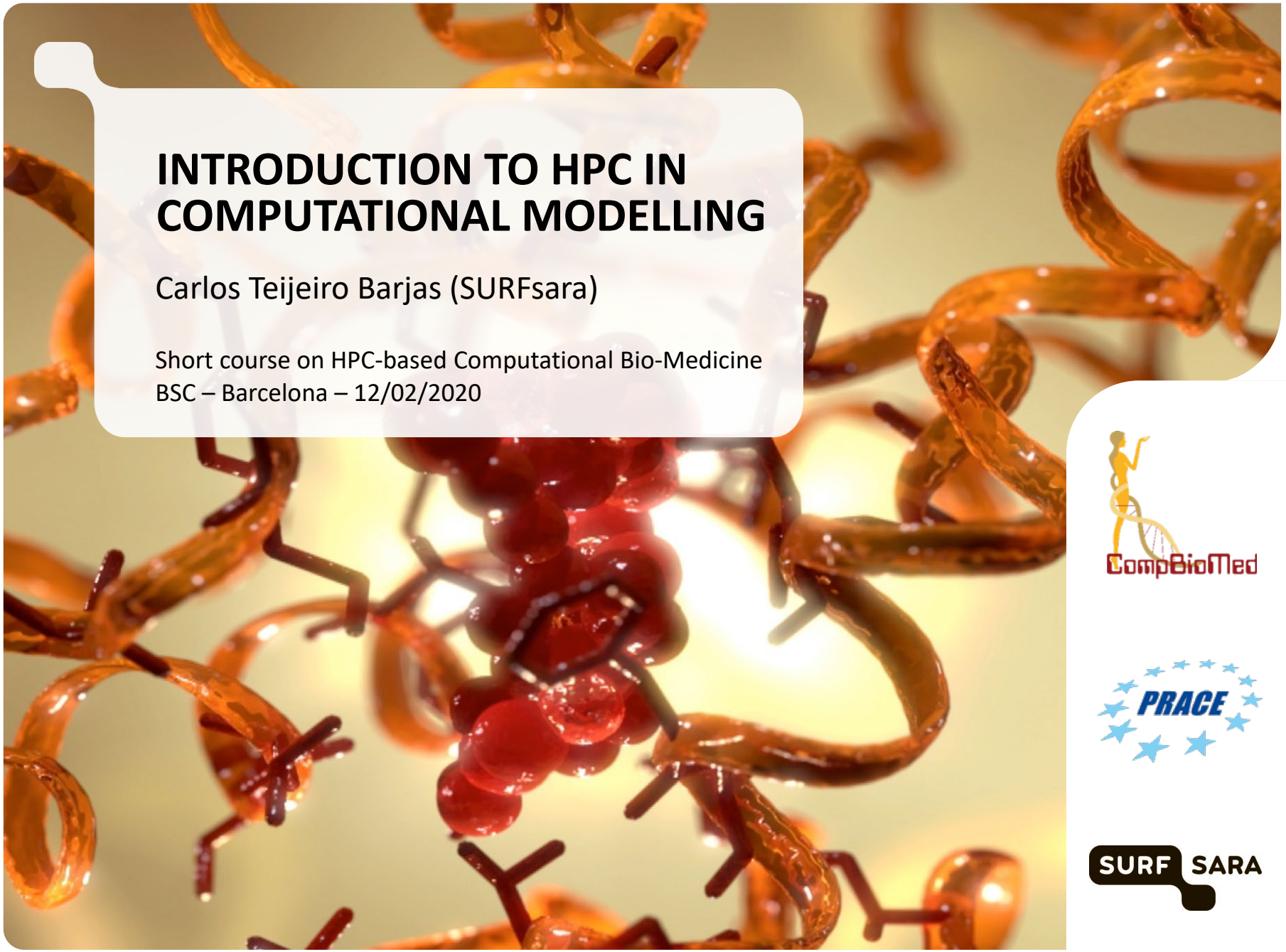

INTRODUCTION TO HPC IN COMPUTATIONAL MODELLING

Carlos Teijeiro Barjas (SURFsara)

Short course on HPC-based Computational Bio-Medicine
BSC – Barcelona – 12/02/2020

CompBioMed

PRACE

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High Performance Computing at SURFsara

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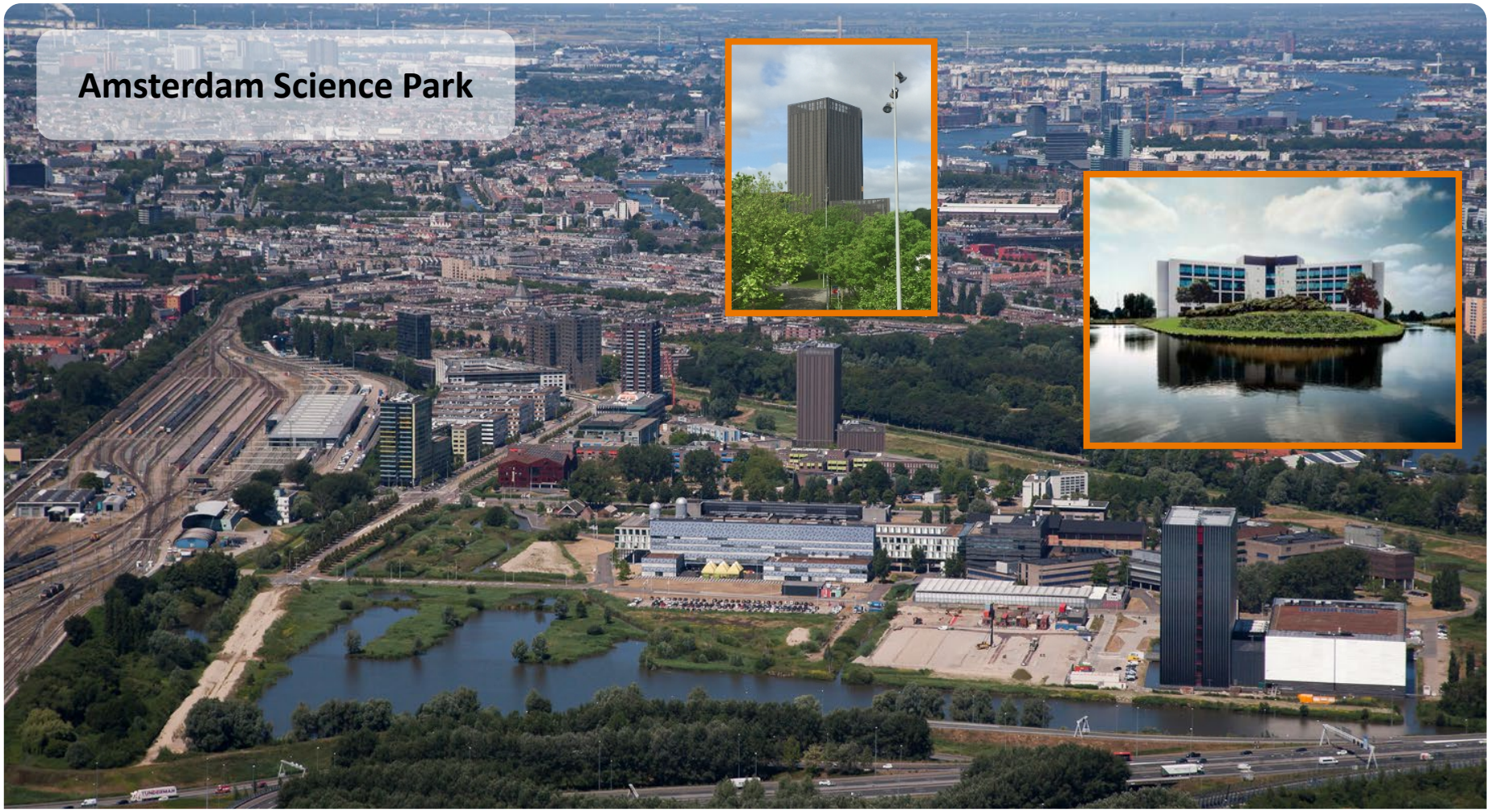
High Performance Computing at SURFsara

