



# High Performance Computing for the VPH

A practical introduction to HPC usage

Marco Verdicchio SURFsara

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 675451.



### **HPC at SURFsara**





HPC Consultant in the Supercomputing Team



Science Park, Amsterdam



- 50% Consultants
- 50% System programmers

### **HPC at SURFsara**

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



Bull sara









# **HPC in CompBioMed**

Cardiovascular

Musculoskeletal

medicine

Neuro

based

medicine

medicine

Molecularly





CompBioMed is a user-driven Centre of
Excellence in Computational Biomedicine, to
nurture and promote the uptake and exploitation
of high performance computing within the
biomedical modelling community. Our user
communities come from academia, industry and
clinical practice.

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# **HPC in CompBioMed**

### **Activities**

- 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).





### **HPC in CompBioMed**



# **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



CompBioMed



Course organized by CompBioMed

# 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 June 2018

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

Rank		1-100	101-200	201-300	301-400	401-500			
	System					Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	Summit - IBM Power Syste Volta GV100, Dual-rail Mel DOE/SC/Oak Ridge Nation United States	em AC922 lanox EDF al Labora	, IBM POWE R Infiniband tory	R9 22C 3.07 , IBM	'GHz, NVIDIA	2,282,54	4 122,300.0	187,659.3	8,806
2	Sunway TaihuLight - Sunw Sunway , NRCPC National Supercomputing China	vay MPP, S Center in	Sunway SW2 Wuxi	6010 260C	1.45GHz,	10,649,60	0 93,014.6	125,435.9	15,371
3	Sierra - IBM Power Syster Volta GV100, Dual-rail Mel DOE/NNSA/LLNL United States	n S922LC lanox EDF	, IBM POWE R Infiniband	R9 22C 3.1G . IBM	Hz, NVIDIA	1,572,48	0 71,610.0	119,193.6	
4	Tianhe-2A - TH-IVB-FEP ( Express-2, Matrix-2000, N National Super Computer China	Cluster, In IUDT Center in	tel Xeon E5- Guangzhou	2692v2 12C	2.2GHz, TH	4,981,76	0 61,444.5	100,678.7	18,482
5	Al Bridging Cloud Infrastr Gold 6148 20C 2.4GHz, NV National Institute of Advan Japan	DIA Tesla	BCI) - PRIM V100 SXM2, strial Science	ERGY CX255 Infiniband and Techn	60 M4, Xeon EDR , <b>Fujitsu</b> ology (AIST)	391,68	0 19,880.0	32,576.6	1,649

VPH2018 - High Performance Computing for the VPH - 4<sup>th</sup> September 2018, Zaragoza, Spain.

# 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



### Is NOT like this...





🖲 🔵 🌒 🏠 zhengi	m — ssh -XY zhengr	m@lisa.surfsara.r	nl — 80×24	
Information:	http://www.surfsa	ra.nl/systems/lis	a/news	8
Last login: Tue Jan 10 ********	) 10:03:12 2017 from *******************	145.100.1.15 ************	*****	
<pre>* Information at: *</pre>	http://www.s	urfsara.nl/system	s/lisa * *	
* Ganglia (host/job) ********	monitoring at: ******************	http://ga *******	nglia.surfsara.nl/ * ********	
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* Questions? * Call or email your a *	dvisor, or contact o	ur helpdesk: help	* desk@surfsara.nl. * *	L
*****	*****	*** last modified	: 10/11/16,07:30 ***	II.
Filesystem Q /home/zhengm 2 zhengm@login1:~\$	)uota Used 100.0 GB 4.67 GB	Avail Use% 195.33 GB 2%	Server fs12	





### 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

### 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

Introduction to HPC in Computational Modelling

# **GETTING STARTED WITH HPC**

### Install UNIX tools on your local machine

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

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

<u>Linux</u> You are already well equipped!

#### **Terminal - Command line**



### 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:

### SSH, or Secure SHell

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



• After successful login





### 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

### You are logged in!



Structure of a unix commands



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

behavior.

• 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

10/40/2/45	nctoboo4@login.noinenctoonctoboo4	INANE (1)	
UNAME(1)	User Commands	UNAME(1)	
NWE	information		
unune - prene system	In ormation		
uname [OPTION]			
DESCRIPTION			
Print certain system	information. With no OPTION, same as -s.		
-a,all			
print all inf	ormation, in the following order, except omit $-p$ and $-i$ if un	sknown:	
-s,kernel-name			
print the ker	nel name		
-n,nodename print the net	work node hostname		
print the ker	nel release		
-v,kernel-version			
print the ker	nel version		
-m,mochine			
print the mac	hine hardware name		
-p,processor print the pro- print the pro- print the pro- print the pro- pro- pro- pro- pro- pro- pro- pro-	cessor type (non-portable)		
i bashara alati			
print the har	dware platform (non-portable)		
-o,operating-syst			
print the ope	rating system		
help display this	help and exit		
version			
output versio	n information and exit		
Manual page uname(1) line	1 (press h for help or g to guit)		

# Linux basic commands - Looking around

• Where I am?

nct00004@login1:~> pwd
/home/nct00/nct00004

• Which files are there?

nct00004@login1:~> ls
bin file1.txt file2.log

```
nct00004@login1:~> ls -l
total 0
drwxr-xr-x 2 nct00004 nct00 4096 May 5 2010 bin
-rw-r--r-- 1 nct00004 nct00 0 Feb 13 01:17 file1.txt
-rw-r--r-- 1 nct00004 nct00 1528 Feb 13 01:17 file2.log
```

• Moving around

nct00004@login1:~> cd ~/subdir

nct00004@login1:~> cd ..

