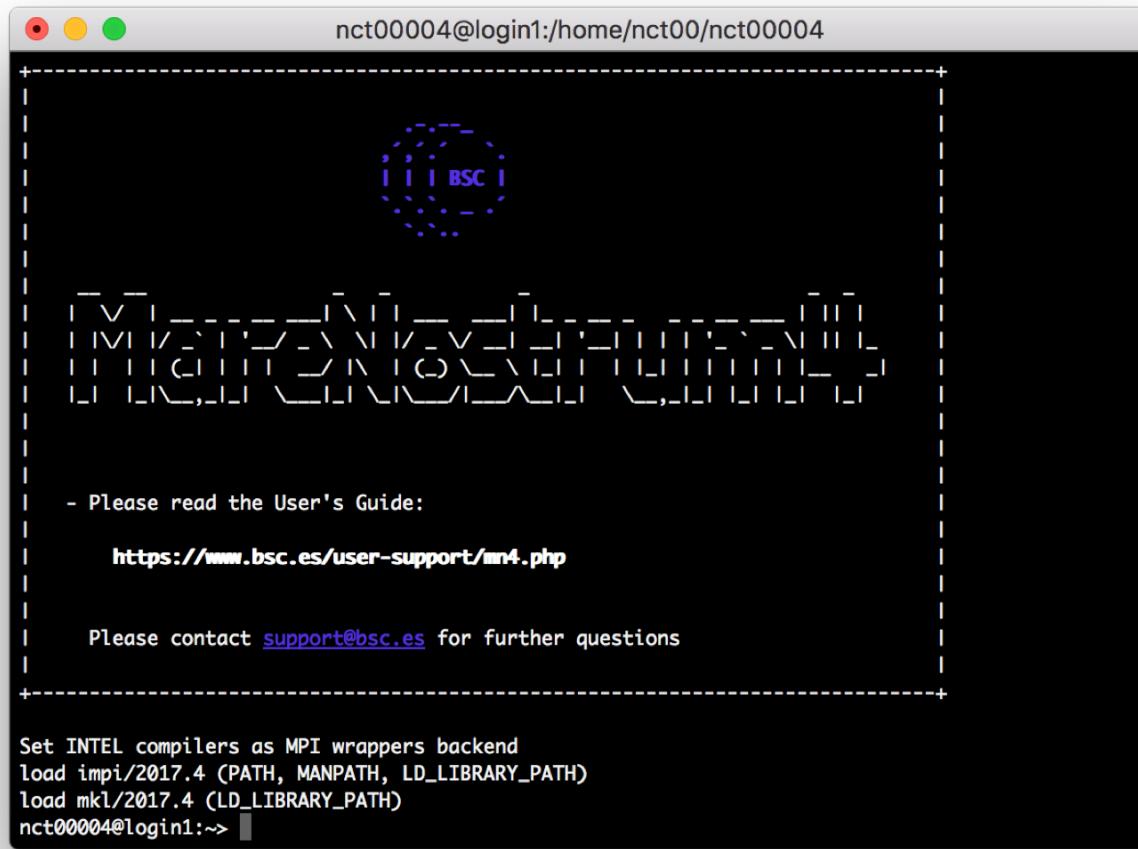
SSH - Authentication and security

- Username/password (Symmetric encryption)
- Public and private keys (Asymmetric encryption)



Login to an HPC system

You are logged in!



Login to an HPC system

MareNostrum4

3456 nodes with a grand total of 165,888 processor cores and 390 Terabytes of main memory.

Compute nodes are equipped with:

- 2 sockets Intel Xeon Platinum 8160 CPU with 24 cores each @ 2.10GHz
- L1d 32K; L1i cache 32K; L2 cache 1024K; L3 cache 33792K
- 96 GB of main memory 1.880 GB/core
 - (216 nodes high memory, 10368 cores with 7.928 GB/core)
- 100 Gbit/s Intel Omni-Path HFI Silicon 100 Series PCI-E adapter
- 10 Gbit Ethernet
- 200 GB local SSD available as temporary storage during jobs

Linux basic commands

Introduction to HPC in Computational Modelling

GETTING STARTED WITH HPC

Linux basic commands

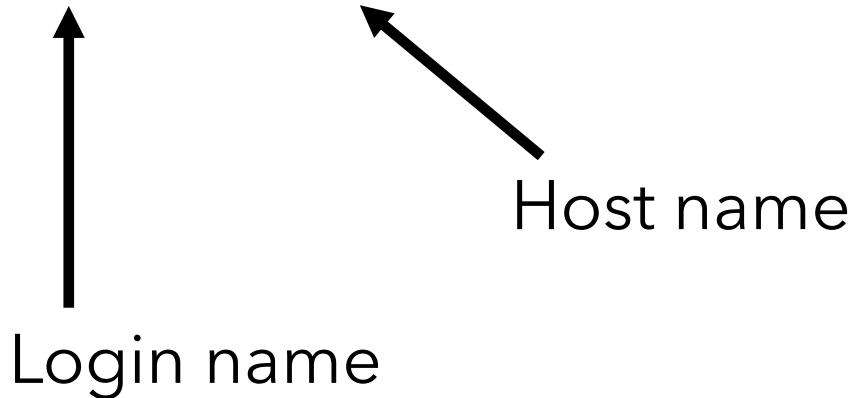
What is UNIX?