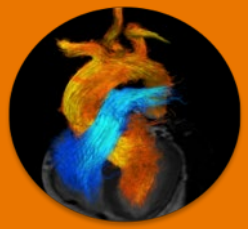


High Performance Computing at SURFsara

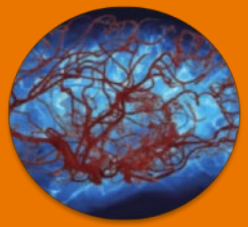
High Performance Computing at SURFsara

- Maintain Cartesius and Lisa
- User support
- Training
- Development and Innovation
- Involvement in EU projects
- After July 2020: officially SURF (!!!)

High Performance Computing in CompBioMed



Cardiovascular medicine



Neuro Musculoskeletal medicine

Molecularly based medicine

CompBioMed

A Centre of Excellence in Computational Biomedicine

- 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).

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SURFsara and HPC in Europe

- HPC resources access, and benchmarking
- Best practices in HPC and trainings

www.prace-ri.eu

- EU Exascale machine based on EU chip (2023)
- Codesign HW/SW

www.european-processor-initiative.eu

- Simplify access to IT services
- Improving service quality

www.eosc-hub.eu

SURFsara and HPC in Europe

- **Convergence of AI and HPC**

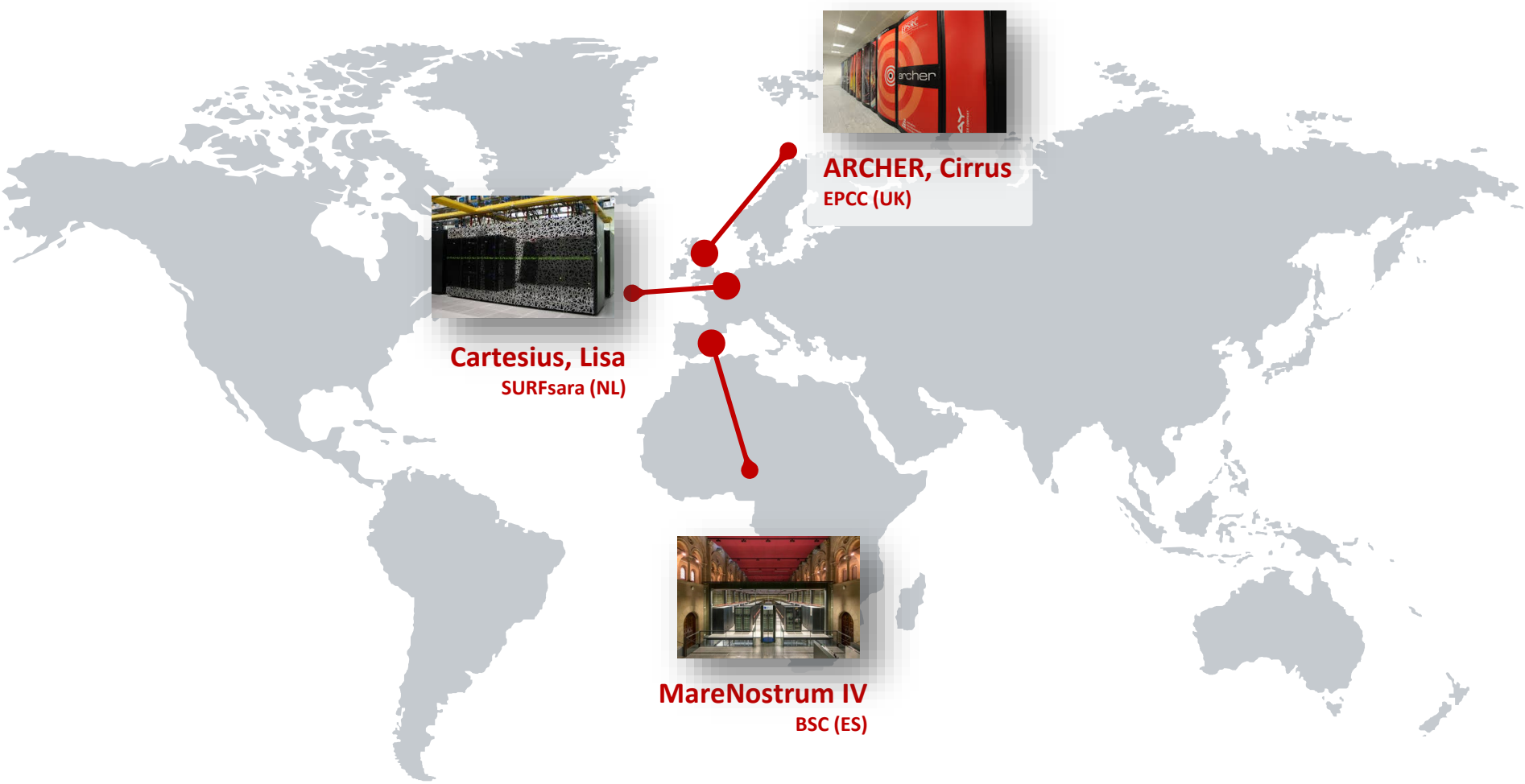
Intel Parallel Compute Centre

www.examode.eu

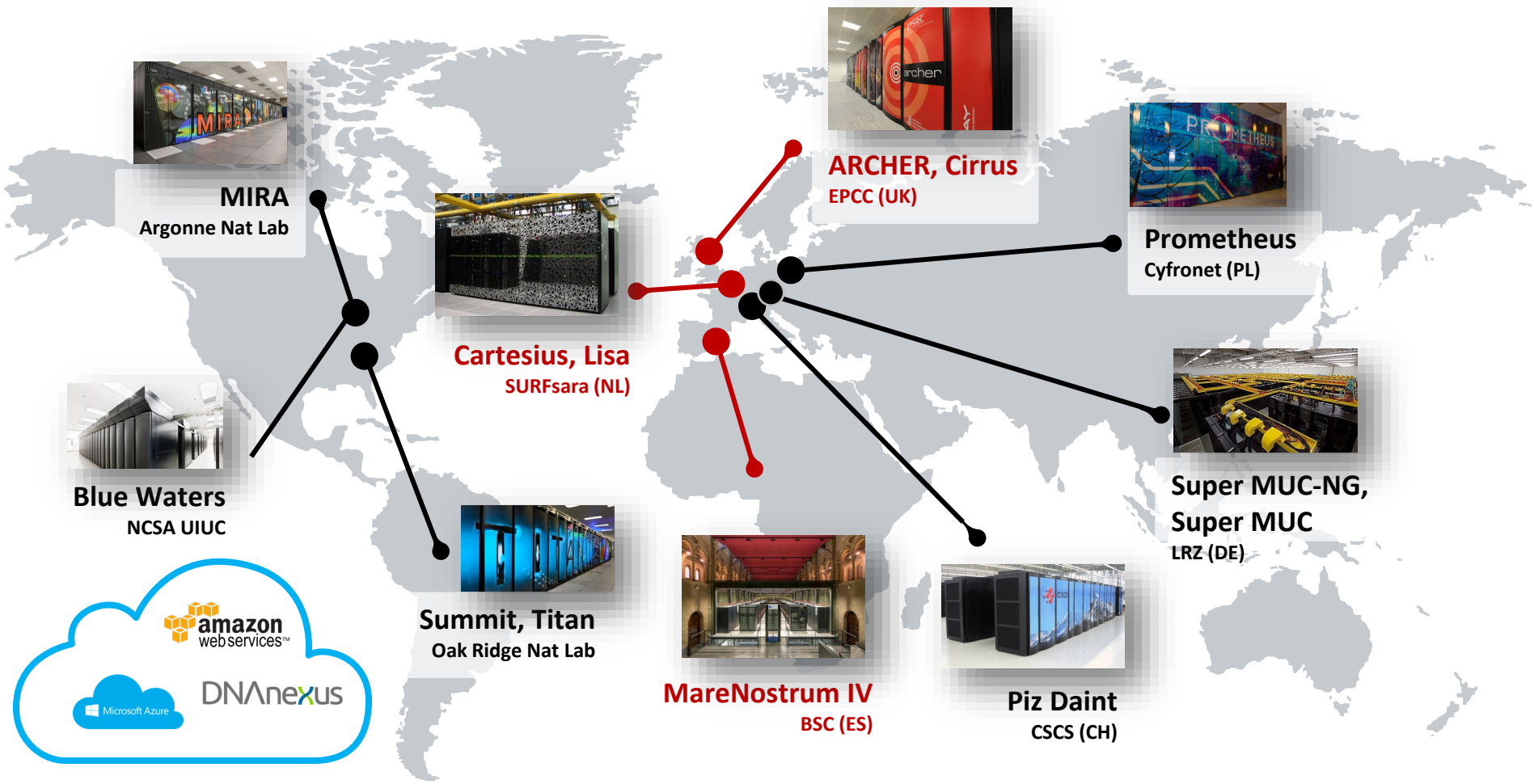
- **Quantum computing**

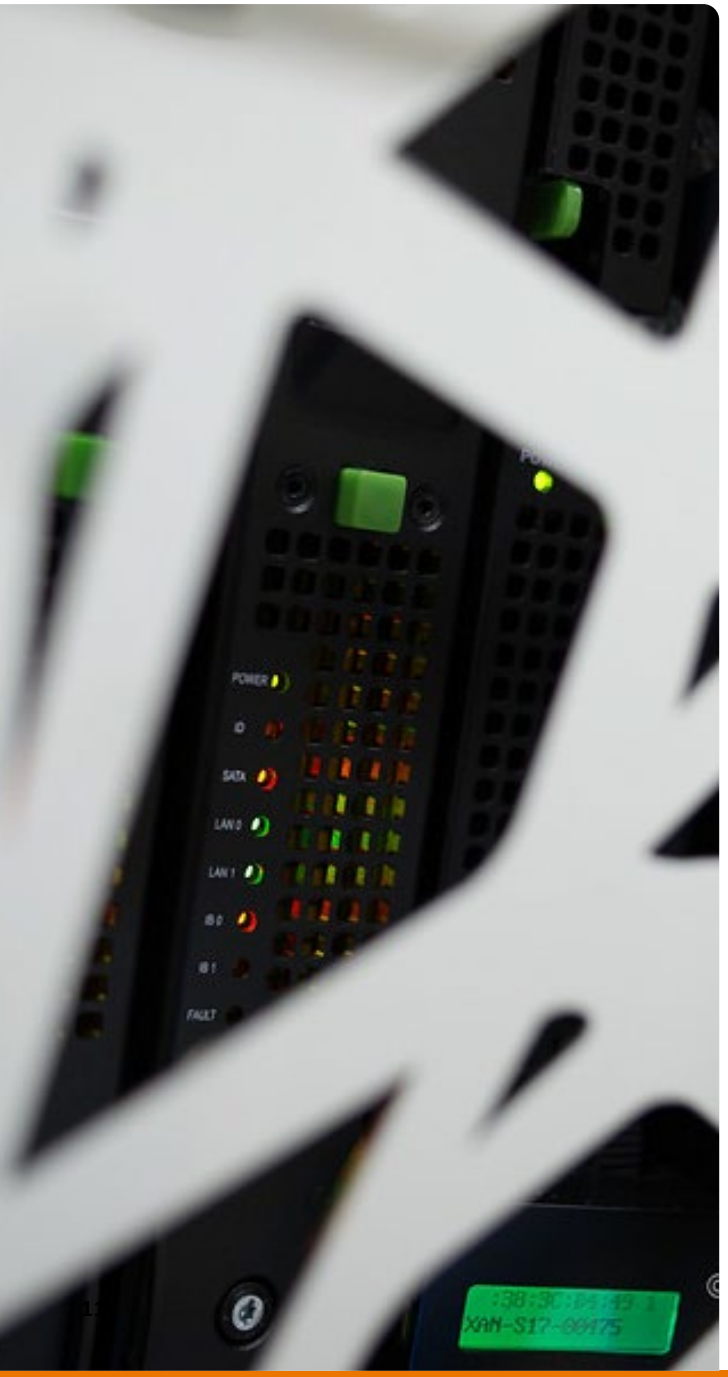
QUANTUM INTERNET ALLIANCE

High Performance Computing in CompBioMed



High Performance Computing in CompBioMed





Outline

What is a Supercomputer?

- Working with an HPC system
- HPC access and usage

More Linux tools

