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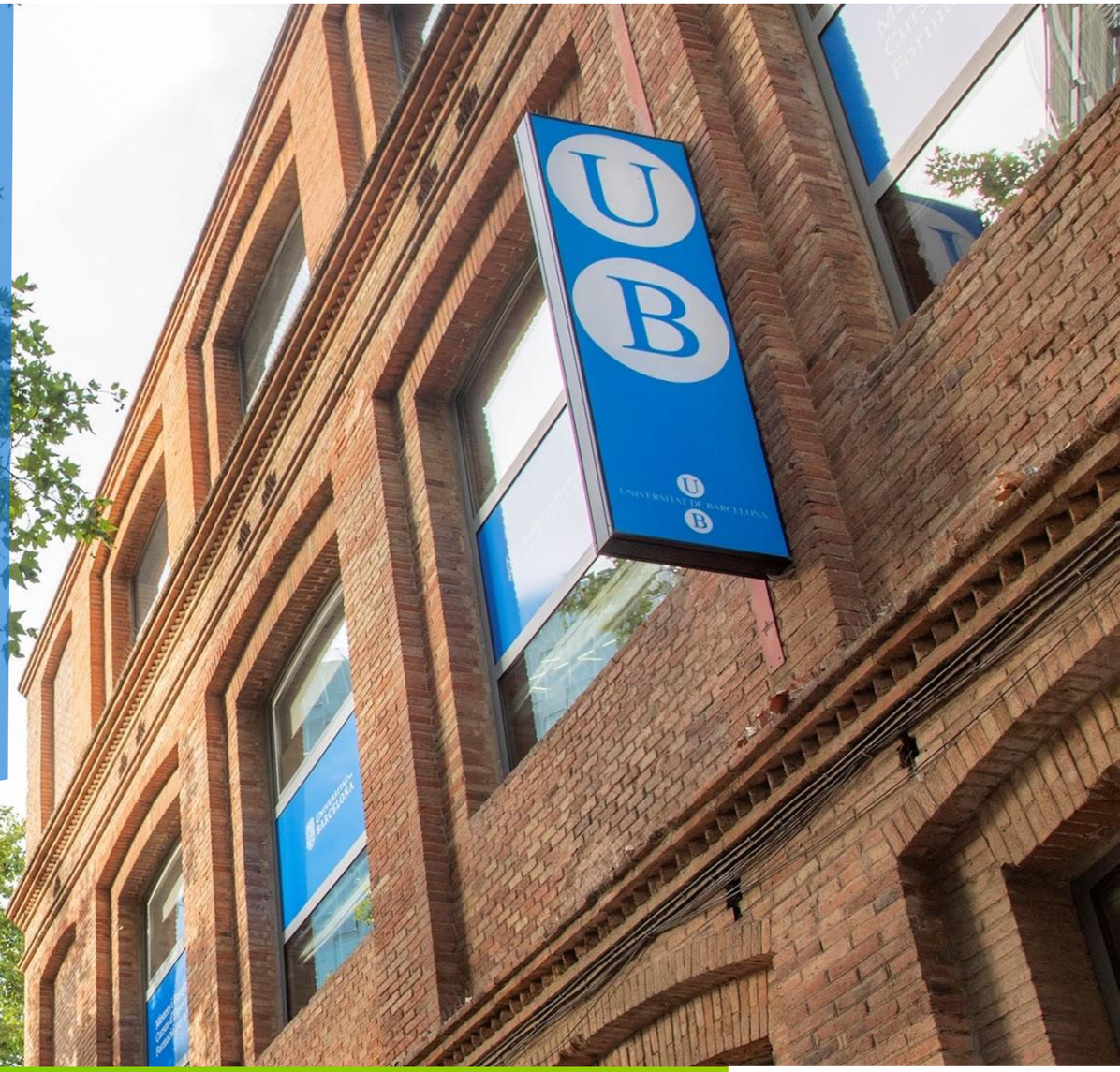
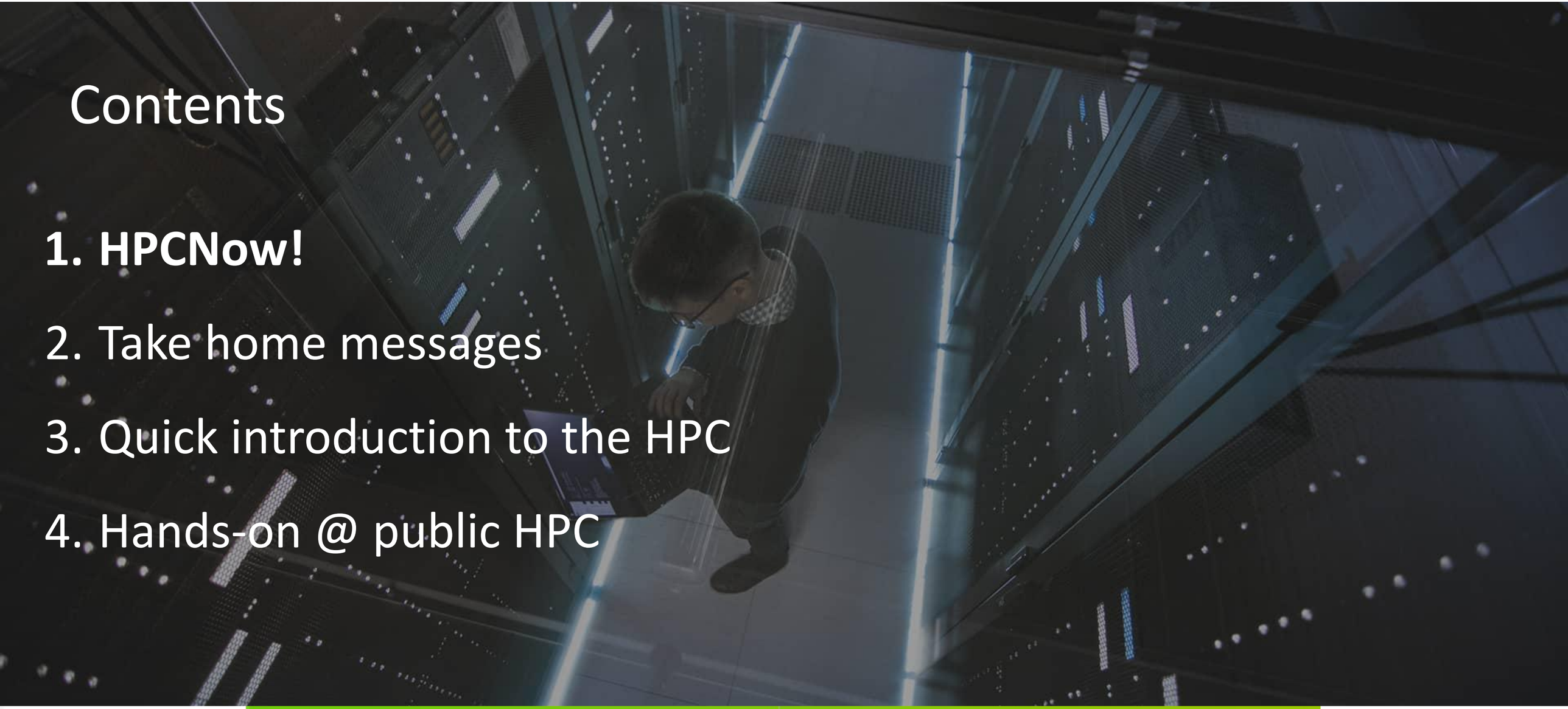
Introduction and Best Practices for High Performance Computing - HPC

Erica Bianco, PhD
Computational Scientist @HPCNow!



HPC Now!



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1. **HPCNow!**
2. Take home messages
3. Quick introduction to the HPC
4. Hands-on @ public HPC


HPC Now!
Advanced supercomputing services for science and engineering
We plan, install & support
You run
www.hpcnow.com

HPC Now!

Services and turnkey solutions adapted to your needs

HPCNow! provides its customers with the best solutions, getting the most out of their systems and maximizing the investment made.

Planning

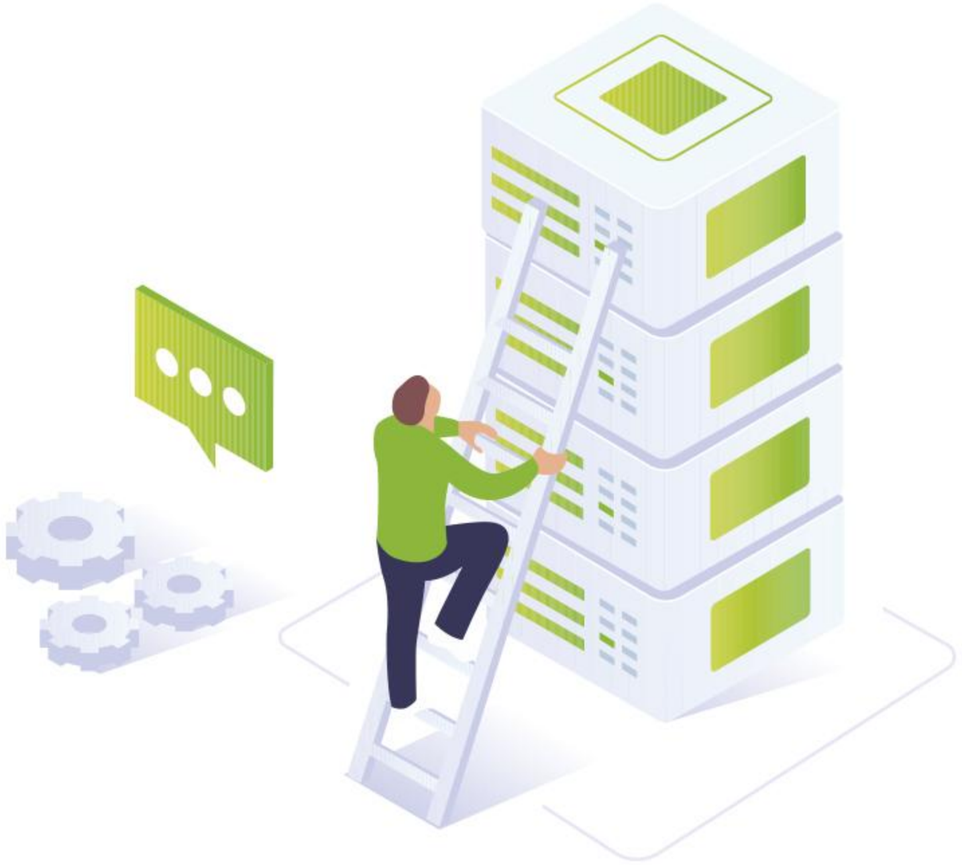
HPCNow! performs detailed planning of all the required components for the optimal performance of an HPC system. On HPC systems already running, also consulting is offered in order to achieve the **best solution to enhance execution and user experience**.

- Consulting
- Solution Design

Installation

HPCNow! takes care of the full installation of an HPC system, **from the hardware to the final application,** including customized training that covers all necessary details for a successful administration and proper use of the resources.