- 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

Linux basic commands

- After successful login

```
nct0004@login1:~>
```



Now the system is ready to accept commands



Linux basic commands

- First command

```
nct0004@login1:~> date  
Wen Feb 14 11:00:00 CET 2018  
nct0004@login1:~>
```

- A little bit more

```
nct0004@login1:~> uname -a  
Linux login1 4.4.103-92.56-default #1 SMP Wed Dec 27 16:24:31 UTC  
2017 (2fd2155) x86_64 x86_64 x86_64 GNU/Linux  
nct0004@login1:~>
```

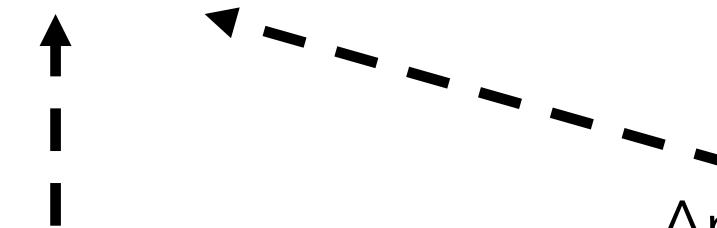
Linux basic commands

- Structure of a unix commands

```
nct00004@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.

- Case-sensitive (everything!)
- Spaces used to separate command, options and arguments

Linux basic commands

- Where to find help?

--help flag

```
nct00004@login1:~> uname --help
```

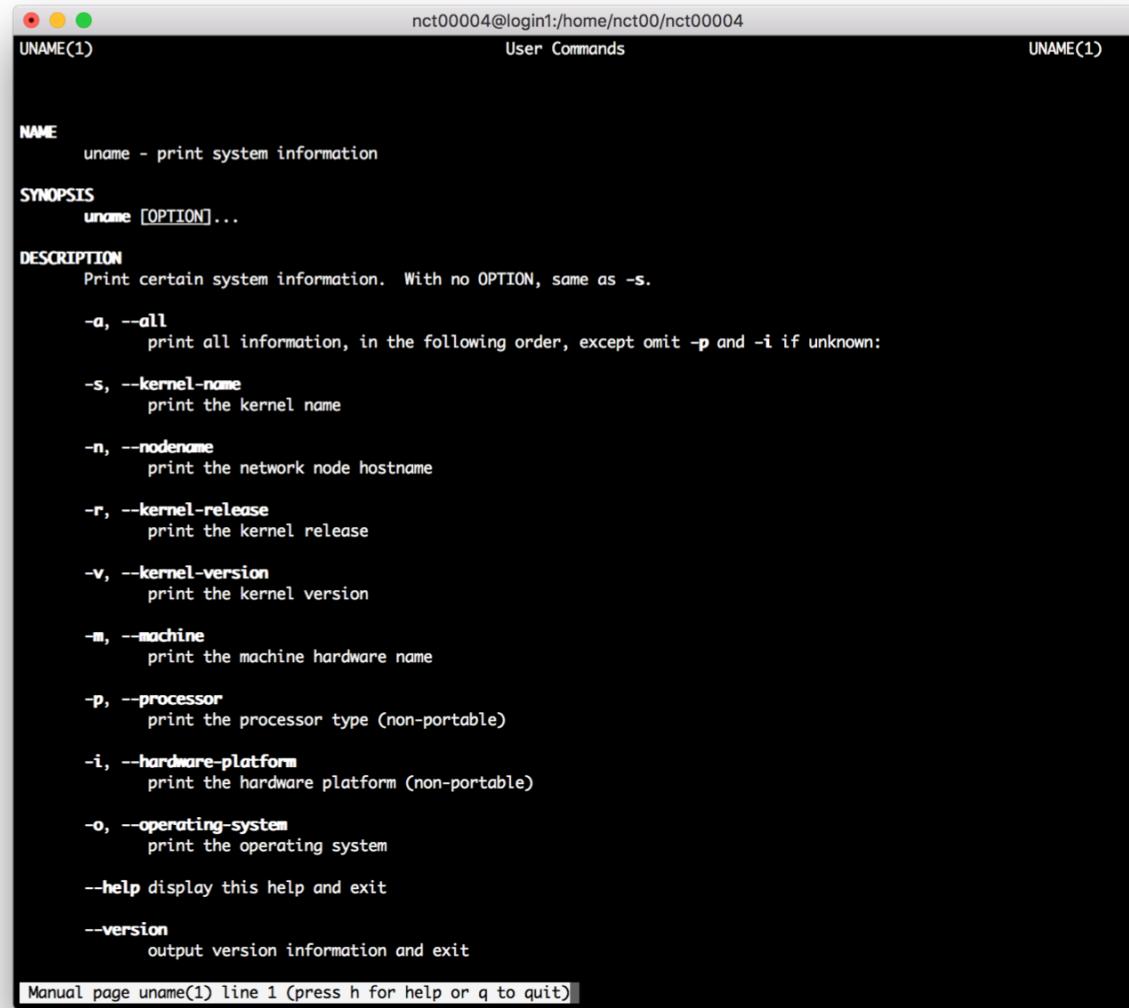
man built-in command

```
nct00004@login1:~> man uname
```

info built-in command

```
nct00004@login1:~> info uname
```

Linux basic commands



```
nct00004@login1:/home/nct00/nct00004
UNAME(1)                               User Commands                               UNAME(1)

NAME
    uname - print system information

SYNOPSIS
    uname [OPTION]...