- Hands-on with cheat sheet
- Linux scripts

Running jobs on a Supercomputer

- Use the batch system
- Running jobs

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What is a Supercomputer?

User Experience

- Multiuser system
- Unix OS
- Optimized software

Compute power

- Many CPUs system
- Specialized hardware
- Low-latency & high bandwidth connections

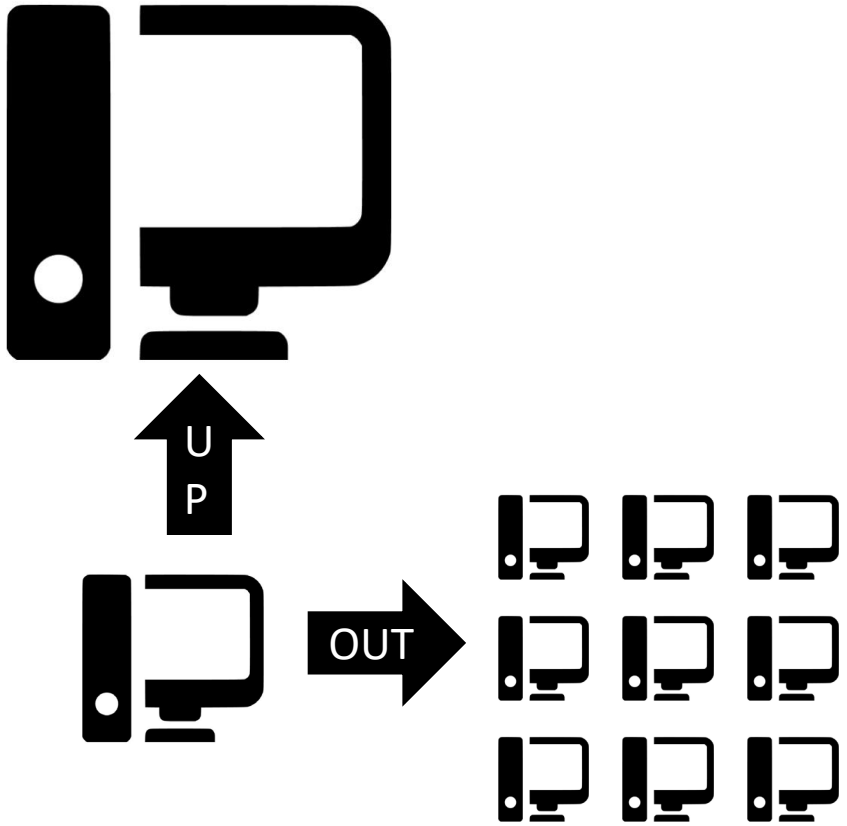
Storage

- Efficient I/O
- Large Memories

What is a Supercomputer?

Why you need a Supercomputer?

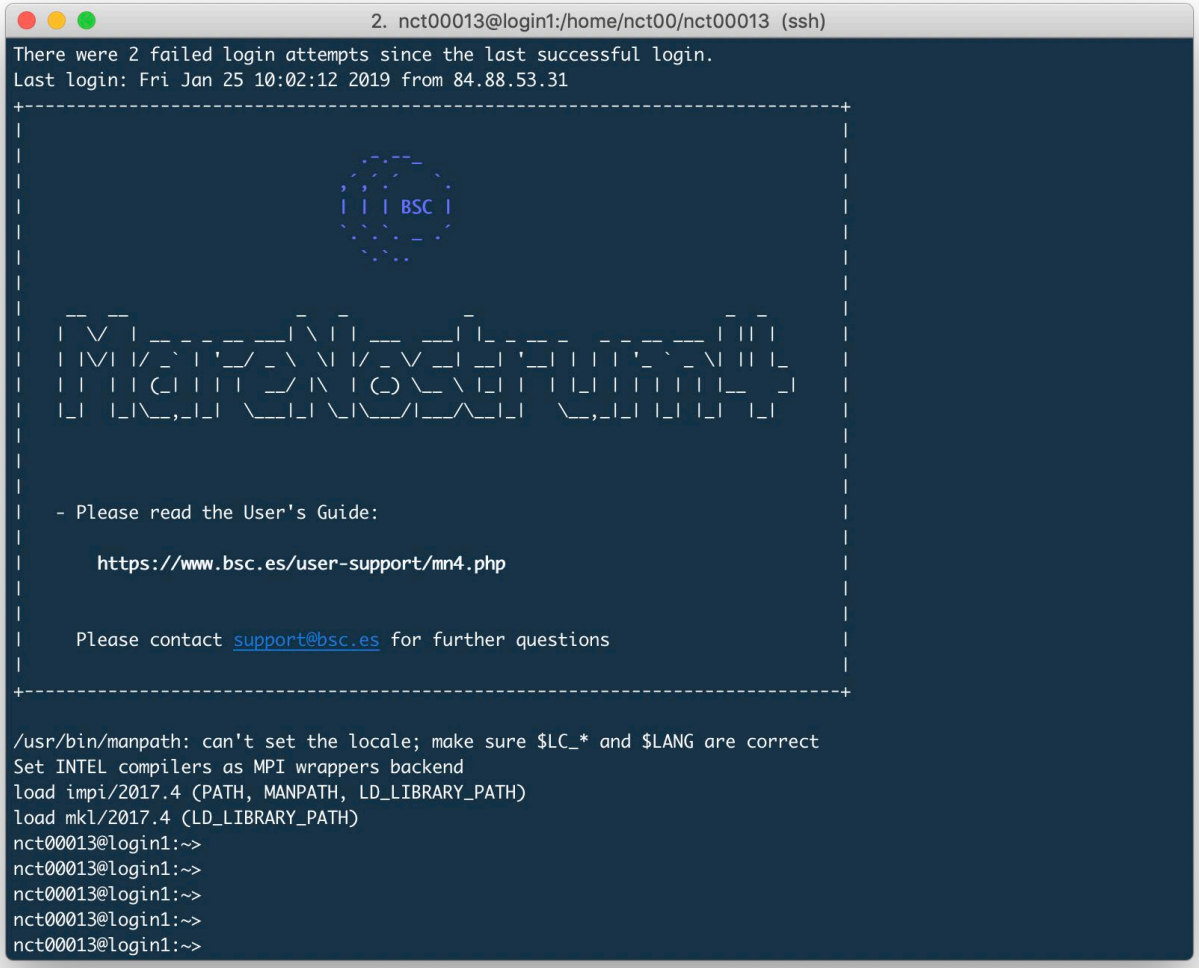
- **Scale up**
  - Faster CPUs
  - Large memories
  - Specialized Hardware/Software
- **Scale out**
  - Large parallel applications
  - Many small- to medium- size jobs