- Infrastucture
- Software
- Training



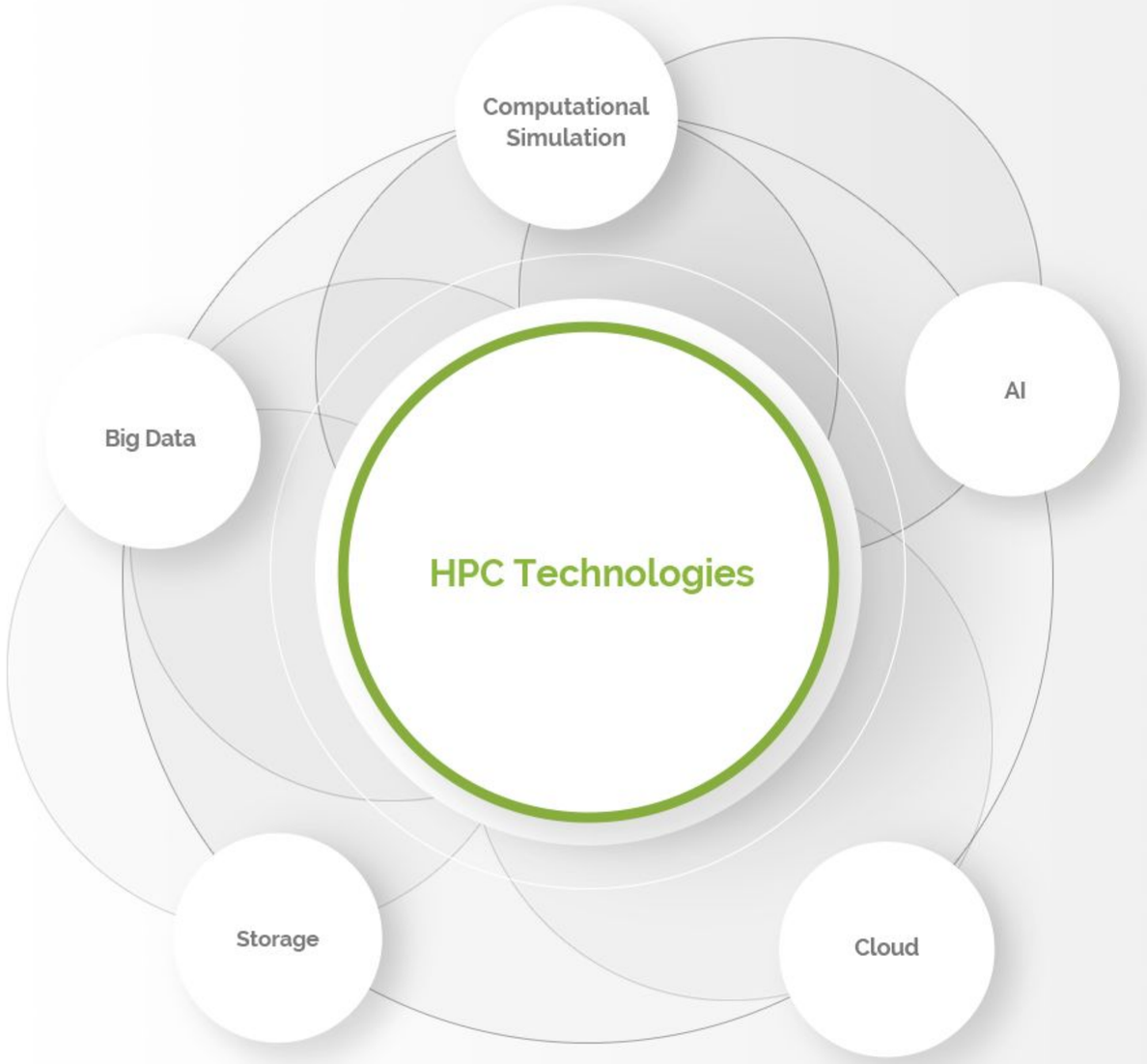
Maintenance

HPCNow! conducts the whole maintenance of an HPC system through its lifetime. It also offers the **best support to the users, advising and resolving any technical issues** that may arise, quickly and efficiently.

- Support
- Managed Services

HPC Now!

Solutions

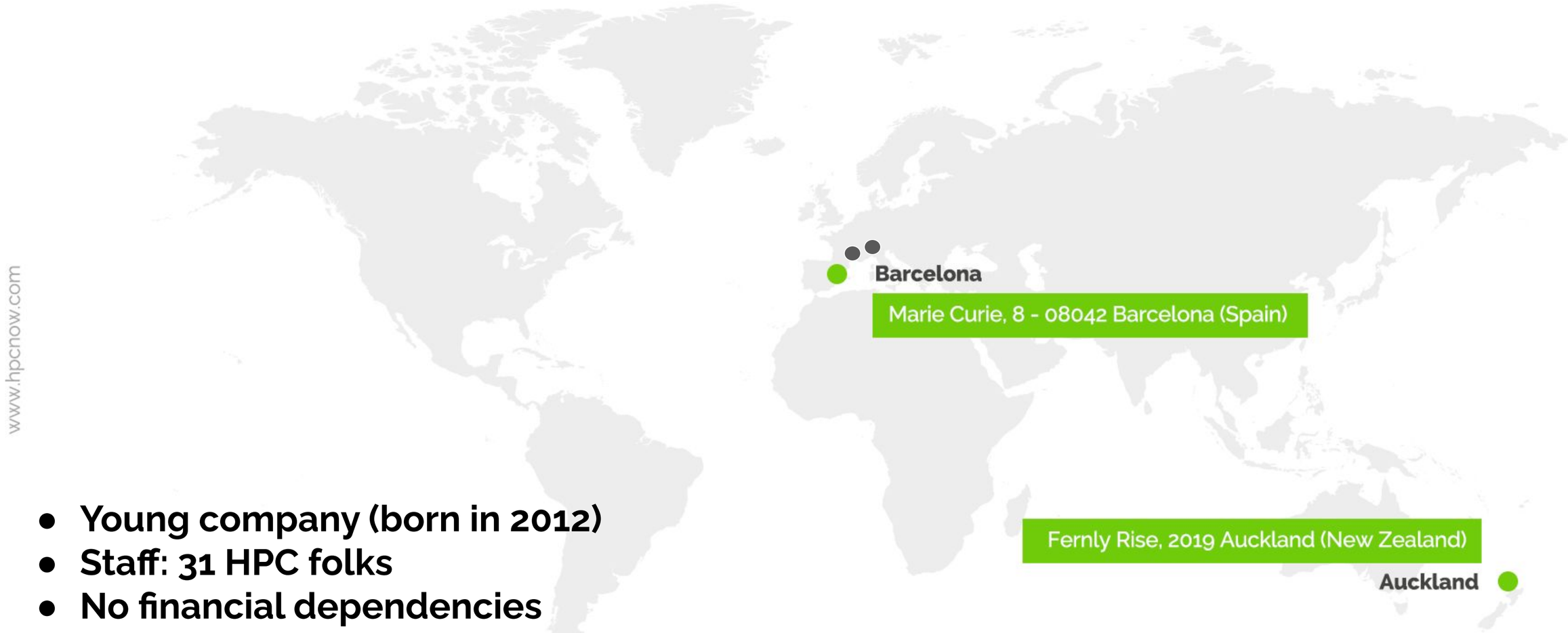


Sectors

HPC technologies are cross-cutting and cover an increasing number of areas. HPCNow! offers services and solutions applicable in all sectors and industries to accelerate and ensure your project success.

Research	Genomics	Energy
Pharma	Automotive	Banking
Biotechnology	Aeronautical	Media

Company



- Young company (born in 2012)
- Staff: 31 HPC folks
- No financial dependencies
- Strong growth
- EU joint venture

doitnow
HPC Services

The company's core values are a deep understanding of the most advanced technologies in HPC along with extensive experience in customer and user support. The similarity of HPC technologies, both technically and commercially, with other growing IT sectors -Big Data, artificial intelligence, cloud computing- allow us to offer solutions in these areas as well.

Providing careful and detailed solutions and the successful customer response to our services has allowed HPCNow! to grow without external funding and to have the means to tackle any new challenge.

+200
years of accumulated experience

+100
satisfied customers in 15 different countries on 5 continents

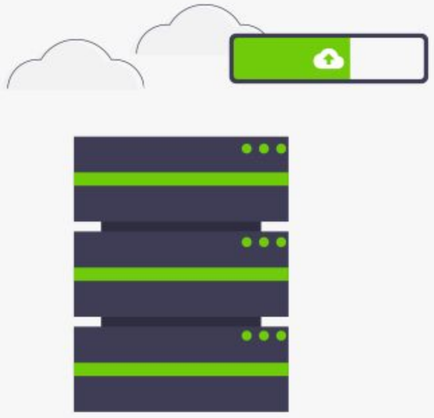
+100
HPC clusters installed

+50
distributed storage solutions deployed

+3.000
users who have received HPC training

We are passionate about new challenges and HPC technologies enthusiasts. Our goal is to take full advantage of supercomputing to provide solutions to our customers' scientific or engineering dares.

User-oriented company



SW & HW & Cloud agnostics

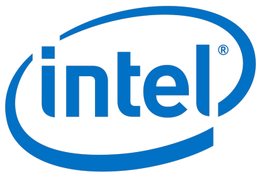
IT + scientific background

HPC services and solutions

- **Customers**

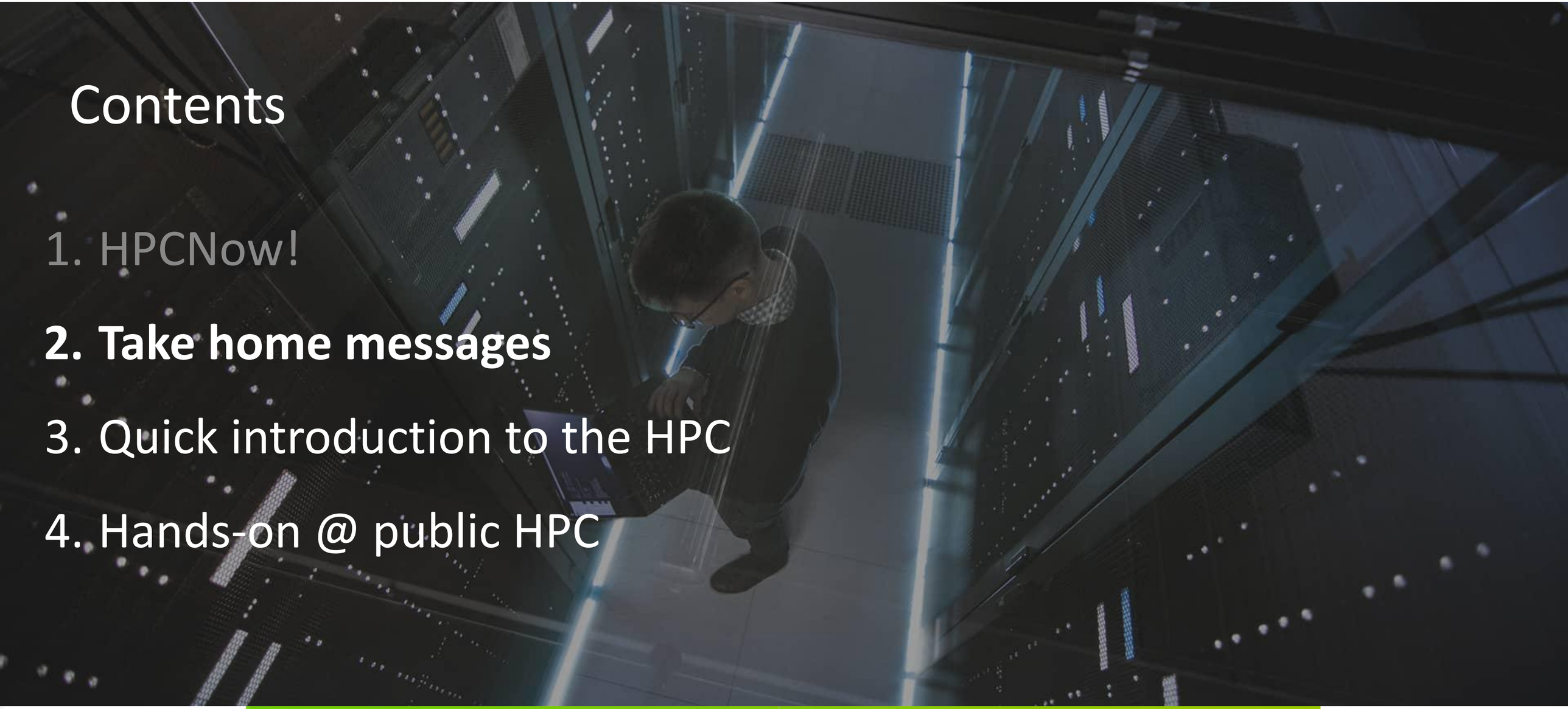
and many more...

