

# Introduction to high-performance computing

Frédéric Wautelet  
CÉCI HPC training 2020

# Outline

MATLAB on  
the cluster

Accelerators/Co-processors

Python for HPC

Slurm workload manager

Share memory (OpenMP)

Message passing (MPI)

Checkpointing

Debugging and profiling

Compilers and libraries

Introduction to GNU/Linux and the command line

Introduction to HPC

- 19/10 - Bernard Van Renterghem, "**Introduction to Linux and the command line**"
- 20/10 - Juan Cabrera, Olivier Mattelaer, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"
- 20/10 - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"
- 20/10 - Damien François, "**Introduction to scientific software development and deployment**"
- 21/10 - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"
- 21/10 - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"
- 22/10 - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"
- 22/10 - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"
- 22/10 - Damien François, "**Introduction to parallel computing**"
- 27/10 - Olivier Mattelaer, "**Introduction to C programming language**"
- 27/10 - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"
- 28/10 - Bernard Van Renterghem, "**Debugging and profiling scientific code**"
- 28/10 - Bernard Van Renterghem, "**Commercial optimized libraries**"
- 29/10 - Orian Louant, "**Parallel programming with MPI**"
- 
- 09/11 - Jérôme de Favereau, "**Introduction to Python**"
- 09/11 - Orian Louant, "**Parallel programming with OpenMP**"
- 10/11 - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"
- 10/11 - Orian Louant, "**Directive Based Parallel programming on GPU**"
- 10/11 - Pieter David, "**Machine learning with Tensorflow: an introduction**"
- 12/11 - Damien François, "**Preparing, submitting and managing jobs with Slurm**"
- 12/11 - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"
- 17/11 - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"
- 18/11 - Damien François, "**Introduction to data storage and access**"
- 18/11 - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"
- 24/11 - Michael Waumans, "**Introduction to BigData tools**"
- 24/11 - Olivier Mattelaer, "**Introduction to code versioning**"
- 25/11 - Damien François, "**Efficient use of Matlab on the cluster**"
- 25/11 - Ariel Lozano, "**Efficient use of Python on the clusters**"