What is a Supercomputer?

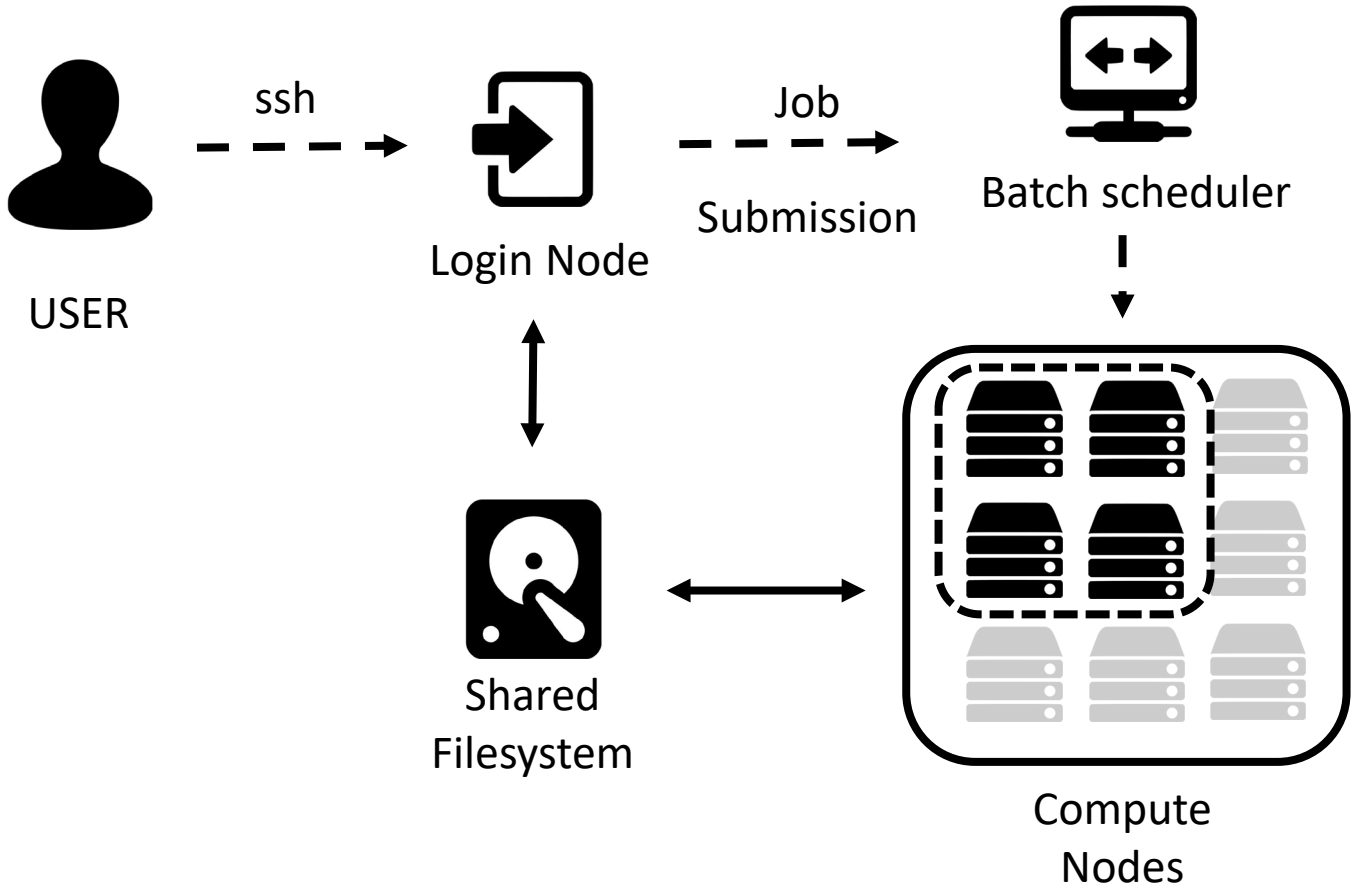
Is NOT like this…

What is a Supercomputer?



What is a Supercomputer?

Working with a Supercomputer

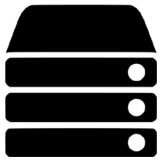


What is a Supercomputer?