- **Partners ecosystem**



- **Contribution to HPC community**

EuroHPC
Joint Undertaking



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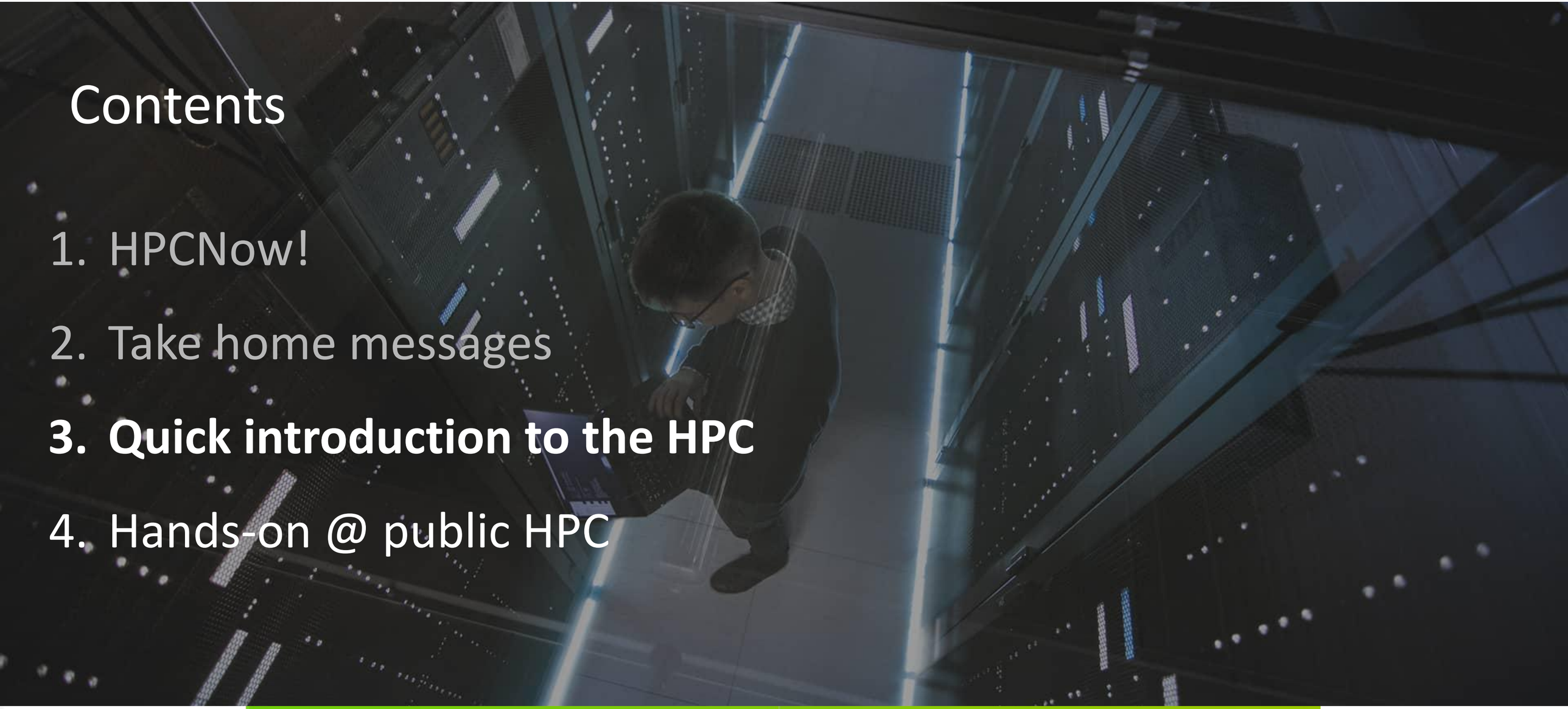
Take home messages

- ★ Basic HPC concepts
  - What does HPC means
  - Why to use an HPC system and how
- ★ How to submit your first jobs successfully to an HPC cluster



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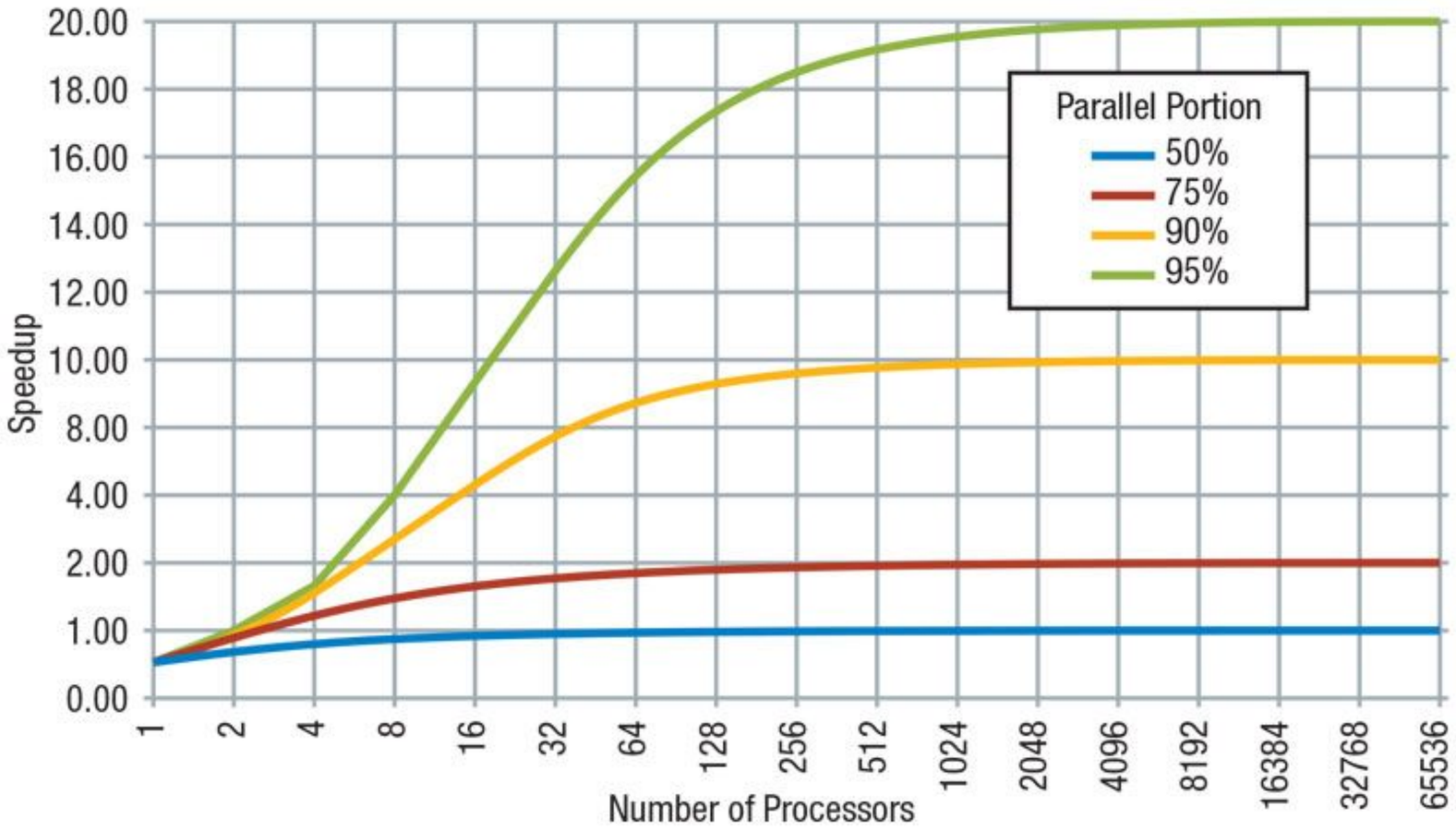
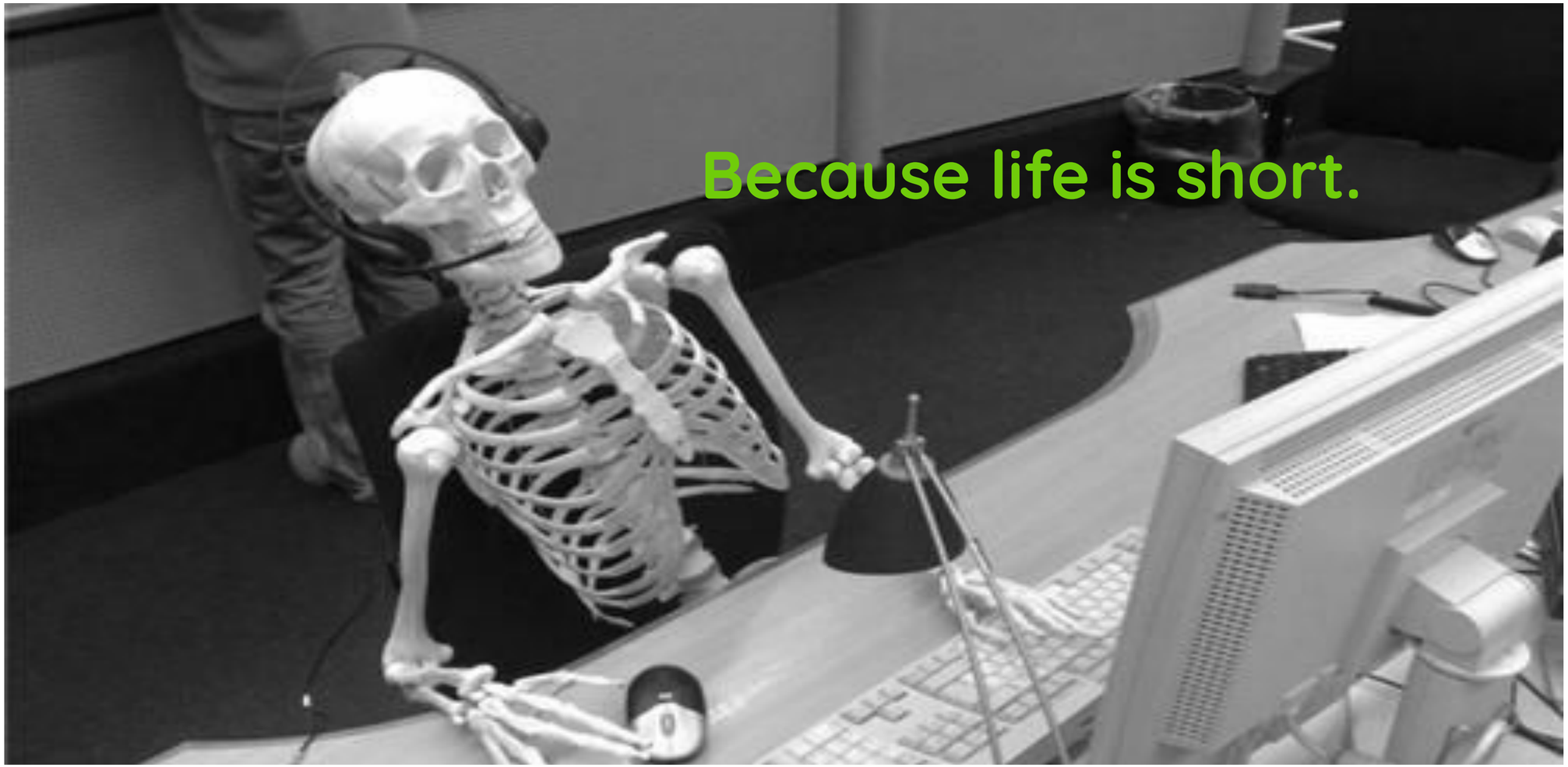
Why use an HPC?

- The key goal is to solve the problems faster.
- Split the work between several processors
- Parallel computing allows to divide the work among multiple CPUs in several compute nodes.
- Ideally, the program will run N times faster by using N processors.
- Unfortunately, in most cases that’s not true.