# Introduction to HPC

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the cluster

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Debugging and profiling

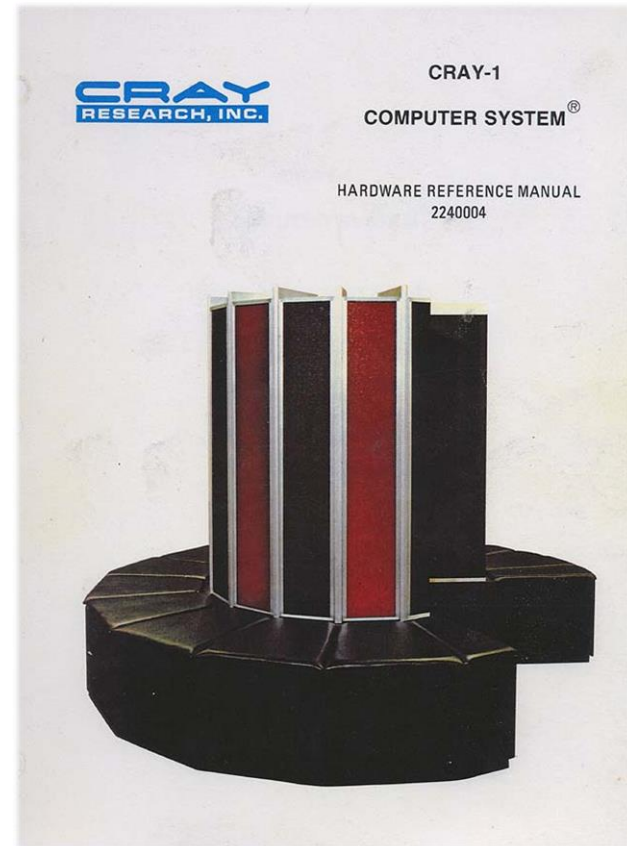
Compilers and libraries

Introduction to GNU/Linux and the command line

Introduction to HPC

# High Performance Computing

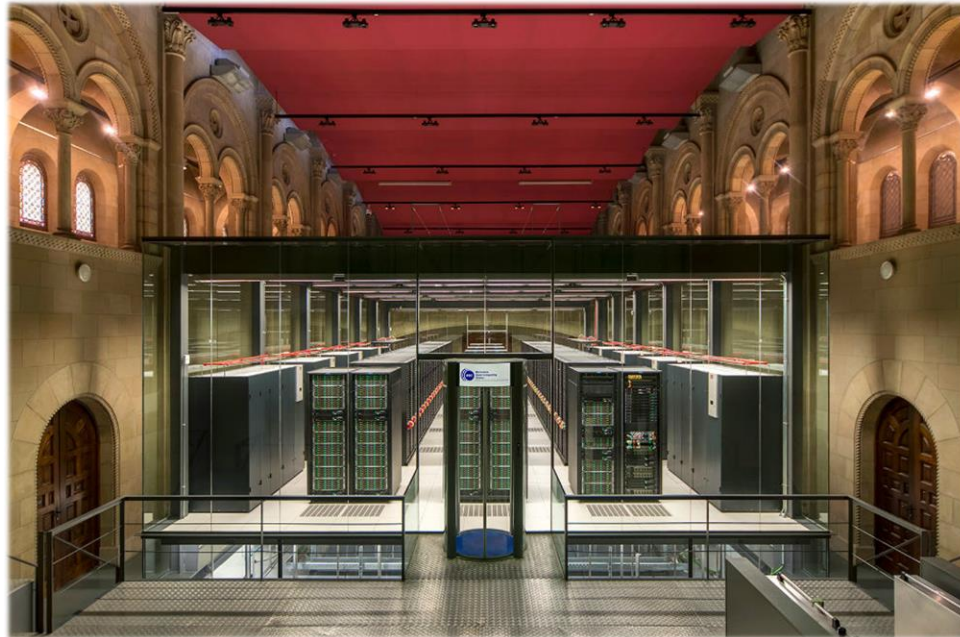
- High-performance computing (HPC) uses supercomputers and computer clusters to solve advanced computation problems.



**Cray-1a (1977)**  
250 MFlops

# Cluster

- A computer cluster is a group of linked computers, working together closely so that in many respects they form a single computer.

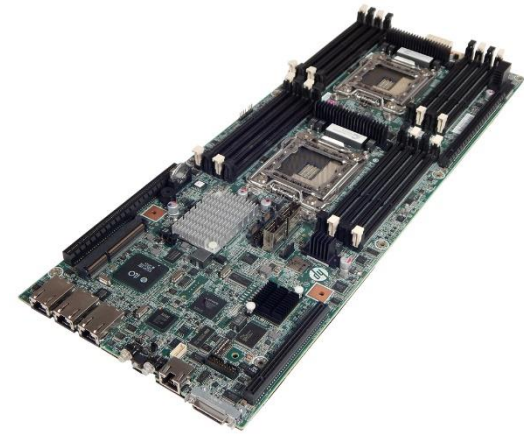


**MareNostrum 4 (2017)**

13.7 PFlops

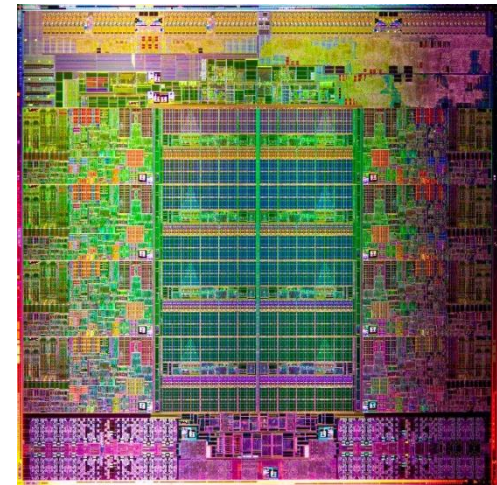
# Nodes and Cores

- Compute node
  - Part of a cluster
  - Equivalent to a high-end workstation



HP SL230s main board

- Core
  - A processor (CPU)
  - Multiple cores per socket



Intel Sandy-Bridge 8-core die

# flop/s

- Floating Point Operations per Second

**Gflop/s =  $10^9$  flop/s**

**Tflop/s =  $10^{12}$  flop/s**

**Pflop/s =  $10^{15}$  flop/s**

**Eflop/s =  $10^{18}$  flop/s**



# TOP500



- Fugaku
  - RIKEN Center for Computational Science, Kobe, Japan
  - TOP500 #1 (June 2020)
  - ~7,300,000 cores
  - 400+ Pflop/s
  - ~30 MW