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

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MORE LINUX TOOLS

Introduction to HPC in Computational Modelling

Getting started with HPC systems

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
- Two essential principles
  - Everything is a file
  - KISS

Getting started with HPC systems

Working with a Supercomputer

1 **Login and transfer files to remote machine**

- ssh, scp/ftp
- Command line, GUI

2 **Prepare your jobs**

- Input + Software
- Job submission script

3 **Submit your job and retrieve output**

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

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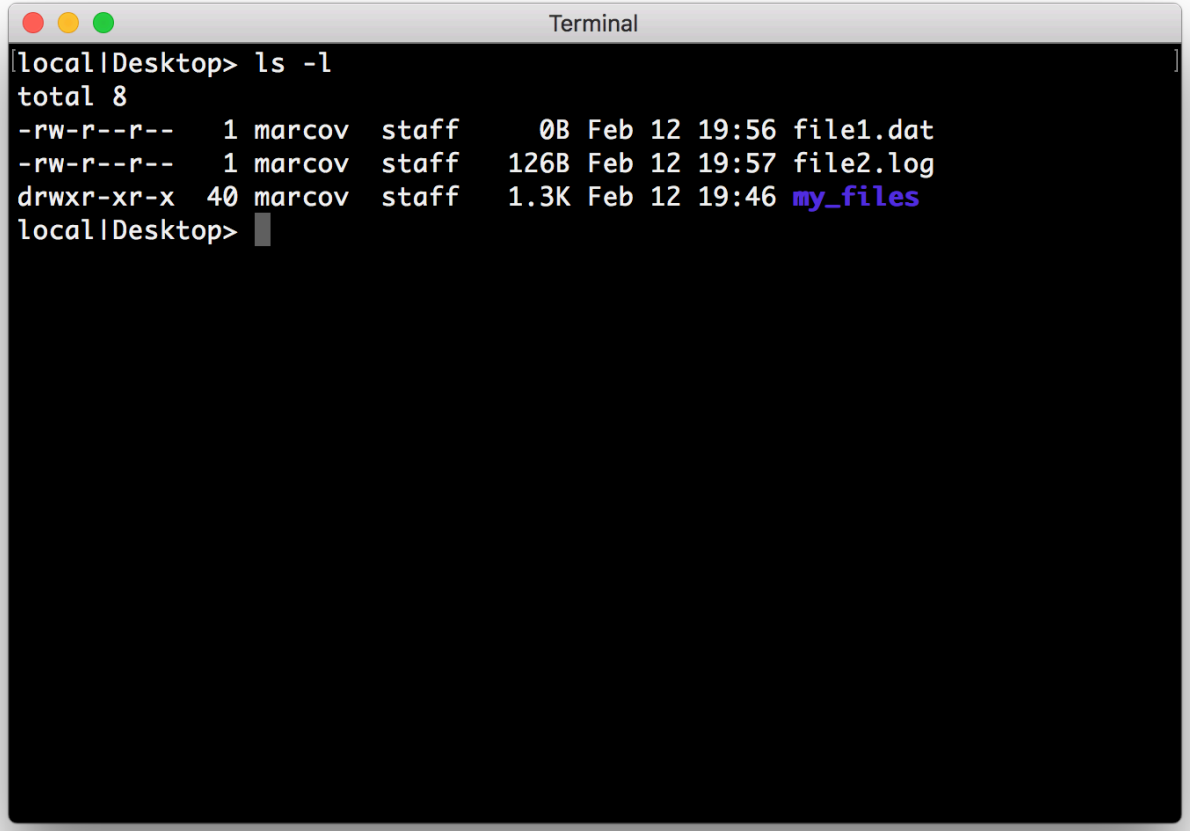
Getting started with HPC systems

Terminal – Working with a Unix system



Getting started with HPC systems

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!

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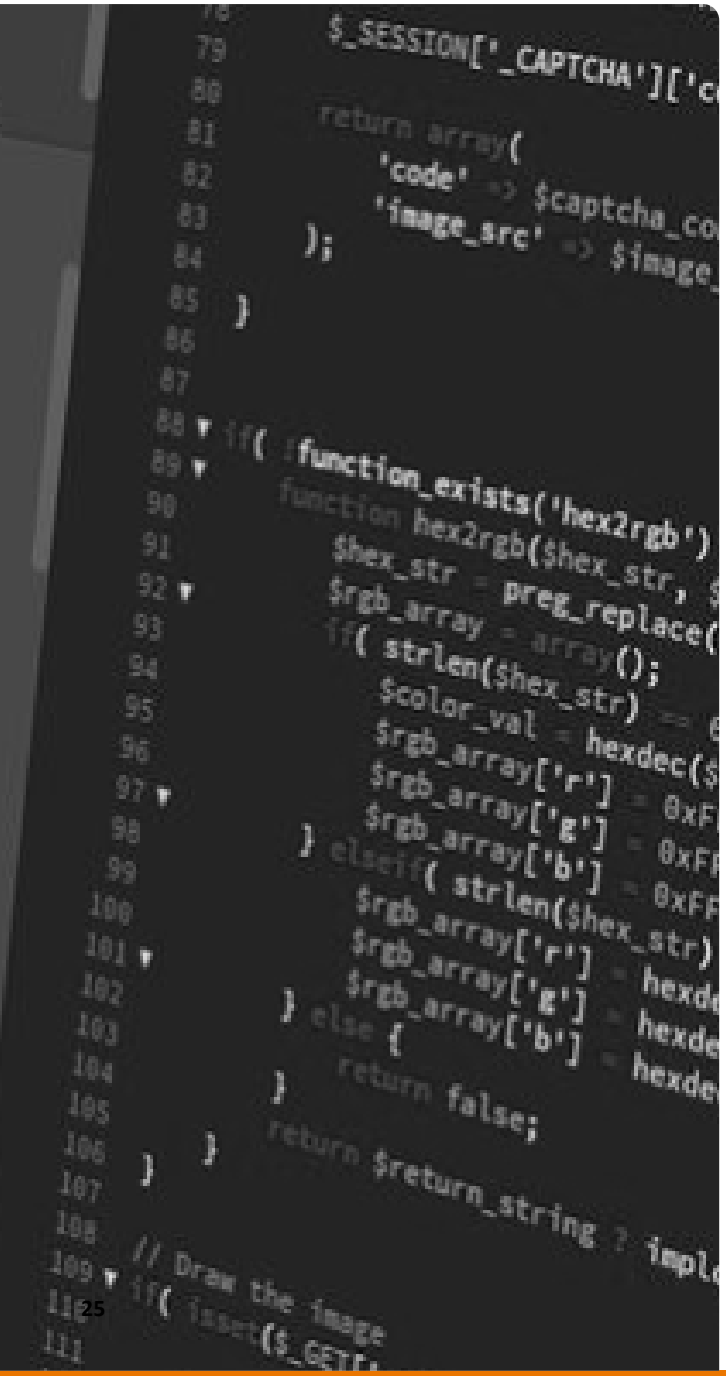

Getting started with HPC systems

- Keep the Linux cheat sheet open:

  https://edu.nl/f4qaf

- Check the material for future hands-on exercises:

  https://edu.nl/mtbvf

- Can you download and transfer the zip file to MareNostrum4 and extract the zip in your home?