DESCRIPTION
    Print certain system information. With no OPTION, same as -s.

    -a, --all
        print all information, in the following order, except omit -p and -i if unknown:
        -s, --kernel-name
            print the kernel name
        -n, --nodename
            print the network node hostname
        -r, --kernel-release
            print the kernel release
        -v, --kernel-version
            print the kernel version
        -m, --machine
            print the machine hardware name
        -p, --processor
            print the processor type (non-portable)
        -i, --hardware-platform
            print the hardware platform (non-portable)
        -o, --operating-system
            print the operating system
    --help display this help and exit
    --version
        output version information and exit

Manual page uname(1) line 1 (press h for help or q to quit)
```

Linux basic commands - Looking around

- Where I am?

```
nct0004@login1:~> pwd  
/home/nct00/nct0004
```

- What files are there?

```
nct0004@login1:~> ls  
bin file1.txt file2.log
```

```
nct0004@login1:~> ls -l  
total 0  
drwxr-xr-x 2 nct0004 nct00 4096 May 5 2010 bin  
-rw-r--r-- 1 nct0004 nct00 0 Feb 13 01:17 file1.txt  
-rw-r--r-- 1 nct0004 nct00 1528 Feb 13 01:17 file2.log
```

Linux basic commands - Moving around

- Changing directory

```
nct0004@login1:~> cd dir/subdir  
nct0004@login1:~/dir/subdir>
```

- Going "on level" up

```
nct0004@login1:~/dir/subdir> cd ..  
nct0004@login1:~/dir>
```

- Going back to home folder (~)

```
nct0004@login1:~/dir/subdir> cd  
nct0004@login1:~>
```

Linux basic commands - Moving around

Path to folders and files

- Relative path

```
nct00004@login1:~> ls dir/mydata.out  
dir/mydata.out
```

- Absolute path

```
nct00004@login1:~> ls ~/dir/mydata.out  
/home/nct00/nct0004/dir/mydata.out
```

Linux basic commands - Files management

- Directories

Create directories

```
nct0004@login1:~> mkdir dir
```

Remove directories (only if empty)

```
nct0004@login1:~> rmdir dir
```

Remove directory and its content (be careful with rm)

```
nct0004@login1:~> rm -r dir
```

Linux basic commands - Files management

- Files

Copy files

```
nct00004@login1:~> cp file1.txt file1.copy
```

Copy files to directories

```
nct00004@login1:~> cp file1.* dir/
```

Move files

```
nct00004@login1:~> mv file1.txt dir/file.txt.new
```

Linux basic commands - Files management

- Files (remote)

Copy files from your local machine to a remote host

```
~> scp file*.txt nct00004@mn1.bsc.es:/home/nct00/nct00004/
```

Copy files from remote host to local machine

```
~> scp nct00004@mn1.bsc.es:/home/nct00/nct00004/dir/mydata.out .
```

Copy folder from your local machine to a remote host

```
~> scp -r dir nct00004@mn1.bsc.es:
```

Linux basic commands

File editing/viewing

- touch: Creates a blank file with a specified name.
- less: View contents of specified file, page by page.
- cat: Display contents of a file.
- head/tail: Displays the first/last 10 lines of a file.

System tools

- history: Display a listing of the last commands you've run.
- find: Search files and directories.
- tar: Compress and extract files.
- top: Display processes running on the system.

...

Bash scripting

What if I want to run many bash commands?

...maybe in a workflow?

- **Bash scripts**

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`

Bash scripting

```
nct0004@login1:~> ls -l
total 0
drwxr-xr-x 2 nct0004 nct00 4096 May  5  2010 bin
-rw-r--r-- 1 nct0004 nct00     0 Feb 13 01:17 file1.txt
```

File permission

Every file/directory has 9 permission bits associated (+ initial to diff):

- 3 user based permission groups: owner(2-4), group(5-7), all users(8-10)
- x3 permission types: read(r), write(w), execute(x)

Permission can be changed with the command **chmod**

```
nct0004@login1:~> chmod u+x simple.sh
```

Training material

The material for this course is available at :

[**http://bit.ly/PATC_HPC**](http://bit.ly/PATC_HPC)

Material for the course Introduction to HPC

The screenshot shows a GitHub repository page for 'Introduction to HPC'. At the top, there are statistics: 6 commits, 1 branch, 0 releases, and 1 contributor. Below this, a dropdown menu shows 'Branch: master' and a 'New pull request' button. To the right are 'Find file' and 'Clone or download' buttons. The main area lists files: 'simple_script.sh' (by mvsurfsara, fixed, 31 minutes ago), 'unix-intro' (by unix-intro, fixed, 31 minutes ago), 'README.md' (updated 20 hours ago), and another 'README.md' (empty). Below the repository details, a section titled 'Introduction to HPC' contains the following text: 'PATC: HPC-based simulations, Engineering and Environment with applications in Bioengineering', 'SURFsara & CompBioMed', 'Examples and exercises for the course Introduction to HPC', and 'Barcelona, 14 Feb 2018'.

6 commits 1 branch 0 releases 1 contributor

Branch: master New pull request Find file Clone or download

mvsurfsara Fixed simple_script.sh Latest commit 762b752 31 minutes ago

unix-intro Fixed simple_script.sh 31 minutes ago

README.md Update README.md 20 hours ago

README.md

Introduction to HPC

PATC: HPC-based simulations, Engineering and Environment with applications in Bioengineering

SURFsara & CompBioMed

Examples and exercises for the course Introduction to HPC

Barcelona, 14 Feb 2018

Training material

The material for this course is available at:

[**http://bit.ly/PATC_HPC**](http://bit.ly/PATC_HPC)

Transfer the zip file to MarenostrumIV