Amdahl's Law

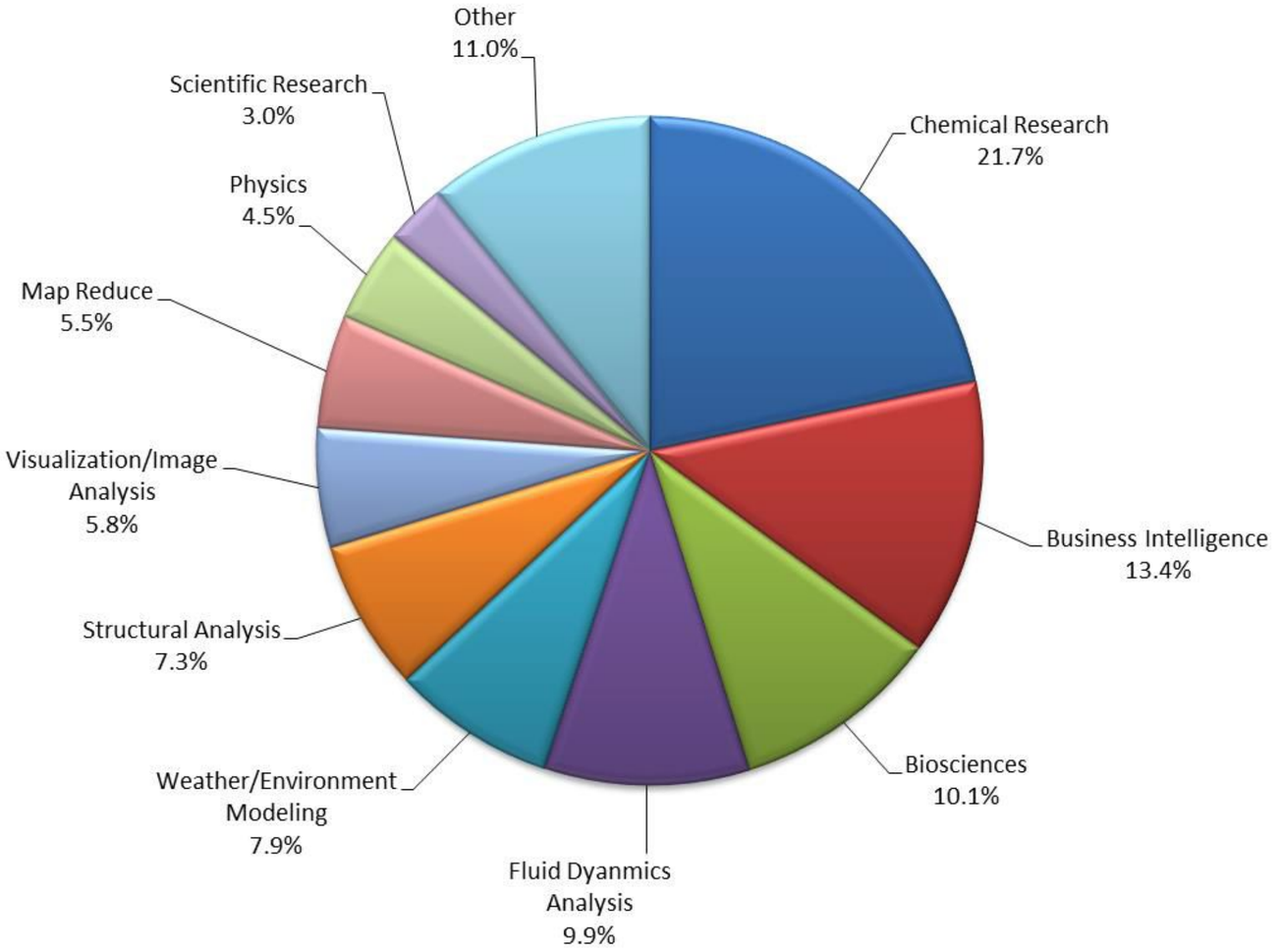

Speedup
20.00
18.00
16.00
14.00
12.00
10.00
8.00
4.00
2.00
1.00
0.00
1
2
4
8
16
32
64
128
256
512
1024
2048
4096
8192
16384
32768
65536
Number of Processors
Parallel Portion
50%
75%
90%
95%

Why to use HPC?



What HPC used for?

- Scientific and Engineering simulations have a need for massive compute power.
- The clock speed of single-core processors can not be faster due power and heat limitations.
- Memory allocated to a single-core is quite limited. Increasing it is very expensive and slow.



Storage: 1 PB = 10^{12} kB = 10^{9} MB = 10^{6} GB = 10^{3} TB.

Main Use Cases for HPC

Clustered (Tightly coupled)

- Fluid dynamics
- Weather forecasting
- Materials simulations
- Crash simulations

- Seismic processing
- Metagenomics
- Astrophysics
- Deep learning

Modest IO requirements

Heavy IO requirements

- Risk simulations
- Molecular modeling
- Contextual search
- Logistics simulations

- Animation and VFX
- Semiconductor verification
- Image processing/GIS
- Genomics

Distributed/Grid (Loosely coupled)

HPC Suitable Work

Suitable Work

- When tasks take too long
- When one server is not enough
- When my problem consumes large amounts of memory

Less Suited Work

- Windows only software
- Interactive software i.e. GUI
- Inefficient, un-optimised software

HPC Parallel execution time

- Single core computation time: computation only.
- Parallel computation time: computation + communication + waiting.
- E.g.writing results (to one file) is often a bottleneck.
- Small problem on many cores: communication cost will dominate.
- Unbalanced load: one core will mainly wait on the other.

Performance

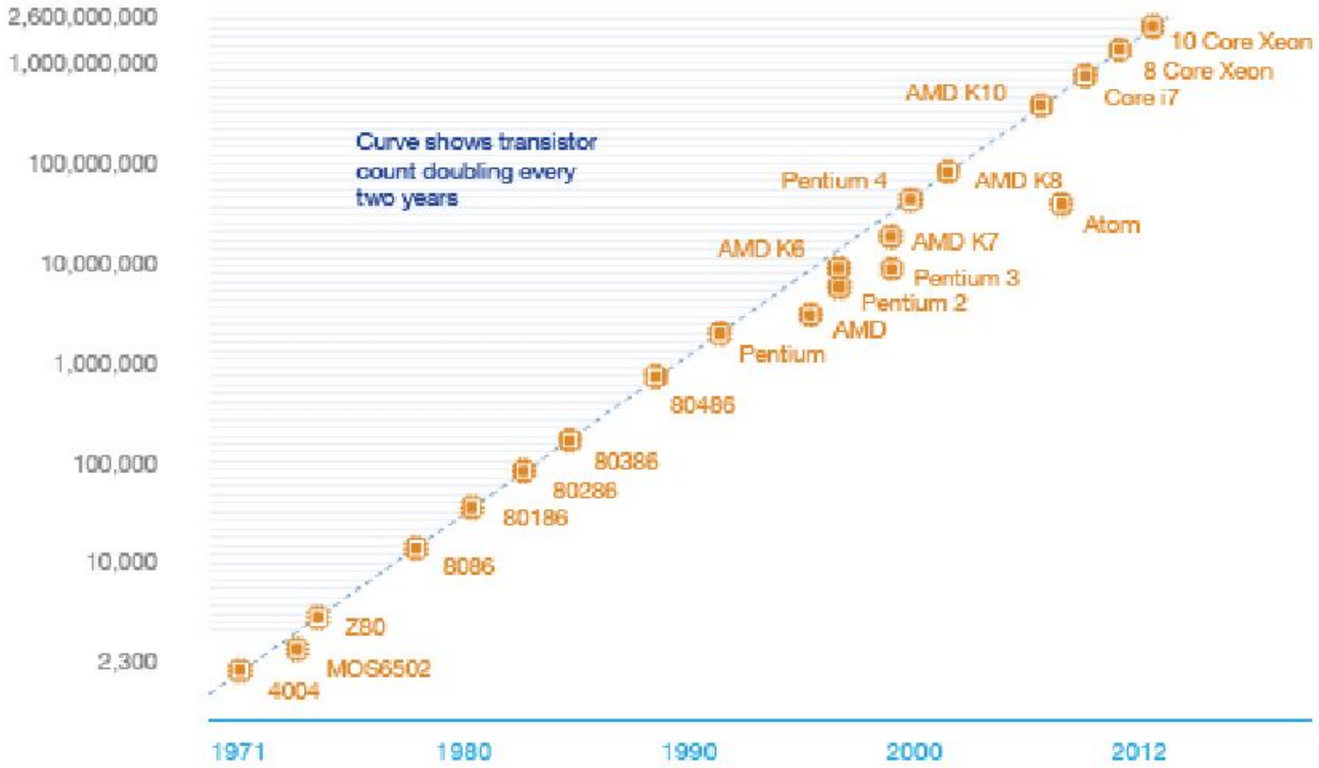
The performance of a program depends on:

- Clock speed
- Floating point unit
- Cache size
- Memory latency
- Memory bandwidth
- IO
- Fabric interconnect

$$\text{FLOPS} = \text{sockets} \times \frac{\text{cores}}{\text{socket}} \times \text{clock} \times \frac{\text{FLOPs}}{\text{cycle}}$$

Moore's law

The number of transistors on a microchip doubles about every two years, though the cost of computers is halved.



It also applies to:

- processor speeds,
- communication speeds,
- storage space on hard disks,
- pixels on a screen.

2014 - DOI:10.1007/978-3-319-04948-9_2

Paradigms in Parallel Programming

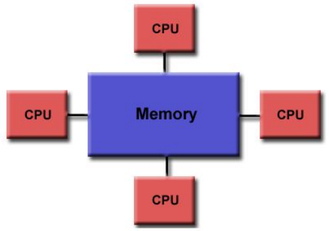
The two parallel programming paradigms most used in HPC are:

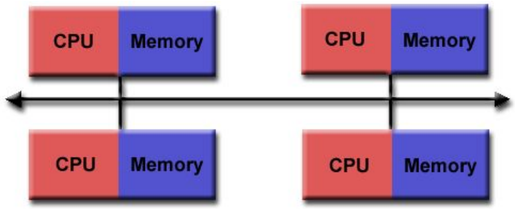
- **OpenMP** for shared memory systems (multithreading): on multiple cores of a single node
- **MPI** for distributed memory systems (multiprocessing): on multiple nodes

Parallel programs are more difficult to write than sequential ones, because concurrency introduces several new classes of potential software bugs, of which race conditions are the most common. Communication and synchronisation between the different subtasks are typically some of the greatest obstacles to getting good parallel program performance.

Architectures

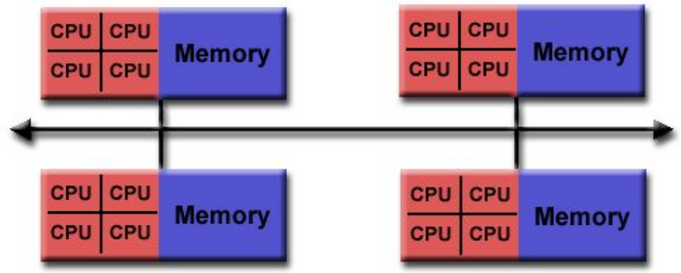
Shared Memory: Memory can be simultaneously accessed by by multiple programs or threads with an intent to provide communication among them or avoid redundant copies. Shared memory is an efficient means of passing data between programs. **OpenMP**





Distributed memory: Defined as a multiprocessor computer system in which each processor has its own private memory. Computational tasks can only operate on local data, and if remote data is required, the computational task must communicate with one or more remote processors through the network. **MPI**

Hybrid: Nowadays, the clusters are composed of multiple compute nodes, where each node has access to a large shared memory in addition to each node's limited non-shared private memory. **OpenMP and MPI**

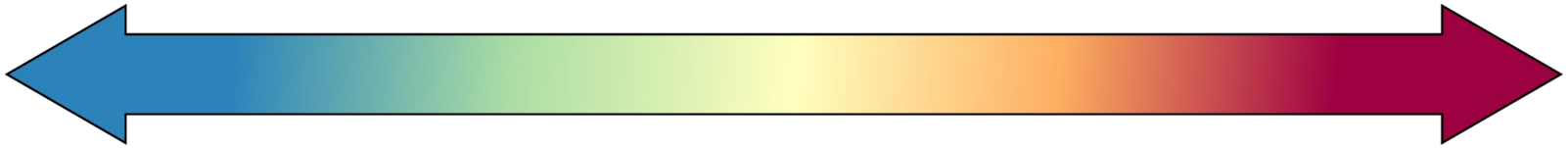


HPC or HTC?