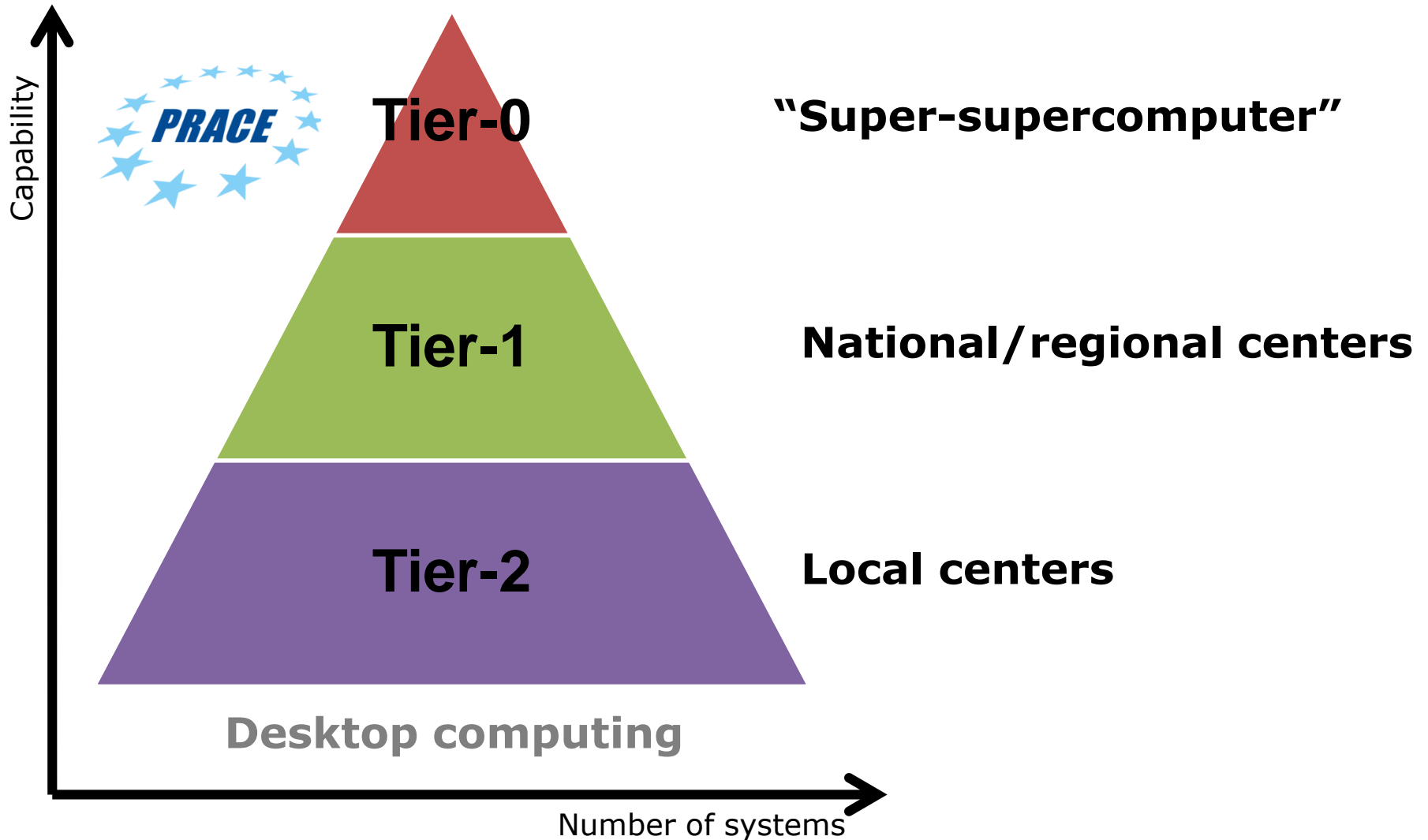
# HPC to Exascale



- Exascale
  - Eflo/s =  $10^{18}$  flo/s
  - Tianhe 3, National Supercomputing Center, Guangzhou, China



# The European HPC ecosystem



# PRACE

- Partnership for Advanced Computing in Europe
- 30 supercomputer in 25 countries
- Call for Proposals for Project Access



# Tier-0



- “super-supercomputers”
- Piz Daint
  - Swiss National Supercomputing Centre (CSCS), Lugano
  - TOP500 #10 (June 2020)
  - ~400,000 cores
  - 27 Pflop/s
  - 2 MW

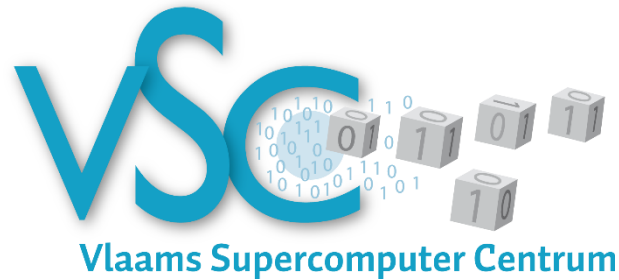


# Tier-1

- Tier-1
  - National and/or regional supercomputers
  - Allows the build-up of the necessary expertise and knowledge required to use a tier-0 supercomputer

# HPC in Belgium

- Vlaamse Gemeenschap/Vlaams Gewest
  - Vlaams Supercomputer Centrum (VSC)



- Fédération Wallonie-Bruxelles
  - Consortium des Équipements de Calcul Intensif (CÉCI)