- Otherwise just copy the files to your home directly:

```
nct00008@login1:~> cp –r
/gpfs/projects/nct00/nct00008/linux-hands-on ~/
```

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Getting started with HPC systems

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"
```

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Getting started with HPC systems

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"
```

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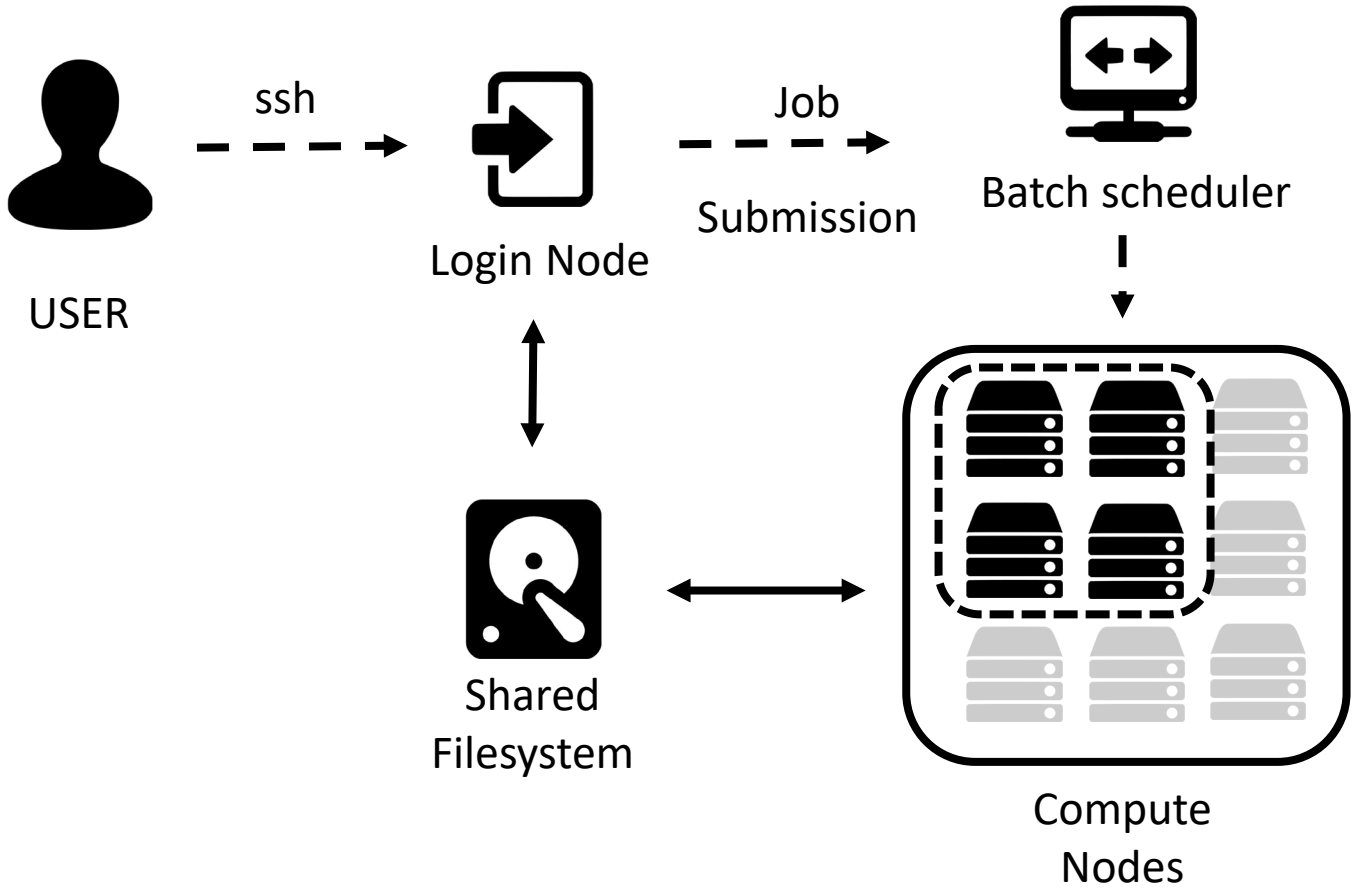
Getting started with HPC systems

Submitting jobs in an HPC system



Getting started with HPC systems

- 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.

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Getting started with HPC systems

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.

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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

```
nct00008@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
```

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Running on a Supercomputer

Submitting and monitoring jobs

Jobs are submitted and controlled using SLURM commands

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

```
nct00008@login1:~> sbatch <job script>
```

- shows all the submitted jobs ant their status:

```
nct00008@login1:~> squeue
```

- remove the job from the queue system:

```
nct00008@login1:~> scancel <jobid>
```

- un a command on the cluster

```
nct00008@login1:~> srun <command>
```

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Running on a Supercomputer

Queues

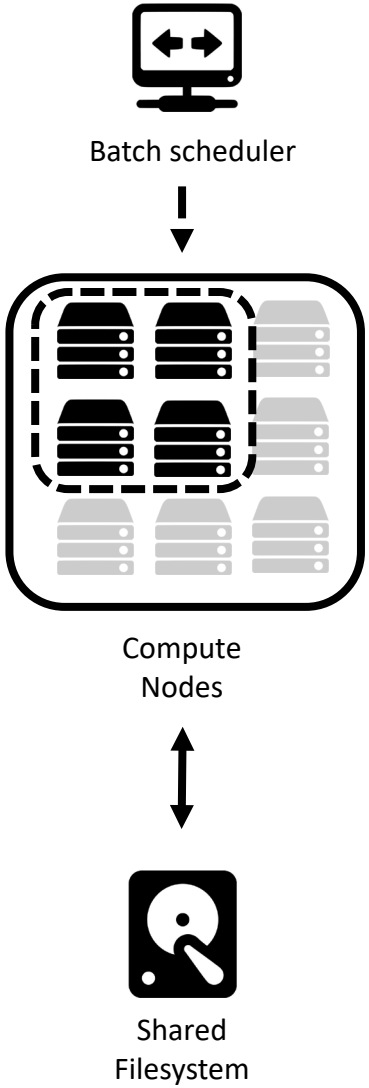
- There are several queues present in the machines and different users may access different queues.
- **`bsc_queue`** shows information of the available queues