High Performance (Capability)

High Throughput (Capacity)

Parallel methods



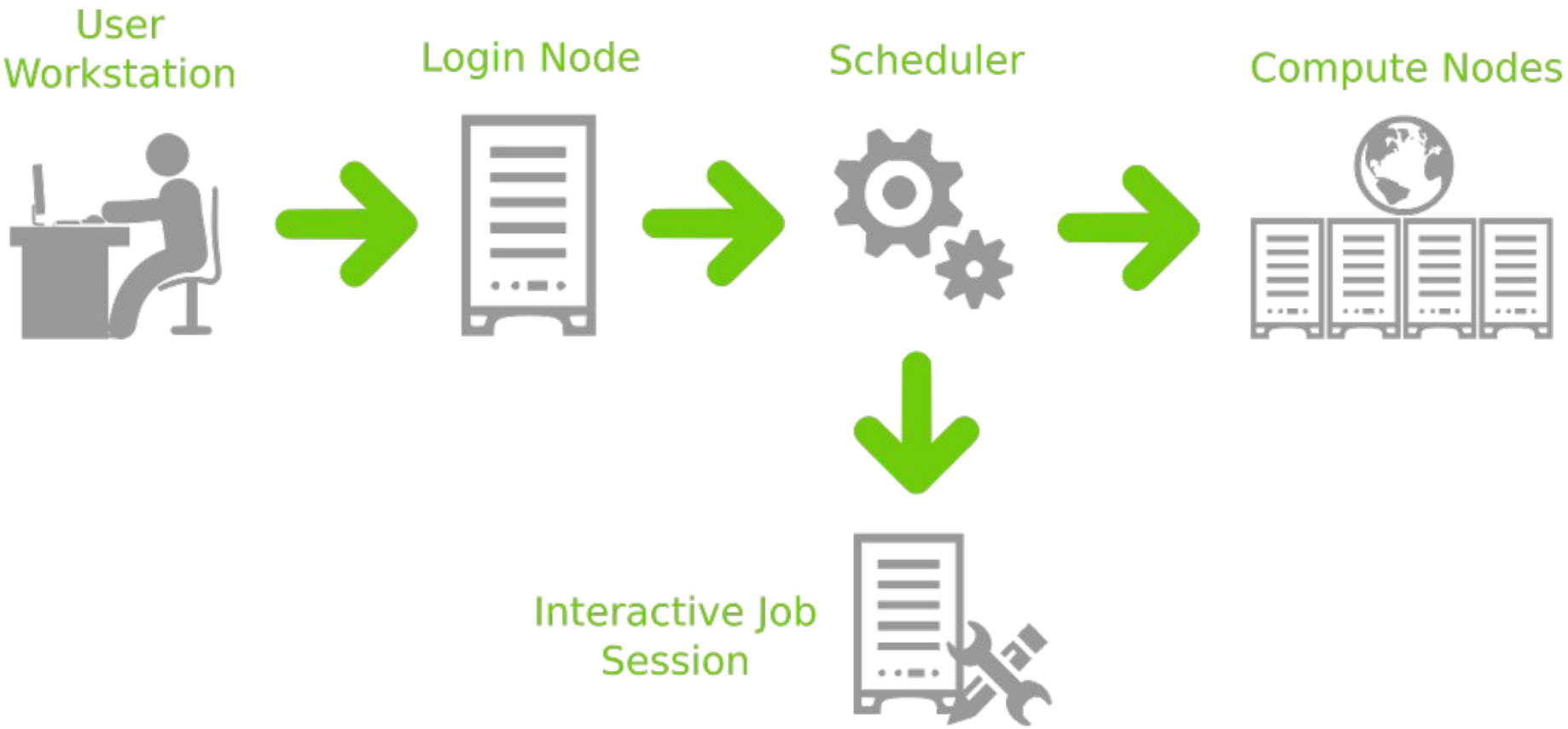
Parametric methods

Fine-grained Applications
- **Many-node**
- **Few concurrent runs**
- **High interconnect use**

Course-grained Applications
- **Single-node**
- **Many concurrent runs**
- **No interconnect use**

User Workflow

On a HPC system you send your script to the queue to be run and use the computational resources



Difference between Desktop Computer and HPC

- No Graphical User Interface (GUI)
- Programs are executed in batch mode
- Resources are shared between multiple users

- Workstation
- Local Server

Local

- Cloud HPC
- HPC Provider Company
- HPC Public Center

Remote

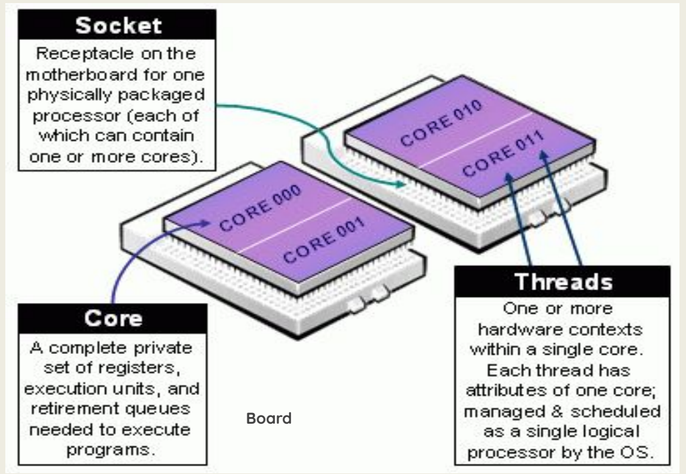
HPC schema

Rack

Node

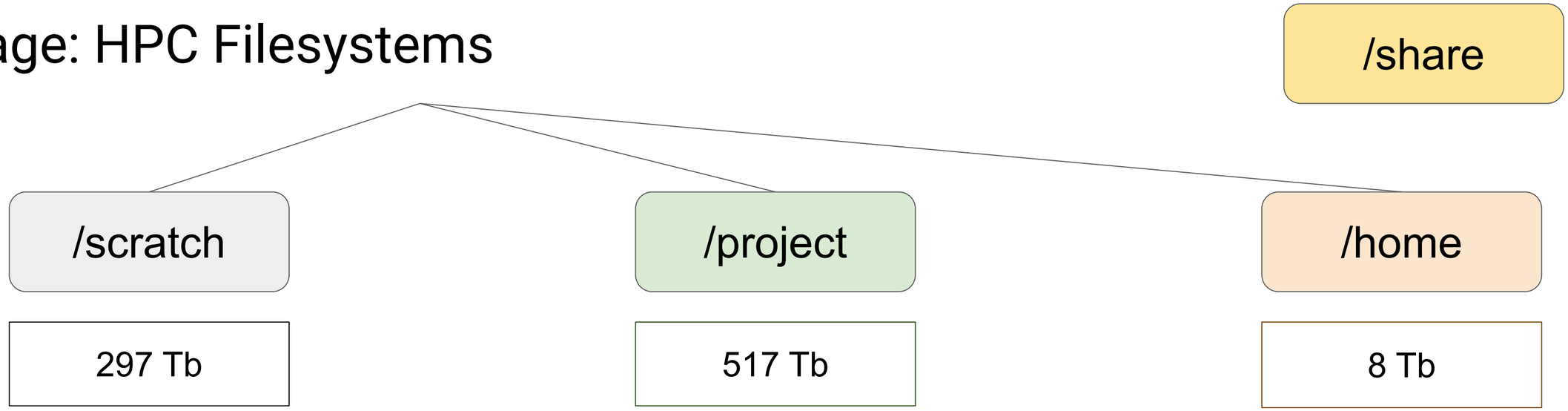
Memory

Disk



Data Center

Storage: HPC Filesystems



/scratch	/project	/home
No quota (but we are a lot of users) short term storage **temporary and working files** faster I/O share files between users	No quota (but we are a lot of users) long term storage (slow I/O) **important files storage** share files between users of the same lab	individual quota: 50 Gb to store scripts and small files symbolic links for project and scratch

https://www.eessi-hpc.org/

Software Applications on an HPC

HPC have shared appstacks and local installed applications.

EESSI is an example of a shared appstack across multiple centers

Environment Modules

Configuring Environment:

- Environment Modules package allows for dynamic modification of the user environment
- Modulefiles contain the required information to configure the shell for an application software
  - Loaded / unloaded dynamically
  - Useful in managing different versions of applications

Lmod cheat-sheet

```
man $MODULENAME ## or module help
module list ## currently loaded modules
module avail ## modules available to be loaded
module show $MODULEFILE.lua ## see exactly what a given modulefile will do to
the environment
module load $MODULENAME ## add a module to the environment
module unload $MODULENAME ## remove a module from the environment
module switch $MODULENAME $NEW_MODULENAME
module purge ## unload all active modules
```

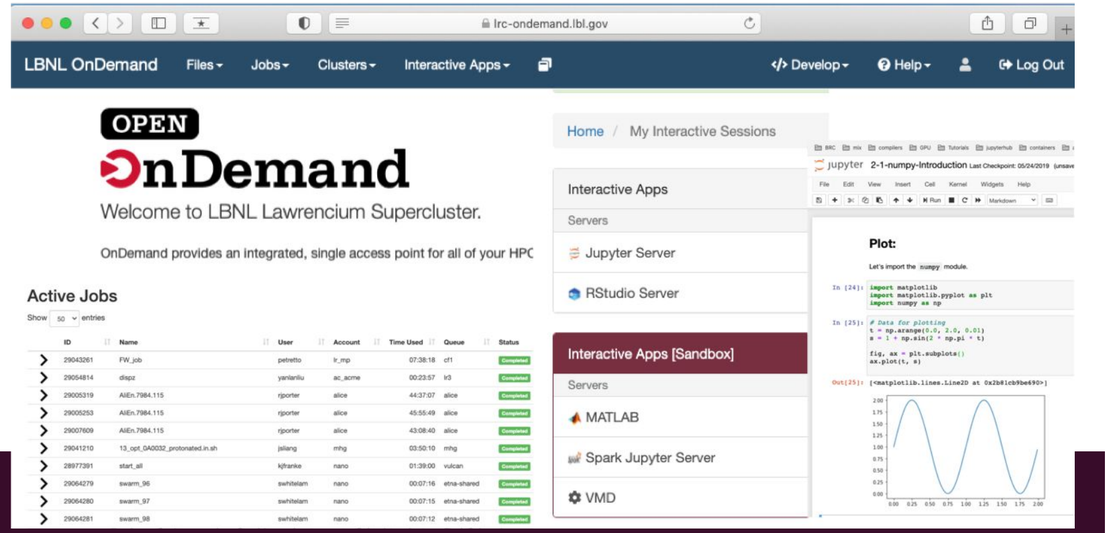
Load a module:

```
[ hpcnow1 ] pirineus7:~ $ which R
/usr/bin/which: no R in (/opt/gold/bin:/…:/usr/sbin)
[ hpcnow1 ] pirineus7:~ $ module load R
[ hpcnow1 ] pirineus7:~ $ which R
/prod/apps/R/4.0.2/bin/R
[ hpcnow1 ] pirineus7:~ $ R

R version 4.0.2 (2020-06-22) -- "Taking Off Again"
Copyright (C) 2020 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

.
.
.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

>
```

Accessing resources: SSH connection

- Linux - use a terminal
- Windows - use a terminal emulator
  - Putty
  - MobaXterm
  - windows powershell
  - WSL (Windows Subsystem Linux)
  - Virtual Machine

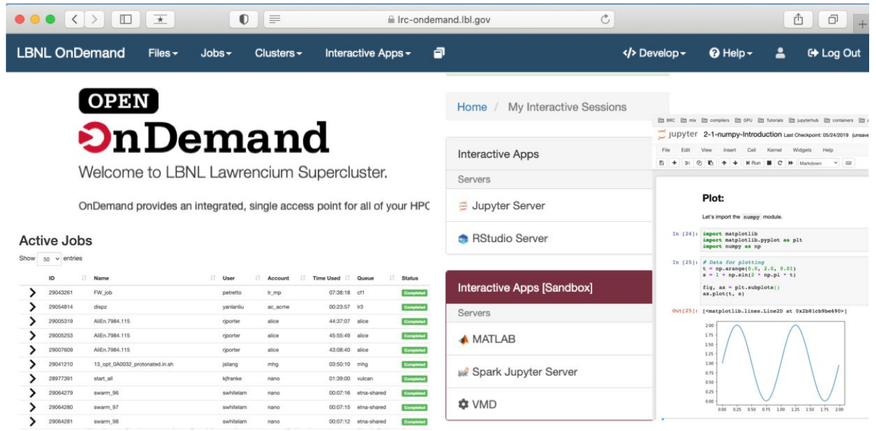
- webportal




```
ssh $USER@$IP -p $PORT
```

Accessing resources: move files from/to remote clients

- GUI (Graphical User Interfaces):
  - WinSCP
  - MobaXterm
  - FileZilla
  - smb mounts, if available
  - webportal
- CLI (Command Line Interfaces):

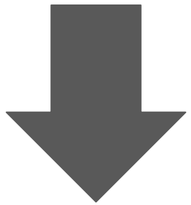



```
scp -oPort $PORT /folder/XX $USER@$IP:/folder/YY

## or

sftp -P $PORT $USER@$IP
```

Compiling

Running interactive jobs

- **never** compile, work or execute jobs on the login node
- **never** ssh directly into computing nodes



USE INTERACTIVE COMMAND
or
LAUNCH THE JOB TO THE QUEUE

Login nodes dos and don'ts

The login nodes are NOT used for:

- running batch jobs
- performing IO intensive operations
- pre and post processing simulations and/or analysis
- visualize data
- performing memory intensive operations

The login nodes are used for:

- access to the cluster
- access to your home and project directories
- upload your data and/or the code
- download the results
- submit and manage batch jobs
- initiate an interactive job session