# Vlaamse Gemeenschap Vlaams Gewest

- Tier-1: BrENIAC
  - KU Leuven
  - 16,000 cores
  - ~600 Tflop/s
  - 5.5 M€



- Tier-2
  - Clusters available in UA, VUB, UGent, KU Leuven and UHasselt



# Fédération Wallonie-Bruxelles

- Tier-1: Zenobe

- CENAERO
- 14,000 cores
- ~300 Tflop/s
- 5.5 M€

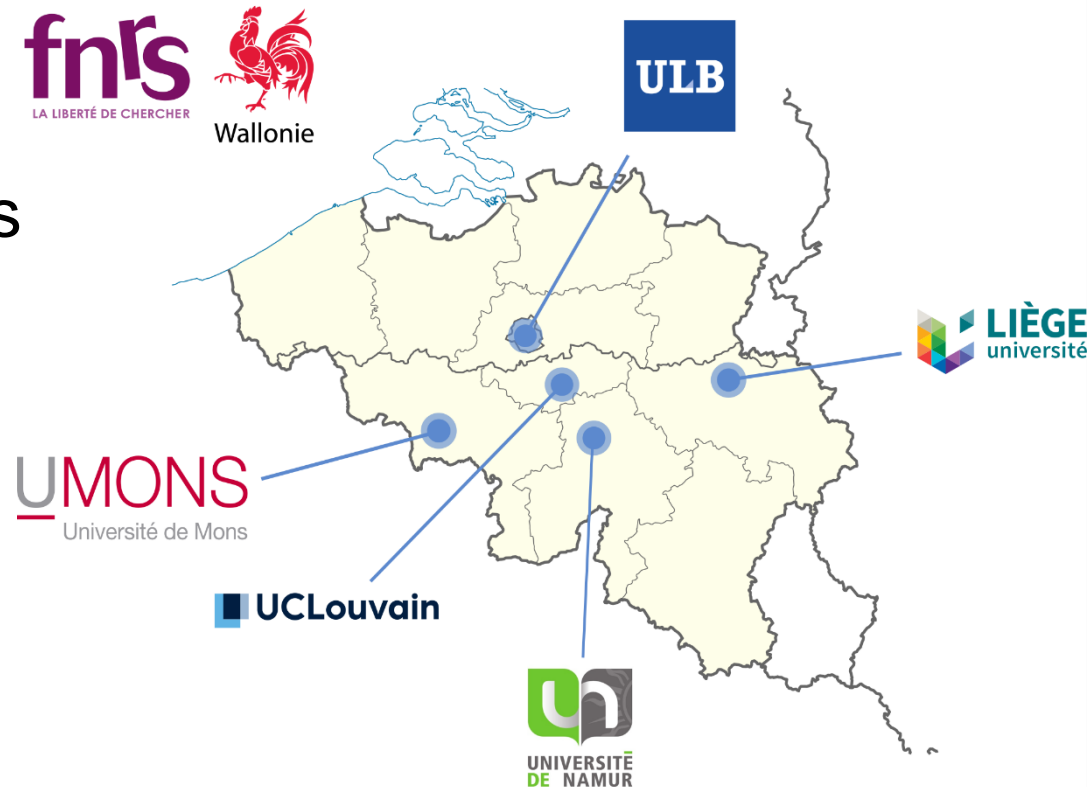


- Tier-2: CÉCI

- UCLouvain
- ULB
- ULiège
- UMONS
- UNamur
- 100+ Tflop/s



- Consortium des Équipements de Calcul Intensif
- Five universities
- Tier-2 HPC clusters