```
~> scp IntroHPC_PATC_CBM-master.zip nct00004@mn1.bsc.es:
```

(Windows users can use MobaXterm or Winscp)

Extract the zip in your home:

```
nct00004@login1:~> unzip IntroHPC_PATC_CBM-master.zip
```

Bash scripting

Simple bash script

unix-intro/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"
```

Bash scripting

Standard input, output and error

Every program (bc, shell, ...) has three predefined input/output associated:

- Standard input (stdin): normally your keyboard
- Standard output (stdout): normally your screen
- Standard error (stderr): normally your screen

These can be redirected to a file or to another command.

```
nct00004@login1:~> echo "3/0" | bc > calc.log
```

Bash scripting - Ex

Simple bash script

unix-intro/simple.sh

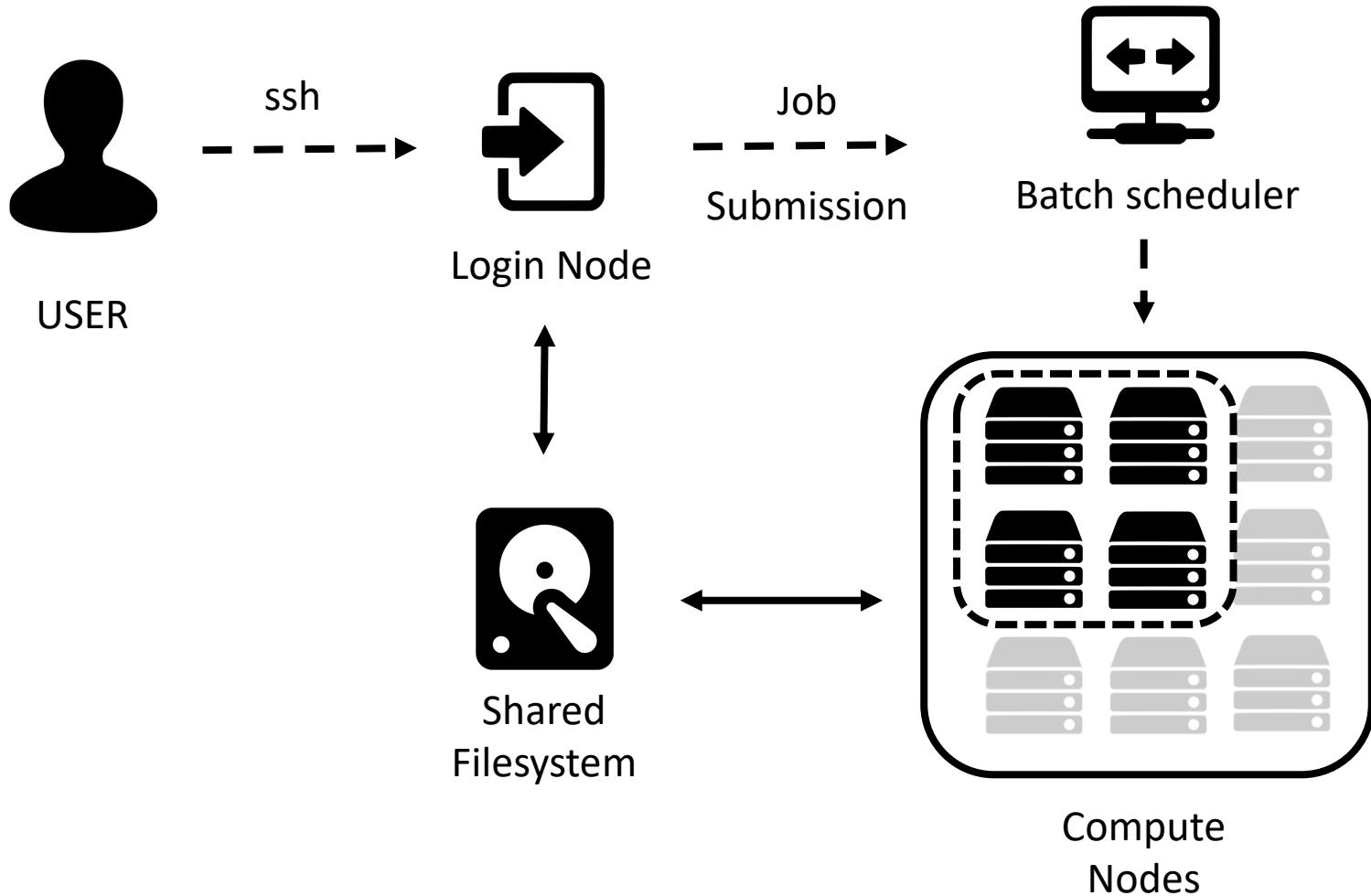
More complicated bash script

unix-intro/advanced.sh

Introduction to HPC

RUNNING JOBS

Batch system



Batch system

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.