Workload Schedulers

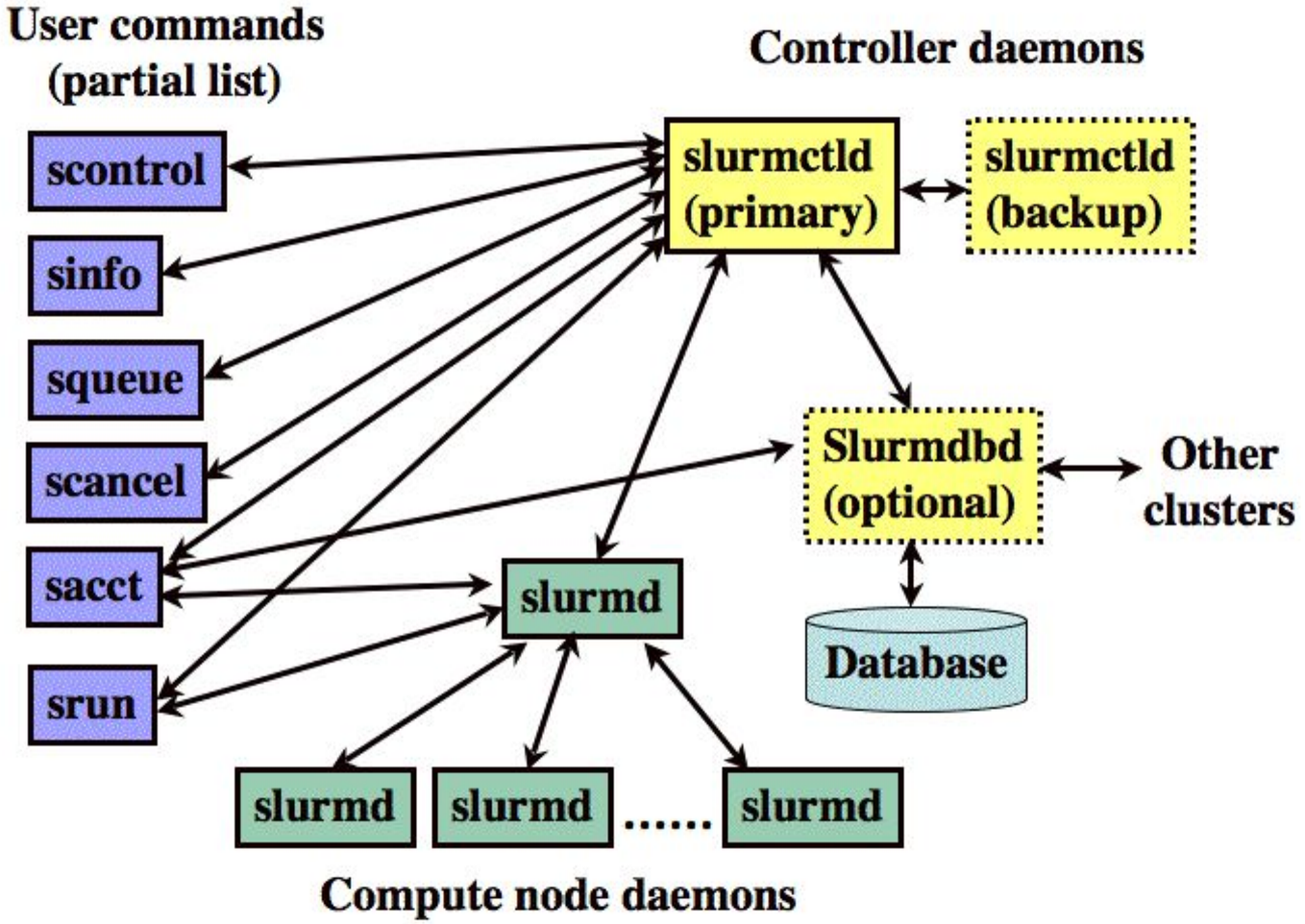
- LSF(IBM Spectrum) --- OpenLAVA
- SGE
- PBS Pro (Altair)
- HTCondor
- Slurm

Slurm as a workload manager

Slurm is an **open-source workload manager** designed for Linux clusters of all sizes. It provides three key functions. First it **allocates exclusive and/or non-exclusive access to resources** (computer nodes) to users for some duration of time so they can perform work. Second, it provides a framework for starting, executing, and monitoring work (typically a parallel job) on a set of allocated nodes. Finally, it arbitrates contention for resources by managing a queue of pending work.

Slurm's design is very modular with dozens of optional plugins. In its simplest configuration, it can be installed and configured in a couple of minutes (see Caos NSA and Perceus: All-in-one Cluster Software Stack by Jeffrey B. Layton). More complex configurations can satisfy the job scheduling needs of world-class computer centers and rely upon a MySQL database for archiving accounting records, managing resource limits by user or bank account, or supporting sophisticated job prioritization algorithms

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


User commands
(partial list)
Controller daemons
scontrol
sinfo
squeue
scancel
sacct
srun
slurmctld
(primary)
slurmctld
(backup)
Slurmdbd
(optional)
Other
clusters
Database
slurmd
slurmd
slurmd
slurmd
.....
Compute node daemons

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slurm workload manager

Slurm cheat-sheet

Command	Description
sacct	Displays accounting data for all jobs.
salloc	Allocate resources for interactive use.
sbatch	Submit a job script to a queue
scancel	Signal jobs or job steps that are under the control of SLURM (cancel jobs or job steps)
scontrol	View SLURM configuration and state
sinfo	View information about SLURM nodes and partitions
sstat	Display statistics of jobs (data from sinfo, squeue and scontrol).
smap	Graphically view information about SLURM jobs, partitions, and set config. param
squeue	View information about jobs located in the SLURM scheduling queue.
srun	Run a parallel job

HPC Now!

Partitions examples

	Time(H)	Priority	Job Preemption
interactive	9	High	none
gui	-	Urgent	none
gui-extra	-	10	none
short	0,5	100	none
medium	48	50	none
large	120	25	Job suspension
extra	-	10	Job suspension

Slurm submit script header example

“sbatch script.slurm” to send the job

```
#!/bin/bash
#SBATCH -J GPU_JOB
#SBATCH --time=01:00:00 # Walltime
#SBATCH -A hpcnow # Project Account
#SBATCH --ntasks=4 # number of tasks
#SBATCH --ntasks-per-node=2 # number of tasks per node
#SBATCH --mem-per-cpu=8132 # memory/core (in MB)
#SBATCH --cpus-per-task=4 # 4 OpenMP Threads
#SBATCH --gres=gpu:2 # GPUs per node
#SBATCH -C kepler ml GROMACS/4.6.5-goolfc-2.6.10-hybrid
srun mdrun_mpi -------
```

Enter the interactive queue or submit the job to the queue

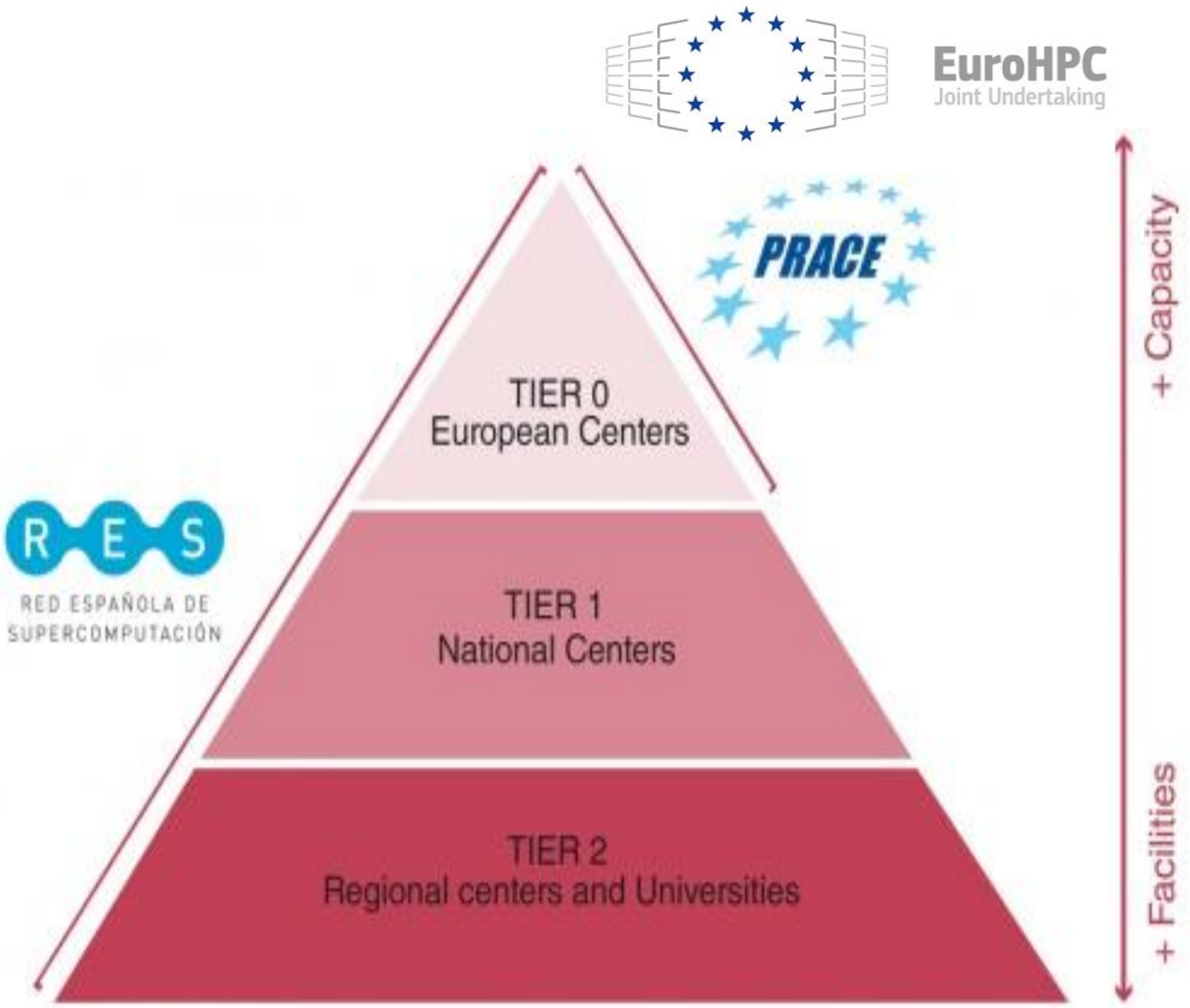
Interactive queue:

```
salloc --time 1:00:00 srun --pty bash
```

Submit to the queue:

```
sbatch slurm-parallel-example.slm
```

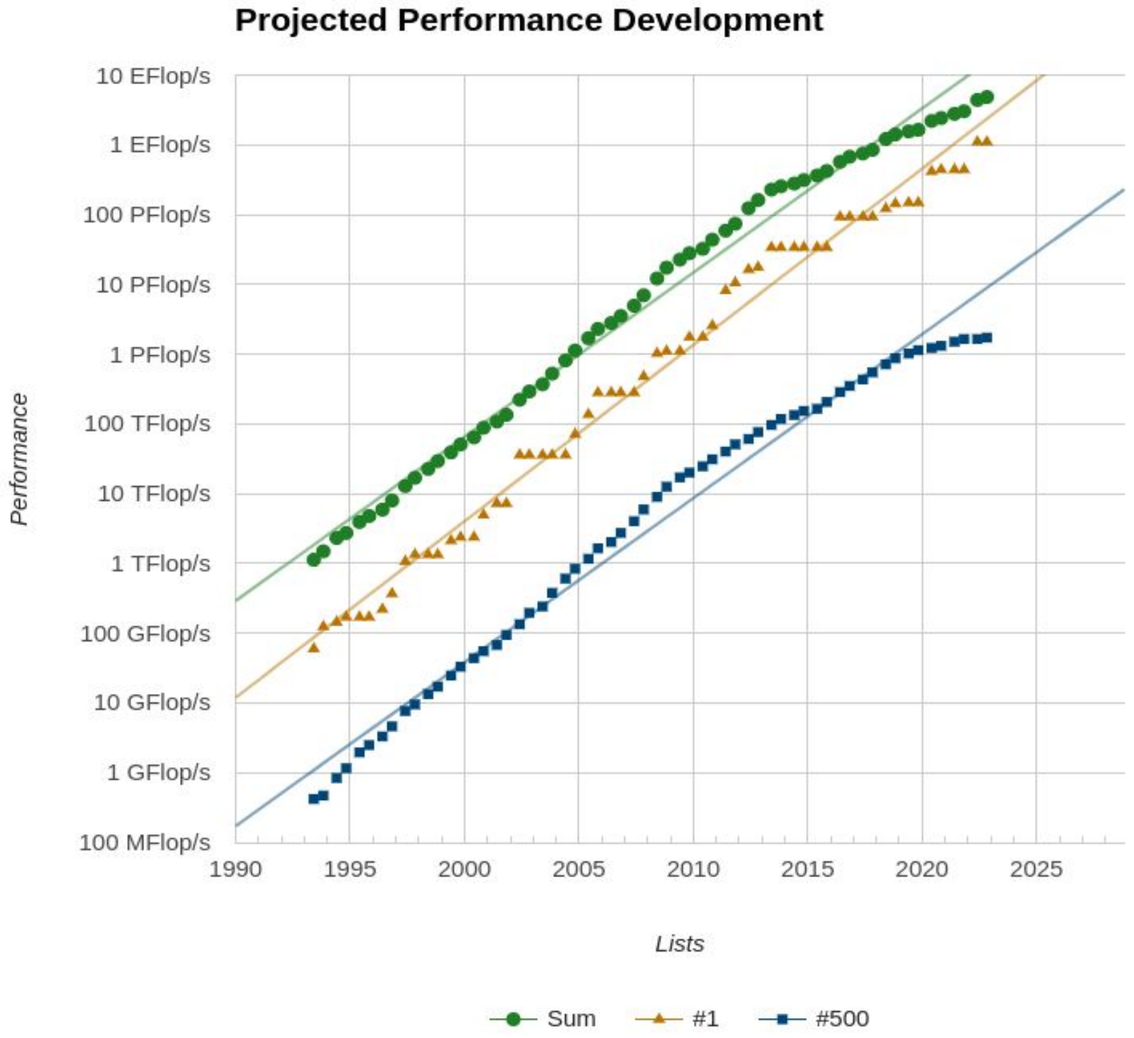
HPC Public centers



TOP 500: Linpack benchmark

www.top500.org

TOP 500
The List.