**Lemaitre 3**  
**2008 cores**  
 Skylake  
 Haswell

95 GB RAM

100Gb/s OPA

**Q2 2018**



**NIC5**  
**4672 cores**  
 Epyc

1 TB RAM

100Gb/s IB

**Q4 2020**



**Vega**  
**2112 cores**  
 Bulldozer

256 GB RAM

10Gb/s IB



**Hercules 2**  
**1536 cores**  
 Sandybridge  
 Epyc

2 TB RAM

10 GbE

**Q3 2019**



**Dragon 2**  
**592 cores**  
 Skylake  
 Tesla V100

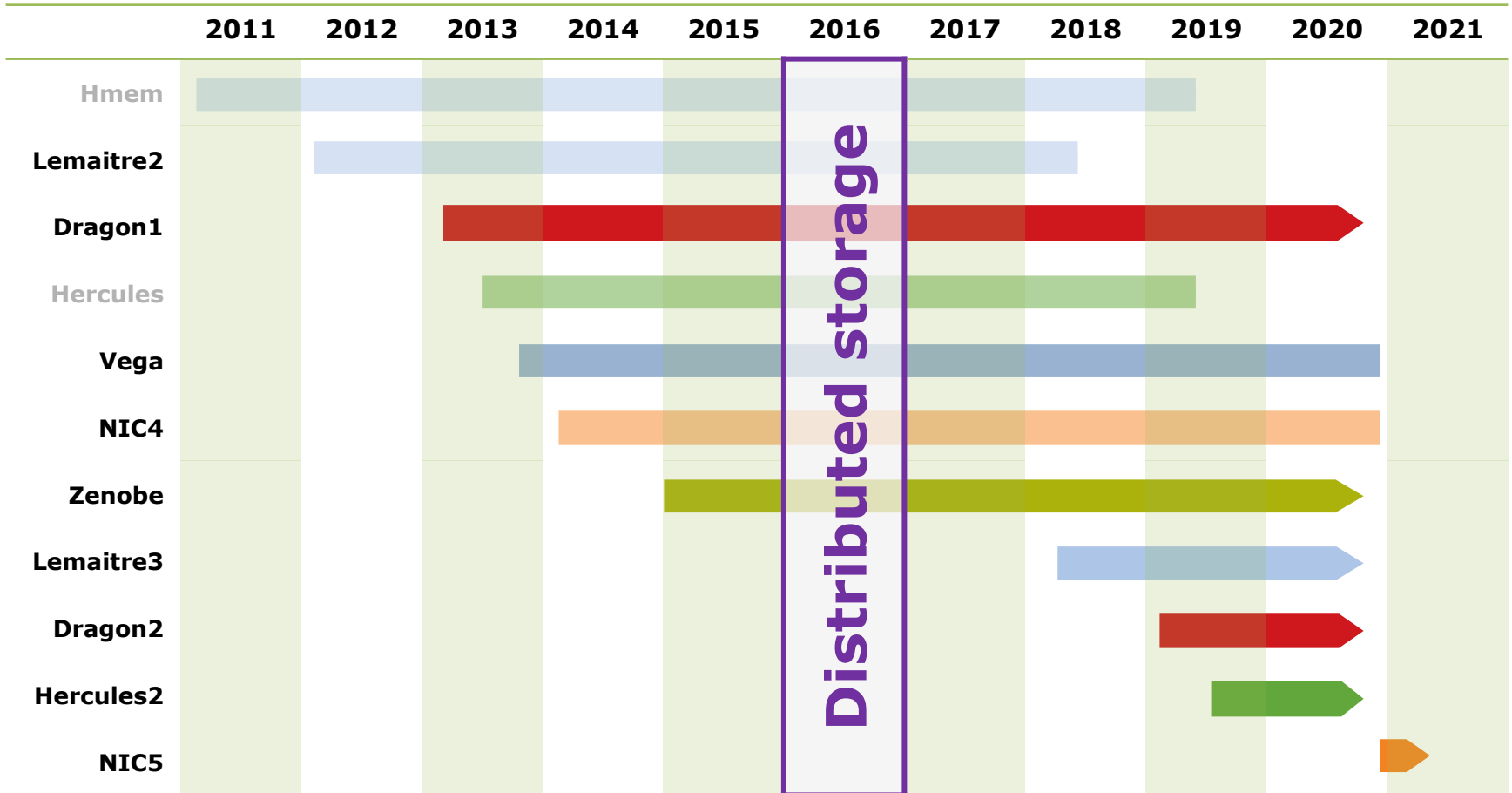
384 GB RAM

10 GbE