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 packges
- 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

```
nct00008@login1:~> module avail

nct00008@login1:~> module avail python

nct00008@login1:~> module load siesta (SUCCESS…?)

nct00008@login1:~> module load …

nct00008@login1:~> module load python/2.7.14

nct00008@login1:~> module unload siesta

nct00008@login1:~> module list
```

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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
```

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Running on a Supercomputer

- Play with the material!

https://edu.nl/mtbvf

- … and keep the cheat sheet around for extra help

https://edu.nl/f4qaf

- unix
  - bash scripts and basic Unix commands
- batch
  - simple submissions scripts to start using SLURM
- parallel
  - advanced submissions scripts to run parallel applications

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)

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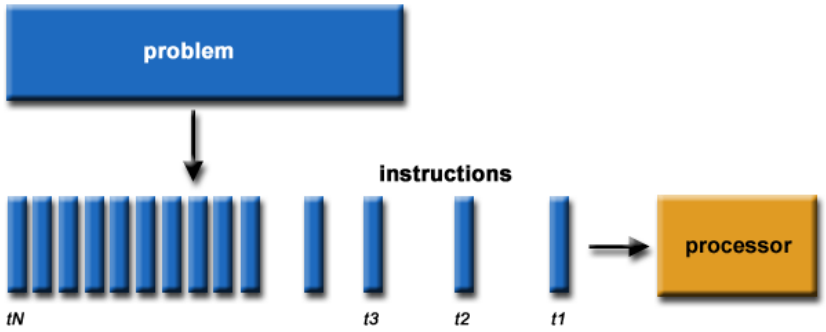
Running on a Supercomputer

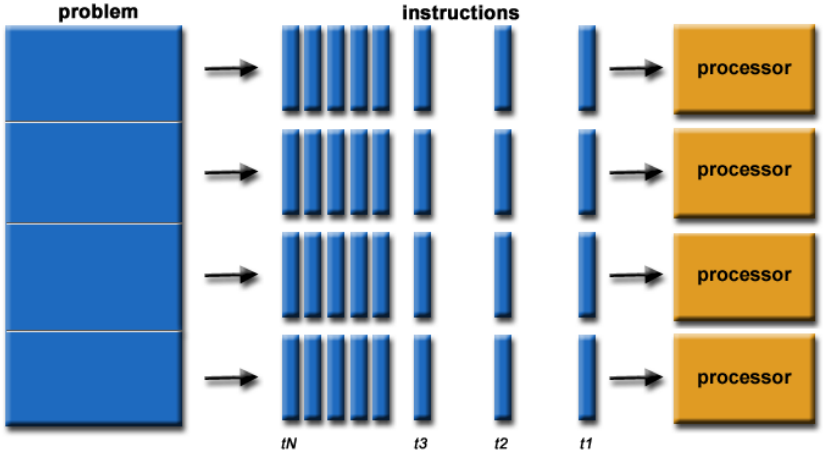
Serial computing

- 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.

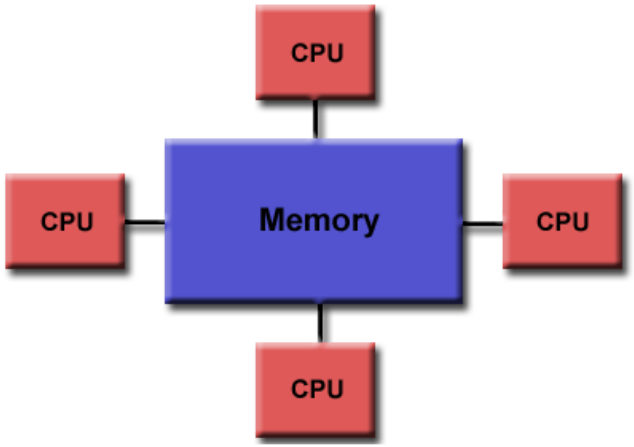


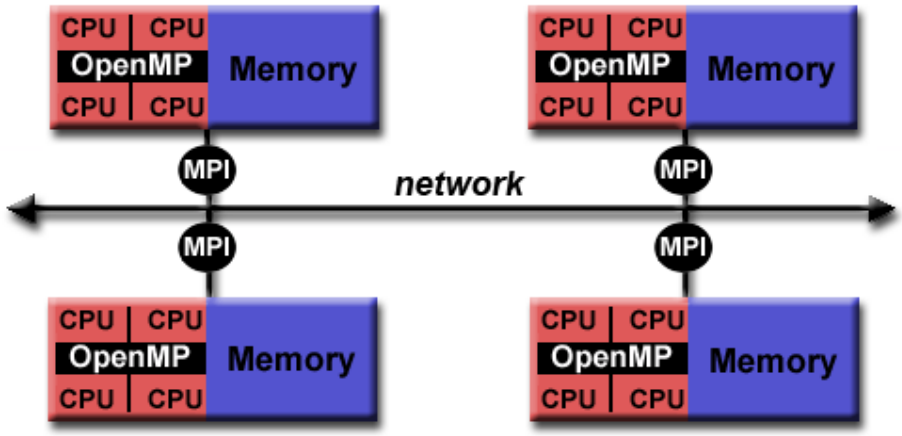
credits: https://computing.llnl.gov/tutorials/parallel_com

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





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One last step…

- Get ready for the real hands-on example: hemodynamics with HemoCell!
  - Please copy the required files to your home directory

```
nct00008@login1:~> cp /gpfs/projects/nct00/nct00008/DATA_HEMOCELL/HemoCell-master.zip ~/.
nct00008@login1:~> cp /gpfs/projects/nct00/nct00008/DATA_HEMOCELL/palabos_dev.tgz ~/.
```

  - Enjoy the next sessions!

Acknowledgements

Marco Verdicchio + SURFsara advisors

BSC support