Batch system

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.

Batch system

- **Queues**

There are several queues present in the machines and different users may access different queues.

```
nct00004@login1:~>bsc_queues
```

QUEUE	NAME	MAX TIME	MAX PROC
	debug	02:00:00	768
	interactive	02:00:00	4
	training	2-00:00:00	768

Batch system

- **Submitting jobs with SLURM**

The method for submitting jobs is to use the SLURM **sbatch** directives directly.

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

```
nct00004@login1:~> sbatch <job script>
```

- shows all the submitted jobs ant their status:

```
nct00004@login1:~> squeue
```

- remove the job from the queue system:

```
nct00004@login1:~> scancel <jobid>
```

- run a command on the cluster

```
nct00004@login1:~> srun <command>
```

Batch system

- **SLURM Job directives**

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

#SBATCH --nodes=<num>	request for <num> compute node
#SBATCH --ntasks=<num>	the number of processes to start
#SBATCH --time=DD-HH:MM:SS	total wall clock time of the job
#SBATCH --qos=<queue>	requesting a specific queue
#SBATCH --task=<queue>	requesting a specific queue
#SBATCH --output=<file>	name of the file where std out is printed
#SBATCH --tasks-per-node=<num>	
#SBATCH --cpus-per-task=<num>	

Batch system - Ex1

SLURM sequential

batch-sys/slurm1.sub

SLURM multinode

batch-sys/slurm2.sub

Software stack

Some software packages require certain settings in your user environment, like paths and environment variables.

Environment Modules

- Provide lots of useful software packages
- In many different versions
- Maintained by experts
- Optimized for the architecture
- Programming and scripting languages: Python, R, Matlab
- Compilers for C, C++, Fortran
- Specialized libraries (MKL, OpenMPI)
- Scientific codes

Software stack

Useful module commands

module avail	list modules
module avail python	list all installed versions of python
module load python	load the default python version
module load python/2.7.13	load a specific version of python
module unload python	unload python
module list	list currently loaded modules

MarenostrumIV uses **Lmod**, a Lua-based module system (TACC)

Software stack

Let's try it...

- List the default loaded modules

```
nct0004@login1:~> module list
```

```
Currently Loaded Modules:
```

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

- Which python I am using?

```
nct0004@login1:~> which python
```

```
/usr/bin/python
```

```
nct0004@login1:~> python --version
```

```
Python 2.7.13
```

Software stack

- Check which python is installed

```
nct0004@login1:~> module av python  
----- /apps/modules/modulefiles/tools -----  
ANACONDA/5.0.1_python2    python/2.7.13      python/3.6.3_ML  
python/2.7.13_ML           python/3.6.1 (D)
```

Where:

D: Default Module

Use "module spider" to find all possible modules.

Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".

Software stack

- List the default loaded modules

```
nct0004@login1:~> module load python
load python/3.6.1 (PATH, MANPATH, LD_LIBRARY_PATH, C_INCLUDE_PATH,
CPLUS_INCLUDE_PATH, PYTHONHOME)
```

- Check is working

```
nct0004@login1:~> which python
/apps/PYTHON/3.6.1/INTEL/bin/python
nct0004@login1:~> python --version
Python 3.6.1
```

Have a look at all the software installed on MarenostrumIV with:

module avail

Software stack

nct00004@login1:/home/nct00/nct00004									
----- /apps/modules/modulefiles/applications -----									
3DNA/2.3	bedops/2.4.26	fhi-aims/171221	mc/4.8.19	picard/2.10.2	siesta/4.1-b3	(D)			
ARNOLD/mtoa_2.0.1	bedtools/2.25.0	flashpca/2.0	mcl/14-137	plumed/2.1.5	singularity/2.3.1				
CDO/1.7.2	blast/2.6.0	gate/7.0	meld/3.16.4	plumed/2.1.5	singularity/2.4.2	(D)			
CDO/1.8.2_ts	blat/36	gate/8.0	(D) meme/4.12.0	plumed/2.3.2.libmatheval	spark4hpc/1.0.0				
CDO/1.8.2	(D) bowtie2/2.3.2	geant4/9.6.p01	mmseqs/2017.07.11	plumed/2.3.2	salite/2017.07.10				
CMOR/3.2.3	bwa/0.5.9	geant4/10.03.p01	(D) modeller/9.19	plumed/2.3.3.libmatheval	(D) swig/3.0.12				
GAMESS/20151214	bwa/0.7.15	(D) gem/13-20121106	namd/2.9.plumed	pplacer/1.1.alpha19	turbonvc/2.1.2				
GMSH/3.0.4	cfitsio/3.410	geos/3.6.1	namd/2.12-tcl	prodigal/2.6.3	underworld/master-aug2017				
R/2.15.0	circos/0.69-5	gmt/4.5.16	namd/2.12	(D) qe-gipaw/6.2	underworld/1.7.0				
R/3.4.0	(D) cp2k/4.1_plumed	gmt/5.4.2	(D) nasm/2.13.01	quantumespresso/6.1-environ	underworld/2.2.2b-py				
TADbit/0.2	cp2k/4.1_plumed-2.3.3	grace/5.1.25	ncl/6.4.0	quantumespresso/6.1-hdf5-environ	underworld/2.2.2b	(D)			
abinit/8.4.1	cp2k/4.1	(D) grib/1.14.0	nco/4.2.3_netcdf-4.2	quantumespresso/6.1-hdf5	vasp/5.2.12				
abinit/8.6.1	(D) cp2k/5.1	gromacs/5.1.4-plumed-libmatheval	nco/4.2.3	quantumespresso/6.1	vasp/5.3.5				
amber/12	cpmd/4.1	gromacs/5.1.4-plumed	nco/4.6.7	(D) quantumespresso/6.2	vasp/5.4.1				
amber/14_plumed	crystal/14	(D) gromacs/5.1.4	ncview/2.1.8	raremetal/4.14.1	vasp/5.4.4	(D)			
amber/14	crystal/17	gromacs/2016.4-double	nektar++/4.4.0	raxml/8.2.11	vcftools/0.1.13				
amber/16	(D) cube/4.3.5	gromacs/2016.4-plumed	nwchem/6.6	repeatmasker/2.6.0	vmd/1.9.3				
ambertools/12	dsrc/2.0.2	gromacs/2016.4	(D) octave/4.2.1	root/5.34.36	vtk/8.0.0				
ambertools/17	(D) esmf/7.0.0	hmmer/3.1b2	octopus/7.1	root/6.10.08	(D) vtk/8.0.1	(D)			
ant/1.10.1	esmf/7.1.0	(D) igv/2.3.94	openbabel/2.3.1	rosetta/2017.08.59291	weeder/2.0				
bash/4.4.12	fastqc/0.11.5	imp/2.8.0	openfoam/4.0	(D) rpmcmc/0.2	wgridb/0.2.0.6c				
bazaar/2.7.0	fhi-aims/131208	julia/0.6.0	openfoamx/3.8	samtools/1.5-dnanexus	wrf/3.9				
bbtools/36.37	fhi-aims/161219	lammps/31Mar2017	paraview/5.4.0	samtools/1.5	(D)				
bcftools/1.6	fhi-aims/170710	(D) mafft/7.3.10	siesta/4.1-b2						
----- /apps/modules/modulefiles/compilers -----									
gcc/4.8.5	gcc/5.4.0	gcc/7.2.0 (D)	intel/2017.1	intel/2017.6	intel/2018.1	java/tu80	java/8u144		
gcc/4.9.4	gcc/7.1.0	go/1.9.2	intel/2017.4 (L,D)	intel/2018.0	java/latest	java/8u131 (D)	java/8u151		
----- /apps/modules/modulefiles/environment -----									
bsc/1.0 (L)	fabric/1.5.0	impi/2017.1	impi/2017.6	impi/2018.1	mvapich2/2.3b	openmpi/1.10.7	opt/flags		
fabric/1.4.2 (D)	fabric/1.5.3	impi/2017.4 (L,D)	impi/2018.0	lmod/icase	openmpi/1.10.4 (D)	openmpi/3.0.0	transfer/1.0		
----- /apps/modules/modulefiles/libraries -----									
HYPRE/2.11.2	boost/1.66.0.py3	hdf5/1.8.19 (D)	libjpeg-turbo/1.5.2	mkl/2018.0	netcdf/4.5.0-ts	petsc/3.7.6-complex	trilinos/12.10.1		
arpack/96	elpa/2017.05.0003	hdf5/1.10.1-ts	libpng/1.6.29	mkl/2018.1	netcdf/4.5.0	petsc/3.7.6-real (D)	udunits/2.2.25		
atlas/3.10.3	fftw/2.1.5	hdf5/1.10.1	libxc/4.0.3	mpc/3.2.0	openssl/1.1.0f	rdkit/2016.03.4	uuid/1.6.2		
boost/1.64.0_py2conda	fftw/3.3.6 (D)	healpix/3.31	libyaml/0.1.7	netcdf/3.6.3	petsc/3.1-p8-complex	rocksdb/5.5.1	vcflib/0817		
boost/1.64.0_py2	gda/2.2.1 (D)	htslib/1.5	metis/5.1.0	netcdf/4.2	petsc/3.1-p8-real	slepc/3.7.4-complex	zlib/1.2.11		
boost/1.64.0_py3 (D)	gda/2.2.3	jasper/1.900.1	mkl/2017.1	netcdf/4.4.0	petsc/3.4.3-complex	slepc/3.7.4-real (D)			
boost/1.64.0	gsl/2.4	libevent/2.1.8	mkl/2017.4 (L,D)	netcdf/4.4.1.1 (D)	petsc/3.4.3-real	szip/2.1.1			
----- /apps/modules/modulefiles/tools -----									
ALYA-MPIO-TOOLS/default	COMPSS/Trunk	COMPSS/2.1_rc1709	DTT/18.0.1 (D)	PARAVER/latest	gpi2/1.3.0	parallel_studio/2017.4	scons/2.5.1		
ANACONDA/5.0.1_python2	COMPSS/TrunkCarlos	COMPSS/2.1	DIMENAS/latest	greasy/latest	perl/5.26_threads	tmux/2.6			
ANACONDA/5.0.1 (D)	COMPSS/TrunkJavi	COMPSS/2.2_rc1801	DIMENAS/5.3.3	cmake/3.8.2	hwloc/2.0.0	perl/5.26	(D)		
BASICANALYSIS/latest	COMPSS/TrunkJEA	COMPSS/2.2	DIMENAS/5.3.4	(D) cmake/3.9.6	llvm/5.0.0	python/2.7.13_ML			
BASICANALYSIS/0.3.1 (D)	COMPSS/TrunkJupyter	DATACLAY/Trunk	EXTRAE/latest	dlb/git	ompss/git	python/2.7.13			
CLUSTERING_SUITE/latest	COMPSS/TrunkRamon	DTT/7.0.5	EXTRAE/3.5.1	dlb/1.3	ompss/stable	python/3.6.1 (L,D)			
CLUSTERING_SUITE/2.6.6 (D)	COMPSS/2.0	DTT/7.0.6	EXTRAE/3.5.2 (D)	dlb/2.0	ompss/17.12 (D)	python/3.6.3_ML			
COMPSS/release	(D)	COMPSS/2.1_rc1707	DTT/7.1	MERGESVCALLERS/10-2016	gatk/3.8-0	papi/5.5.1	ruby/2.4.2		