**Q1 2019**

**10920 cores total**

# The CÉCI upgrade



LA LIBERTÉ DE CHERCHER

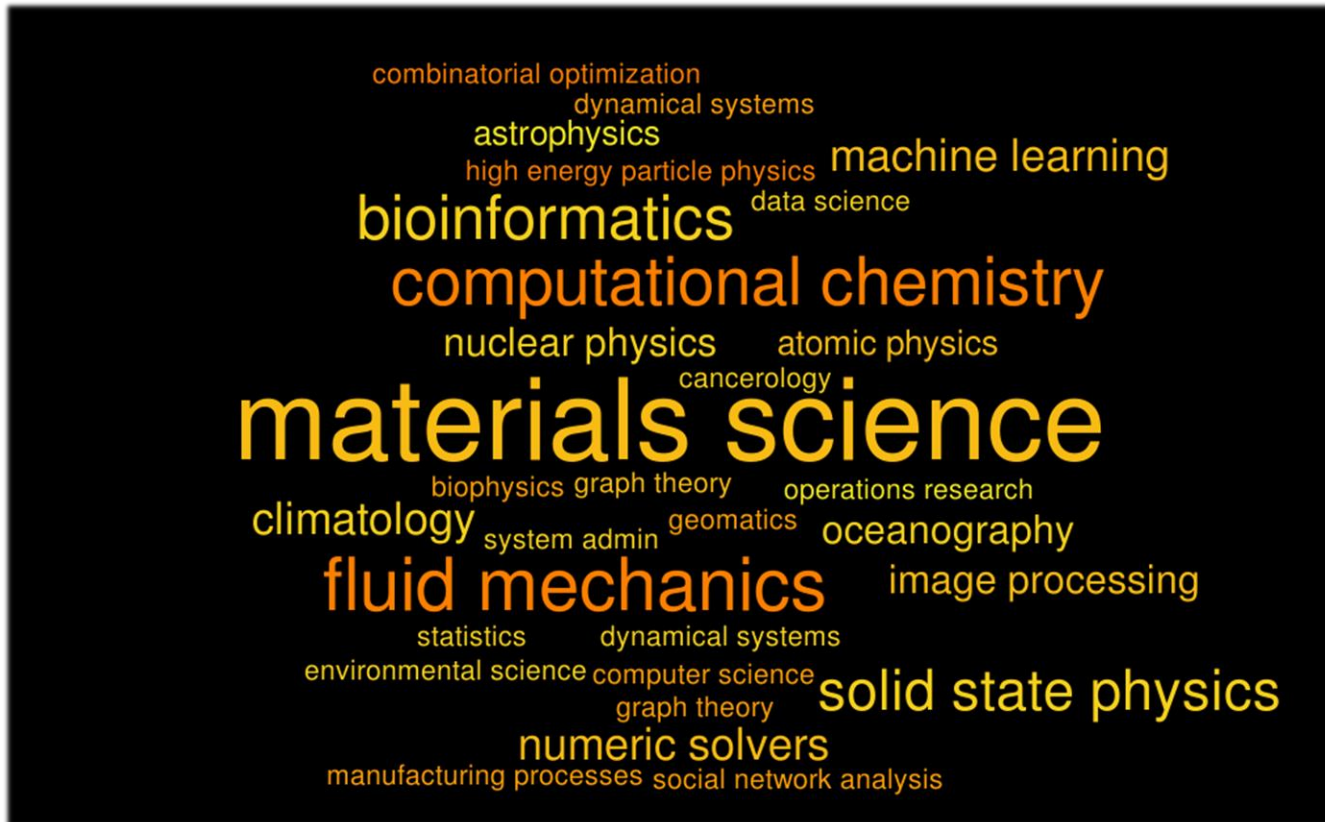


RÉGION WALLONNE



# Users

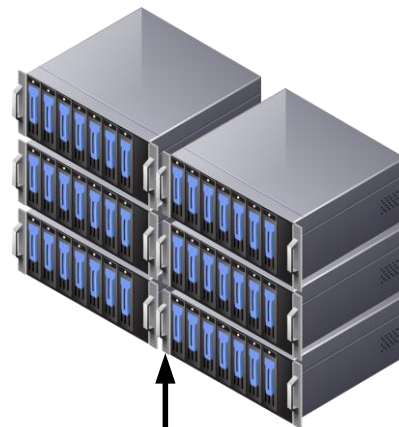
- 400+ actives users
- Fields of applications



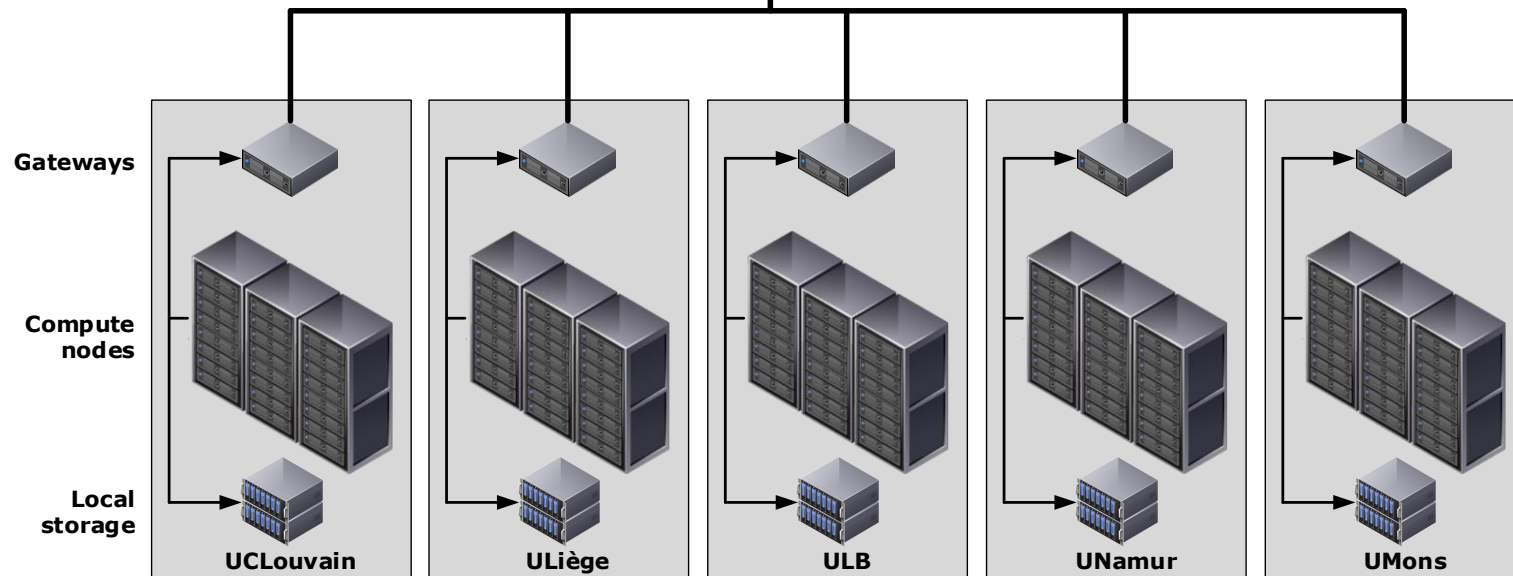
# CÉCI distributed storage



- Distributed storage solution
- Visible from all the frontends and compute nodes of all CÉCI clusters
- 400 TB net