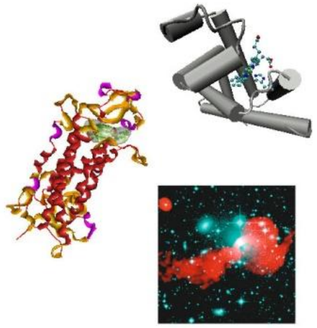


HPC Public Center: CSUC

- SSH Connection
- Different architectures (SMP, DMP)
- MPI and OpenMP
- Software is already installed
- Slurm Scheduler
- Pay-per-use access (When the job is running)

CSUC

Càlcul Científic	Comunicacions	Portals i Repositoris	e-Administració	Promoció
CAP SDF	ANELLA CIENTÍFICA Red IRIS Node Catalunya CATNIX	TDX RECERCAT RACO RECYT mdx padicat CALAIX	Arxiu Certificació Logs Registre Vot	TERAFLOP JOCS TAC TSIUC



Operacions i Seguretat



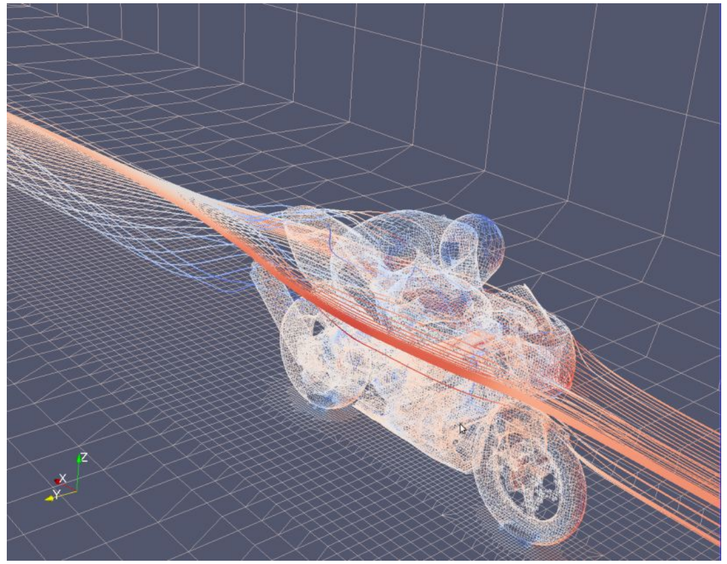


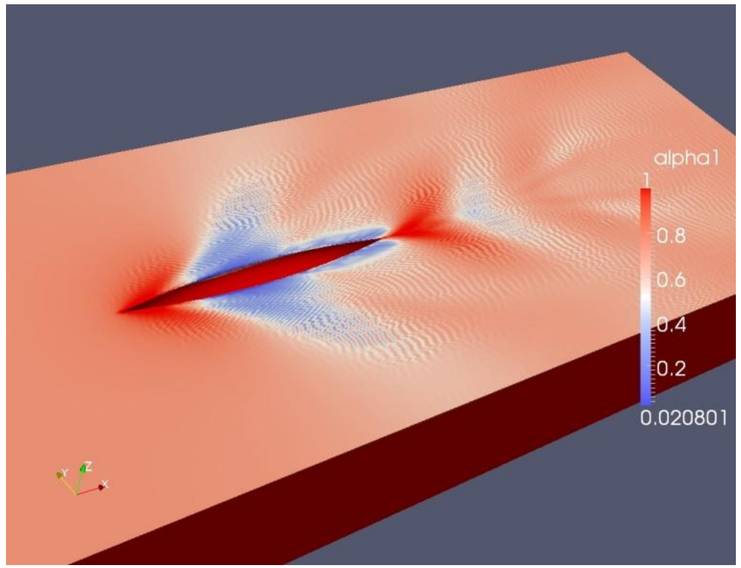


CSIRT
EC-UR
ER-CESCA
SAH
SED
S24x7

Càlcul Científic

- ✓ Proveeix de Càlcul d'Altes Prestacions (CAP) a la comunitat científica i industrial.
- ✓ Gestiona el Servei de Disseny de Fàrmacs (SDF), que ofereix eines per modelitzar molècules d'interès biològic.





Maquinari d'Emmagatzematge

Collserola (2014)

- **10 nodes**
  - Coprocessador Intel Phi
  - 24 (2 cpus amb 12 cores) a 2.6 GHz
  - Memòria
  - Collserola1 -> 512 GB
  - Collserola2-9 -> 256 GB
  - Nodes interconnectats amb Infiniband (56 Gbps).

Bull Sequana X800 - Canigó (2018)

- **Memòria compartida**
  - 384 cores a 2.7 GHz
  - 9 TB memòria
  - 40 TB emmagatzematge
  - Connectada amb Infiniband (100 Gbps) a clúster BeeGFS (emmagatzematge compartit /scratch).

Maquinari d'Emmagatzematge

Bull Sequana X550 - Pirineus 2 (2018)

- **Clúster heterogeni**
- **46 nodes estàndard**
  - 48 cores (2 cpus de 24 cores) a 2.7 GHz
  - 192 GB memòria
  - 4 TB emmagatzematge
- **6 nodes FAT**
  - 48 cores (2 cpus de 24 cores) a 2.7 GHz
  - 384 GB memòria
  - 4 TB emmagatzematge
- **4 nodes amb 2 GPU's**
  - 48 cores (2 cpus de 24 cores) a 2.7 GHz
  - 192 GB memòria
  - 4 TB emmagatzematge
  - GPU's:
    - 3584 nuclis CUDA
    - 12 GB de memòria
    - Rendiment de 4,7 Tflop/S
- **4 nodes amb processadors Intel KNL 7250**
  - 68 cores a 1,4 GHz
  - 384 GB memòria
  - 4 TB emmagatzematge

Tots els nodes estan interconnectats a clúster BeeGFS (emmagatzematge compartit /scratch) mitjançant Infiniband (100 Gbps).

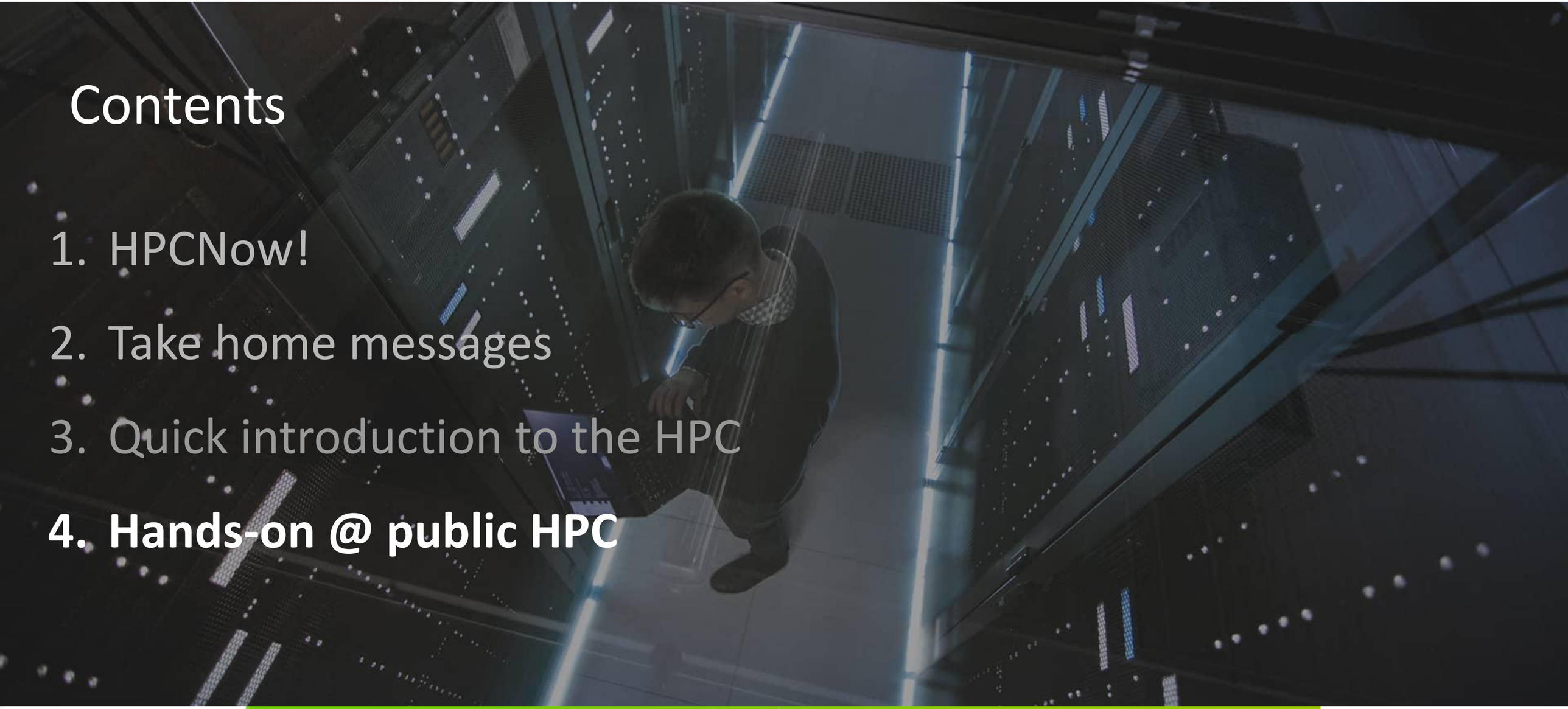
Aquesta serà la màquina per defecte on s'enviaran tots els càlculs que no tinguin requeriments especials.

Best practices

- NEVER run scripts outside of Workload scheduler
- Use the short or interactive queue to test your simulations
- Work on `/shared or /scratch` for light i/o jobs
- Work on `/tmp` for intensive i/o jobs
- Store temporary files on `/scracth`
- Move important files to `/projects`

Books

- Introduction to high-performance scientific computing (2nd edition), by Victor Eijkhout, Lulu, 2015
- Introduction to High Performance Computing for Scientists and Engineers, Hager, Wellein, CRC Press, 2010.
- High Performance Computing, Sterling, Anderson, Brodowicz, Morgan Kaufmann, 2017.