File systems

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!

MarenostrumIV

- Root filesystem: Is the filesystem where the operating system resides.
- GPFS filesystems: GPFS is a distributed networked filesystem which can be accessed from all the nodes and Data Transfer Machine.
- Local hard drive: Every node has an internal hard drive (\$TMPDIR).

File systems

The IBM General Parallel File System (GPFS) is a high-performance shared-disk file system providing fast, reliable data access from all nodes of the cluster to a global filesystem.

- **/apps:** Over this filesystem will reside the applications and libraries that have already been installed on the machine.
- **/gpfs/home:** This filesystem has the home directories of all the users, and when you log in you start in your home directory by default. It is highly discouraged to run jobs from this filesystem.
- **/gpfs/projects:** In addition to the home directory, there is a directory in /gpfs/projects for each group of users. This space is intended to store data that needs to be shared between the users of the same group or project.
- **/gpfs/scratch:** Each user will have a directory over /gpfs/scratch. Its intended use is to store temporary files of your jobs during their execution.

Batch system - Ex2

Running python on MarenostrumIV

run-jobs/python_seq.sub

run-jobs/pairwise.py

- Using a system installed software (modules)
- Make appropriate usage of disk space (scratch)

Parallel jobs

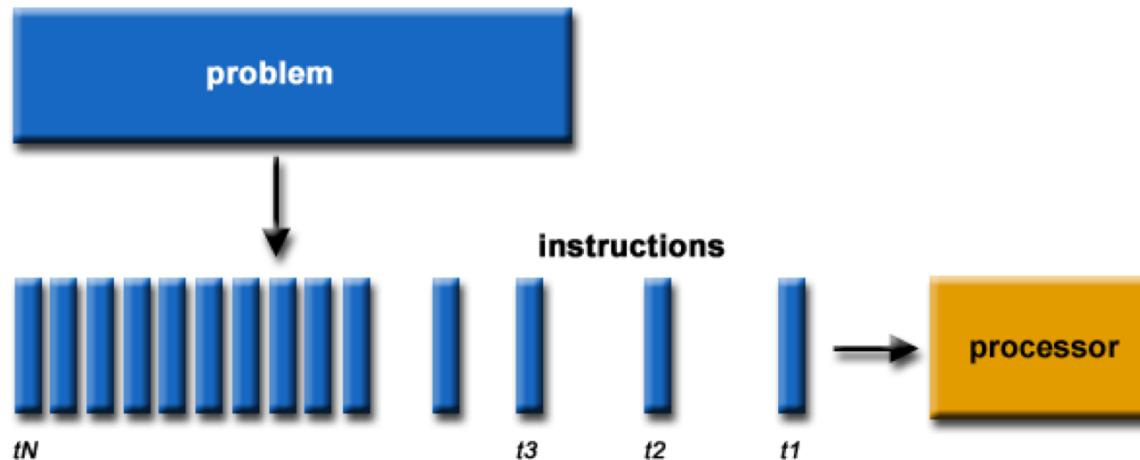
Introduction to HPC in Computational Modelling