IBM  
Spectrum  
Storage

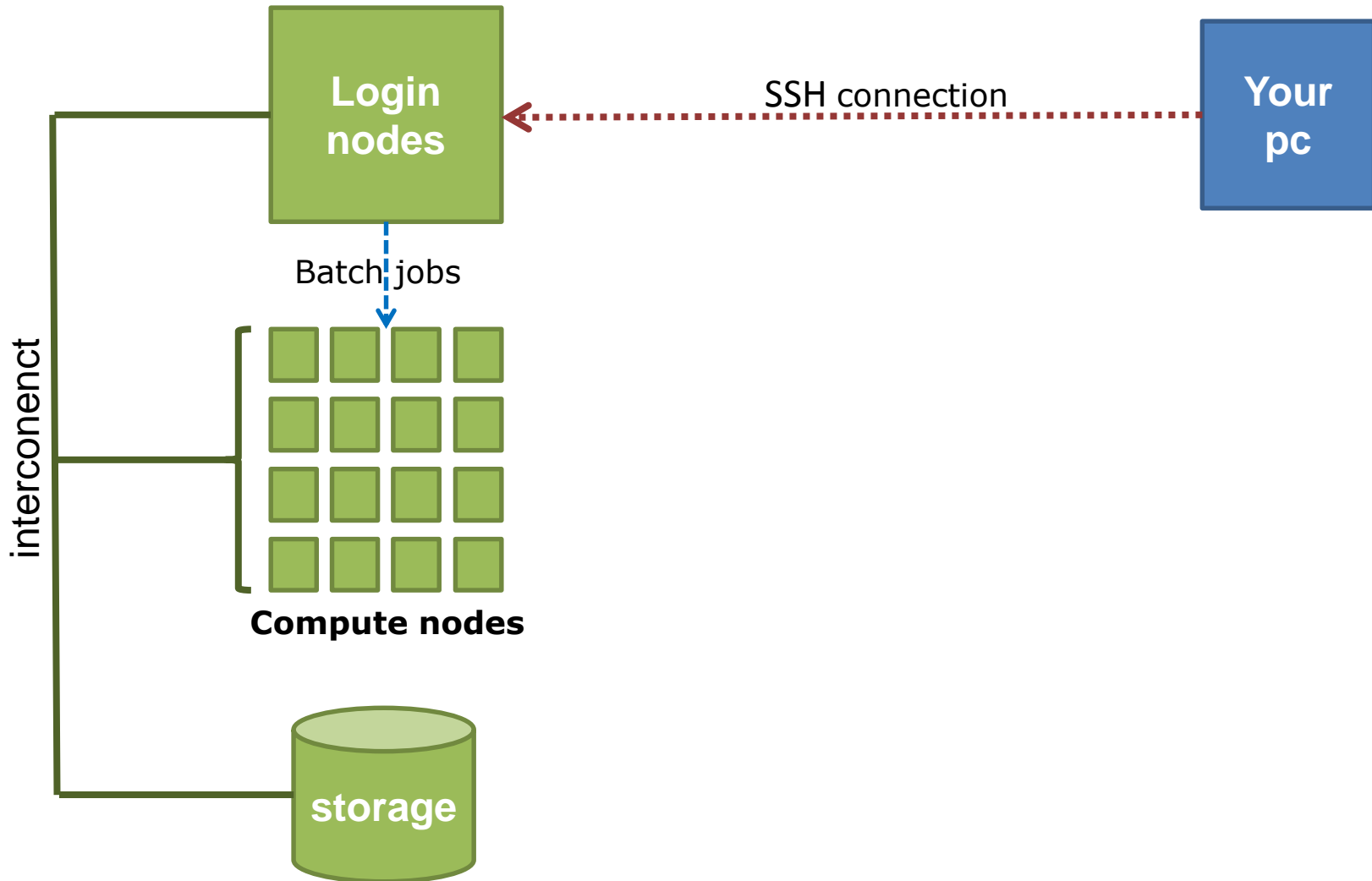


# CÉCI distributed storage



- Common storage directories for all CÉCI clusters
- No need to transfer data between clusters with scp
- Common software repository
- Almost all software installed on any cluster are available on all clusters

# A cluster in a nutshell



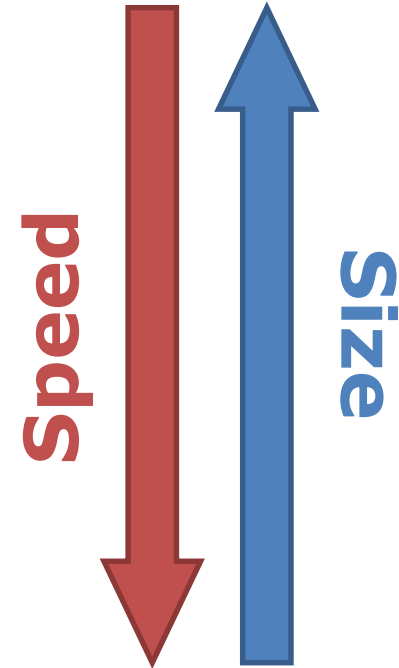


# Login node

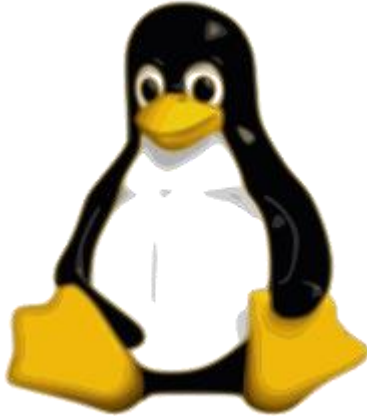
- Submit jobs to batch system
- Manage your files
- Interactive work at small scale
- CÉCI login nodes
  - hercules2.ptci.unamur.be
  - dragon2.umons.ac.be
  - lemaitre3.cism.ucl.ac.be
  - nic4.segi.ulg.ac.be
  - vega.ulb.ac.be