nct00004@login1:~> cd

• Directories

nct00004@login1:~> mkdir dir

nct00004@login1:~> rmdir dir

nct00004@login1:~> rm -r dir

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/nct00004/dir/mydata.out

• Files

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

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

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

• Remote files

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

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

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

The material for this course is available at: <a href="http://bit.ly/HPC\_CBM">http://bit.ly/HPC\_CBM</a>

Transfer the zip file to MarenostrumIV

~> scp IntroHPC\_CBM-master.zip nct00004@mn1.bsc.es:

(Windows users can use MobaXterm or Winscp)

Extract the zip in your home:

nct00004@login1:~> unzip IntroHPC\_CBM-master.zip

#### 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.

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

nct00004@login1:~> ls -l
total 0
drwxr-xr-x 2 nct00004 nct00 4096 May 5 2010 bin
-rw-r--r-- 1 nct00004 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: **u**ser(2-4), **g**roup(5-7), all **o**ther(8-10)
- x3 permission types: read(**r**), write(**w**), execute(**x**)

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

nct00004@login1:~> chmod u+x simple.sh

### Simple bash script

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"

### 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

### Advanced bash script

unix/advanced.sh

#!/bin/bash
# <- this is a comment and everything that follow is ignored
args=\$# # Number of args passed.
if [ \$args = 0 ]
then
 echo "This script needs a number as argument input."
 echo "Ex: ./advanced.sh 10"
 exit
fi</pre>

unix/advanced.sh (cont'd)

```
num=$1 # First argument passed.
echo "The input number is:" $1
echo
cd src
gcc -o ../fact.exe fact.c 1> compile.log 2> compile.err
# Redirect stdout and stderr to files
cd ..
./fact.exe $num | tee fact.log # Pipe output into command
echo
echo "Done"
```

# Introduction to HPC **RUNNING JOBS**

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.



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.

#### • <u>Multiusers, queue system.</u>

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.

### 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>

### **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.

- #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>
- #SBATCH --output=<file>
- #SBATCH --tasks-per-node=<num>
- #SBATCH --cpus-per-task=<num>
- **#SBATCH** -- reservation=VPHSUMMER18

- requesting a specific queue
- name of the file where std out is printed

### slurm.schedmd.com/sbatch.html

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

# 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

### Software stack

### Useful module commands

module availlist modulesmodule avail pythonlist all installed versions of pythonmodule load pythonload the default python versionmodule load python/2.7.13load a specific version of pythonmodule unload pythonunload pythonmodule listlist currently loaded modules

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

### Software stack

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VPH2018 - High Performance Computing for the VPH - 4<sup>th</sup> September 2018, Zaragoza, Spain.

# 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

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

# **Batch jobs**

### batch/slurm1.sub

```
#!/bin/bash
#SBATCH --job-name="test_serial"
#SBATCH --ntasks=1
#SBATCH --time=00:02:00
#SBATCH --workdir=.
#SBATCH --output=serial_%j.out
#SBATCH --error=serial_%j.err
```

echo "Who am I?" whoami echo "Where ?" srun hostname

sleep 600 echo "Ciao"

### batch/slurm2.sub

#!/bin/bash
#SBATCH --job-name="test\_multinode"
#SBATCH --nodes=2
#SBATCH --tasks-per-node=3
#SBATCH --time=00:02:00
#SBATCH --workdir=.
#SBATCH --workdir=.
#SBATCH --output=multinode\_%j.out
#SBATCH --error=multinode\_%j.err

echo "Who am I?" whoami echo "Where ?" srun hostname

sleep 600 echo "Ciao"

### Submitting jobs with SLURM

- submits a "job script" to the queue system:

nct00004@login1:~> sbatch slurm2.sub

- check the status of the submitted jobs:

nct00004	4@login1:~>	> squeue					
JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
2262040	main	test_m	nct00001	PD	0:00	2	(None)

### Introduction to HPC in Computational Modelling

# **RUNNING JOBS**

### 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



```
parallel/python_par.sub
```

wait

```
# Loading python module
module load python/2.7.13
...
for i in 10
    do
        python pairwise.py 2000 &
        done
```

Running python in parallel

Load the appropriate module

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

- <u>Task parallel</u>
  - many independent runs
  - needs orchestration
  - E.g.: monte-carlo, parameter sweeps
- <u>Shared memory</u>
  - 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
  - E.g.: PDE problems, time stepping



Shared memory topology



Distributed memory topology

- <u>Task parallel</u>
  - many independent runs
  - needs orchestration
  - E.g.: monte-carlo, parameter sweeps
- <u>Shared memory</u>
  - 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
  - E.g.: PDE problems, time stepping



Hybrid topology

- <u>Task parallel</u>
  - many independent runs
  - needs orchestration
  - E.g.: monte-carlo, parameter sweeps
- <u>Shared memory</u>
  - 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
  - E.g.: PDE problems, time stepping



Hybrid topology



### **Running an MPI application**

Requires compilers, MPI, HDF5, perl.

nct00004@login1:~> module load hdf5
nct00004@login1:~> module load mpi
nct00004@login1:~> module load perl

The code needs to be compiled and right libraries loaded.

nct00004@login1:~> cd mpi; make

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

~> scp nct00004@mn1.bsc.es:IntroHPC\_CBM-master/mpi/\*.gif .

# **MPI jobs**

### **Running an MPI application**

```
mpi/run_wave (I)
```

```
SCRATCH=/gpfs/scratch/nct00/$USER/$SLURM_JOBID
mkdir -p $SCRATCH || exit 1
cp wave $SCRATCH
...
cd $SCRATCH
```

# **MPI jobs**

### **Running an MPI application**

```
mpi/run_wave (II)
```





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