Contents

1. HPCNow!
2. Take home messages
3. Quick introduction to the HPC
4. **Hands-on @ public HPC**

Hands-on @ CSUC

- Get data from github
- Access login node
- Explore environment
- Execute scripts through SLURM
  1. Serial
  2. OpenMP
  3. MPI
  4. Hybrid

Get data from GitHub

Get the data from GitHub - or from the folder 2023UB-formation

Contains all the scripts to run, a README and the list of command to be run.

```
git clone https://github.com/kErica/2023UB-formation.git
```

Access the cluster

User: curs$NUM [1..23]
Password: c1rs$NUM (for example curs24 password c1rs24)

Change the password at first login: 8 characters, 1 uppercase , 1 lowercase, 1 number, 1 special character.

```
## login

ssh curs$NUM@hpc.csuc.cat -p 2122
```

Access and move the data

Moving the data from source to destination and access CSUC cluster

```
## transfer files
scp -rp -P 2122 2023UB-formation curs$NUM@hpc.csuc.cat:/home/curs$NUM

## or
cd 2023UB-formation
sftp -oPort=2122 <YOUR_USERNAME>@hpc.csuc.cat
mput -R *
```

Explore the environment

In the login node you can see:

- available resources
- scheduler partition
- access storage

```
hpcnow1@login2:/home/hpcnow1>df -h
Filesystem                      Size  Used Avail Use% Mounted on
/dev/vda1                       7.9G  6.7G  1.2G  86% /
devtmpfs                        7.8G     0  7.8G   0% /dev
tmpfs                           7.8G     0  7.8G   0% /dev/shm
tmpfs                           7.8G  641M  7.2G   9% /run
tmpfs                           7.8G     0  7.8G   0% /sys/fs/cgroup
cabreraSas.xe:/cap_prod/prod    3.5T  3.5T   81G  98% /prod
netapp.xe:/vol/cap_nfs/home     7.0T  6.5T  537G  93% /home
netapp.xe:/vol/cap_sdf/sdf      240G  189G   52G  79% /home/sdf
192.168.93.123:/slurm_cap       2.0G     0  2.0G   0% /etc/slurm
192.168.93.122:/cap_dades        10T  4.1T  6.0T  41% /dades
192.168.93.201:/ubbiomed/        25T  8.9T   17T  36% /dades/ubbiomed
beegfs_nodev                     175T  159T   17T  91% /mnt/beegfs
```

Explore the scheduler commands

You can also check the scheduler commands and partitions in login nodes

```
sacct## Displays accounting data for all jobs.
salloc  ## Allocate resources for interactive use.
sbatch  ## Submit a job script to a queue
scancel ## Signal jobs or job steps that are under the control of SLURM (cancel jobs or job
steps)
scontrol  ## View SLURM configuration and state
sinfo## View information about SLURM nodes and partitions
sjstat  ## Display statistics of jobs ( data from sinfo, squeue and scontrol).
smap ## Graphically view information about SLURM jobs, partitions, and set config. param
squeue  ## View information about jobs located in the SLURM scheduling queue.
srun ## Run a parallel job
```

Get an interactive session

Check the options of the application and request 4h of interactive time

```
salloc -h
Usage: salloc [OPTIONS...] [command [args...]]

salloc --time 4:00:00 srun --pty bash

## where installed
interactive -t 4
```

Execute scripts through SLURM

Send a serial job (not parallel) and an array of jobs to the scheduler

```
>cat serial.slm

#!/bin/bash
#SBATCH -J Serial           # Jobname
#SBATCH --ntasks=1          # Processors
#SBATCH --time=10:00        # Walltime
#SBATCH --mem-per-cpu=2G    # memory/cpu
#SBATCH -o serial-%j.out
#SBATCH -e serial-%j.err
#SBATCH --reservation=hpcnow

srun sleep 30
srun echo "My first serial Slurm job"
```

Execute scripts through SLURM

Send a serial job (not parallel) and an array of jobs to the scheduler

```
>cat serial-array.slm

#!/bin/bash
#SBATCH -J Serial           # Jobname
#SBATCH --ntasks=1          # Processors
#SBATCH --time=10:00        # Walltime
#SBATCH --mem-per-cpu=2G    # memory/cpu
#SBATCH -o serial-%j.out
#SBATCH -e serial-%j.err
#SBATCH --reservation=hpcnow

srun sleep 30
srun echo "My first serial Slurm job - ${SLURM_ARRAY_TASK_ID}"
```

Execute scripts through SLURM

Send a serial job (not parallel) and an array of jobs to the scheduler

```
## send a job to the queue
sbatch serial.slm

## send an array of job to the queue
sbatch --array=0-9 serial-array.slm
```

Execute scripts through SLURM

Execute an OpenMP job (parallel, no MPI)

```
>cat openmp.slm

#!/bin/bash
#BATCH -J OMP
#SBATCH --time=10:00       # Walltime
#SBATCH -n 16                # Number of cores
#SBATCH -N 1                 # Number of nodes
#SBATCH --reservation=hpcnow
#SBATCH --mem-per-cpu=800M # memory/cpu

export OMP_NUM_THREADS=16

/home/$USER/2023UB-formation/02-OpenMP/hello > hello.log
```

Execute scripts through SLURM

Execute an OpenMP job (parallel, no MPI)

```
sbatch openmp.slm

## check the output
ls # note that the default outfile is created for slurm
cat hello.log # the output file mentioned in the script
```

Execute scripts through SLURM

Execute an job with different options: **openMP**, hybrid and MPI

```
#!/bin/bash

#SBATCH -J gmx_omp_8
#SBATCH -e gmx_omp_8.%j.err
#SBATCH -o gmx_omp_8.%j.out
#SBATCH -N 1
#SBATCH -n 1
#SBATCH -c 8
#SBATCH --mem-per-cpu=2G
#SBATCH -t 30
#SBATCH --reservation=hpcnow

module load gromacs/2018.3

OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK:-1}

cp ${SLURM_SUBMIT_DIR}/ion_channel.tpr ${SCRATCH}
cd ${SCRATCH}

srun gmx_mpi mdrun -ntomp $OMP_NUM_THREADS -ntomp_pme 0 -s ion_channel.tpr

cp md.log ${SLURM_SUBMIT_DIR}/omp-md.${SLURM_JOB_ID}.log
```

Execute scripts through SLURM

Execute an job with different options: **openMP**, hybrid and MPI

```
sbatch gmx_omp_8.slm

## check the output
## check the errors and logs
```

Execute scripts through SLURM

Execute an job with different options: openMP, **hybrid** and MPI

```
#!/bin/bash

#SBATCH -J gmx_hyb_8
#SBATCH -e gmx_hyb_8.%j.err
#SBATCH -o gmx_hyb_8.%j.log
#SBATCH -N 2
#SBATCH --ntasks-per-node 1
#SBATCH -c 4
#SBATCH --mem-per-cpu=2G
#SBATCH -t 30
#SBATCH --reservation=hpcnow

module load apps/gromacs/2018.3

OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK:-1}

cp ${SLURM_SUBMIT_DIR}/ion_channel.tpr ${SCRATCH}
cd ${SCRATCH}

srun gmx_mpi mdrun -ntomp $OMP_NUM_THREADS -npme 0 -ntomp_pme 0 -s ion_channel.tpr

cp md.log ${SLURM_SUBMIT_DIR}/hyb-md.${SLURM_JOB_ID}.log
```

Execute scripts through SLURM

Execute an job with different options: openMP, **hybrid** and MPI

```
sbatch gmx_hyb_8.slm

## check the output
## check the errors and logs
```

Execute scripts through SLURM

Execute an job with different options: openMP, hybrid and **MPI**

```
#!/bin/bash

#SBATCH -J gmx_mpi_8
#SBATCH -e gmx_mpi_8.%j.err
#SBATCH -o gmx_mpi_8.%j.log
#SBATCH -N 2
#SBATCH -n 4
#SBATCH -t 30
#SBATCH --mem-per-cpu=2G
#SBATCH --reservation=hpcnow

module load apps/gromacs/2018.3

OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK:-1}

cp ${SLURM_SUBMIT_DIR}/ion_channel.tpr ${SCRATCH}
cd ${SCRATCH}

srun gmx_mpi mdrun -ntomp $OMP_NUM_THREADS -npme 0 -ntomp_pme 0 -s ion_channel.tpr

cp md.log ${SLURM_SUBMIT_DIR}/mpi-md.${SLURM_JOB_ID}.log
```

Execute scripts through SLURM

Execute an job with different options: openMP, hybrid and **MPI**

```
sbatch gmx_mpi_8.slm

## check the output
## check the errors and logs
```

Execute scripts through SLURM

Comparison OpenMP,

```
#SBATCH -J gmx_omp_8
#SBATCH -e gmx_omp_8.%j.err
#SBATCH -o gmx_omp_8.%j.out
#SBATCH -N 1
#SBATCH -n 1
#SBATCH -c 8
#SBATCH --mem-per-cpu=2G
#SBATCH -t 30
```

1 node (-N)
1 task (-n) - *default*
8 cpus per task (-c)

hybrid and

```
#SBATCH -J gmx_hyb_8
#SBATCH -e gmx_hyb_8.%j.err
#SBATCH -o gmx_hyb_8.%j.log
#SBATCH -N 2
#SBATCH --ntasks-per-node=1
#SBATCH -c 4
#SBATCH --mem-per-cpu=2G
#SBATCH -t 30
```

2 nodes (-N)
1 task per node (--ntasks)
4 cpus per task (-c)

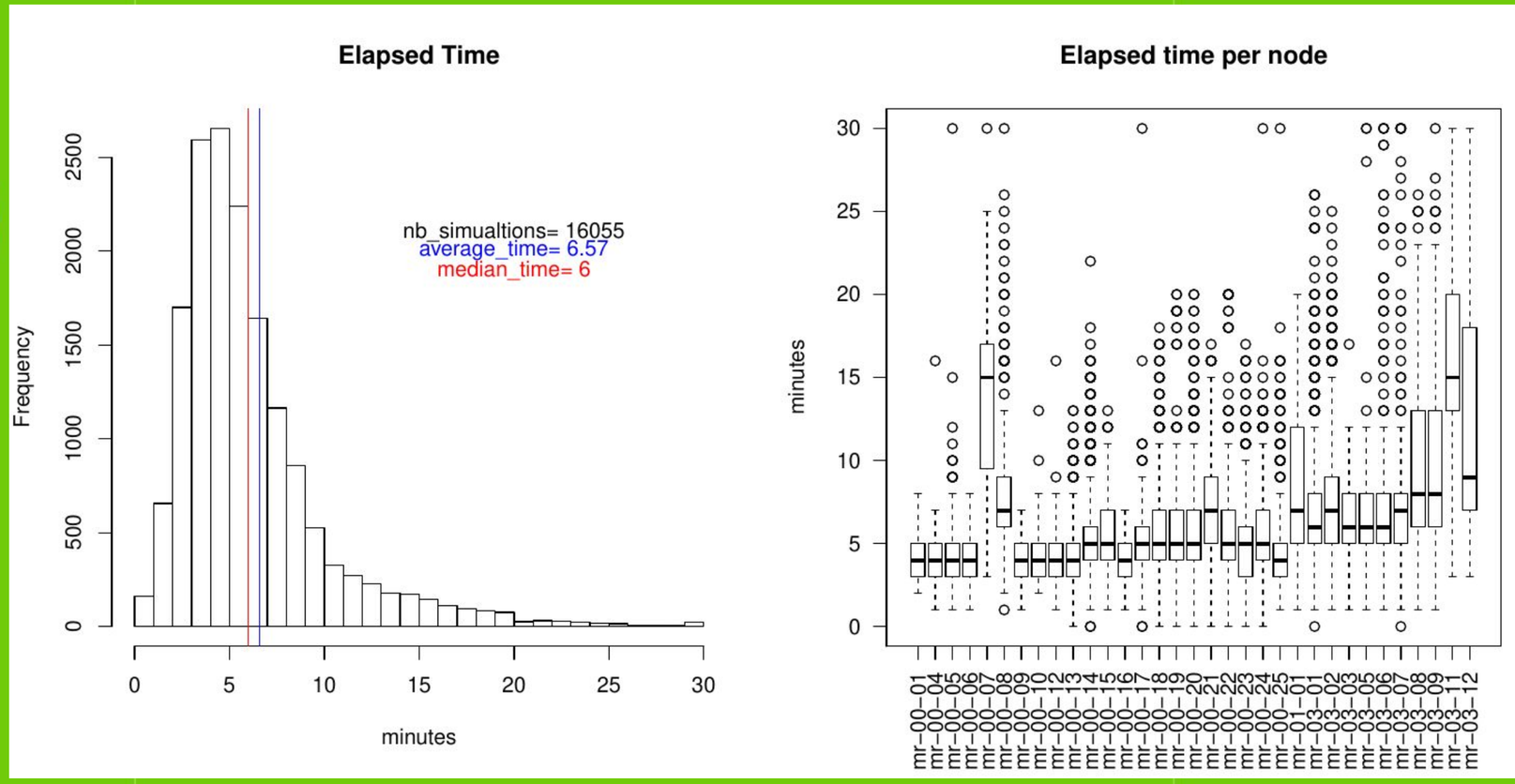
MPI job Slurm parameters

```
#SBATCH -J gmx_mpi_8
#SBATCH -e gmx_mpi_8.%j.err
#SBATCH -o gmx_mpi_8.%j.log
#SBATCH -N 2
#SBATCH -n 4

#SBATCH -t 30
#SBATCH --mem-per-cpu=2G
```

2 nodes (-N)
4 tasks (-n)

Questions?



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