RUNNING JOBS

Parallel jobs

Serial computing

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

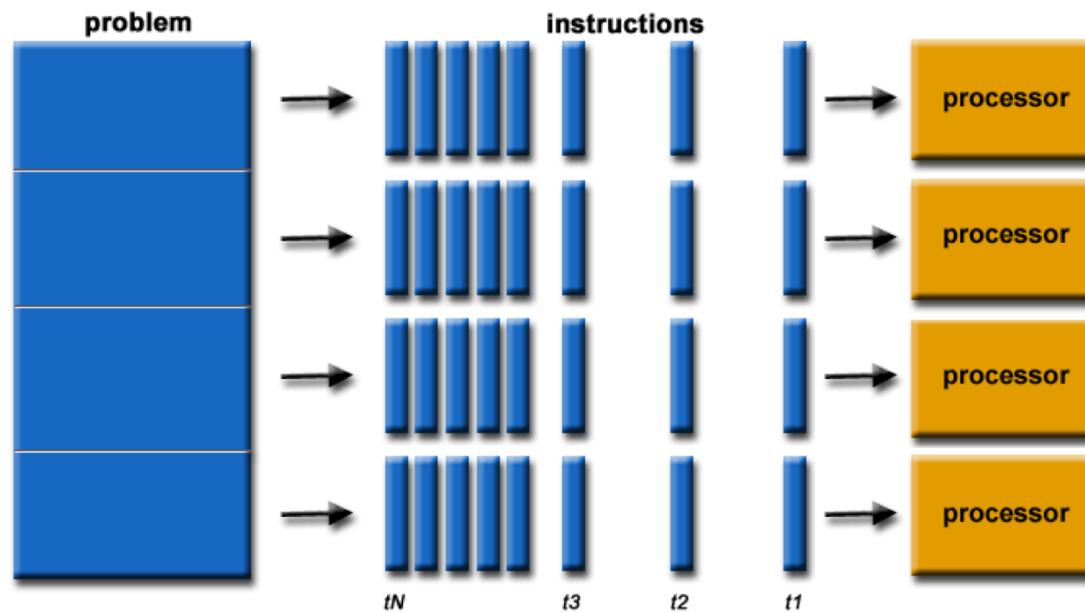


credits: https://computing.llnl.gov/tutorials/parallel_com

Parallel jobs

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

Parallel jobs - Ex

Running python in parallel on MarenostrumIV

batch-sys/python_par.sub

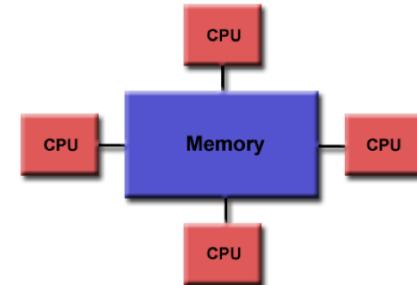
batch-sys/pairwise.py

Exploit background processes in UNIX

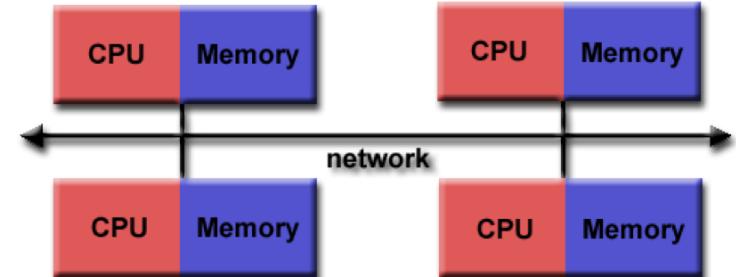
- **&** : at the end of a command put the process in bg and let you continue to work
- **wait** : wait that all the background processes have ended before continue

Parallel jobs

- 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



Shared memory topology

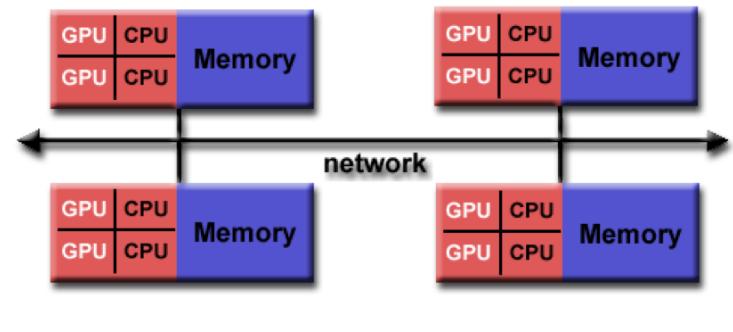


Distributed memory topology

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

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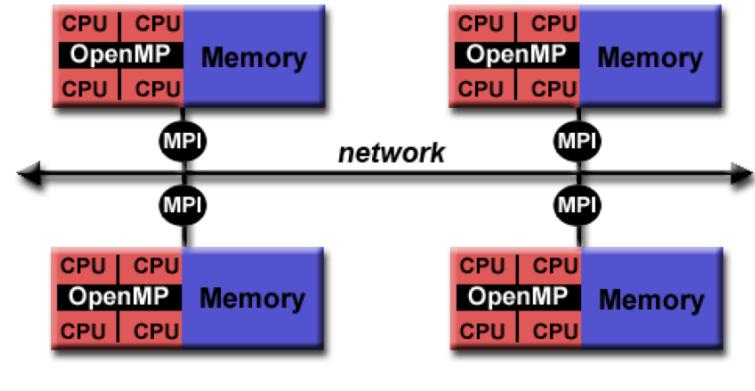


Hybrid topology

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

Parallel jobs

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Hybrid topology

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

Parallel jobs - Ex

Running an MPI application

mpi-ex/run_wave

mpi-ex/Makefile

Uses MPI library to distribute work across multiple node.

The code needs to be compiled and right libraries loaded.

It generates a gif that we need to copy back at the end.

Thank you to my colleagues ...

Caspar van Leeuwen

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