# Four levels of storage

- **\$CECIHOME**
  - 400 TB
  - CÉCI distributed storage
- **\$HOME**
  - Programs and scripts
- **\$WORKDIR**
  - Input and output data
- **\$LOCALSCRATCH or \$GLOBALSCRATCH**
  - Job temporary data



# Operating system



- All CÉCI cluster are running GNU/Linux



# CentOS

- Linux CentOS 7
  - Red Hat Enterprise Linux (RHEL) compatible

# Clusters at CÉCI

The aim of the Consortium is to provide researchers with access to powerful computing equipment ([clusters](#)). Clusters are installed and managed locally at the different sites of the universities taking part in the Consortium, but they are accessible by all researchers from the member universities. A single login/passphrase is used to access all clusters through SSH.

All of them run Linux, and use [Slurm](#) as the job manager. Basic parallel computing libraries (OpenMP, MPI, etc) are installed, as well as the optimized computing subroutines (e.g. BLAS, LAPACK, etc.). Common interpreters such as R, Octave, Python, etc. are also installed. See each cluster's FAQ for more details.

Cluster	Host	CPU type	CPU count*	RAM/node	Network	Filesystem**	Accelerator	Max time	Preferred jobs***
<a href="#">Hercules2</a>	UNamur	<a href="#">Epyc</a> 2 GHz <a href="#">SandyBridge</a> 2.20 GHz	1024 (30 x 32 + 2 x 64) 512 (32 x 16)	64 GB..2 TB	<a href="#">10 GbE</a>	<a href="#">NFS</a> 20 TB	None	15 days	serial / ≡ SMP
<a href="#">Dragon2</a>	UMons	<a href="#">SkyLake</a> 2.60 GHz	592 (17 x 32 + 2 x 24)	192..384 GB	<a href="#">10 GbE</a>	<a href="#">RAID0</a> 3.3 TB	4x <a href="#">Volta</a> V100	21 days	serial / ≡ SMP
<a href="#">Lemaitre3</a>	UCL	<a href="#">SkyLake</a> 2.3 GHz <a href="#">Haswell</a> 2.6 GHz	1920 (80 x 24) 112 (4 x 28)	95 GB 64 GB	<a href="#">Omnipath</a>	<a href="#">FHGFS</a> 580 TB	None	2 days 6 hours	≡ MPI
<a href="#">NIC4</a>	ULiège	<a href="#">SandyBridge</a> 2.0 GHz <a href="#">IvyBridge</a> 2.0 GHz	2048 (120 x 16 + 8 x 16)	64 GB	<a href="#">QDR Ib</a>	<a href="#">FHGFS</a> 144 TB	None	3 days	≡ MPI
<a href="#">Vega</a>	ULB	<a href="#">Bulldozer</a> 2.1 GHz	896 (14 x 64)	256 GB	<a href="#">QDR Ib</a>	<a href="#">GPFS</a> 70 TB	None	14 days	serial / ≡ SMP / ≡ MPI
<a href="#">Hercules*</a>	UNamur	<a href="#">SandyBridge</a> 2.20 GHz	512 (32 x 16)	64..128 GB	<a href="#">GbE</a>	<a href="#">NFS</a> 20 TB	None	63 days	serial / ≡ SMP
<a href="#">Dragon1</a>	UMons	<a href="#">SandyBridge</a> 2.60 GHz	416 (26 x 16)	128 GB	<a href="#">GbE</a>	<a href="#">RAID0</a> 1.1 TB	4x <a href="#">Tesla</a> C2075	41 days	serial / ≡ SMP
<a href="#">Lemaitre2*</a>	UCL	<a href="#">Westmere</a> 2.53 GHz	1380 (115 x 12)	48 GB	<a href="#">QDR Ib</a>	<a href="#">Lustre</a> 120 TB	3x <a href="#">Quadro</a> Q4000	3 days	≡ MPI
<a href="#">Hmem*</a>	UCL	<a href="#">MagnyCours</a> 2.2 GHz	816 (17 x 48)	128..512 GB	<a href="#">QDR Ib</a>	<a href="#">FHGFS</a> 30 TB	None	15 days	≡ SMP

# Hercules 2 @ UNamur


- High memory jobs
  - Up to 2 TB
- Long duration job
  - 15 days
- No multi-node jobs
- Large local scratch
  - Up to 8 TB



# HPC @ UNamur

- Local support :
  - Plateforme Technologique en Calcul Intensif (PTCI)
    - Juan CABRERA
    - Frédéric WAUTELET
  - [ptci-support@unamur.be](mailto:ptci-support@unamur.be)
- Other HPC resources
  - Hyades 2
    - 288 cores total
    - Up to 92 GB RAM per node

# Dragon 2 @ UMons

- High performance SMP nodes
- Very long duration job
  - 40+ days
- GPU
  - 4x  NVIDIA Volta V100
- No multi-node jobs



# HPC @ UMons

- Local support :
  - Sébastien KOZLOWSKYJ  
([Sebastien.KOZLOWSKYJ@umons.ac.be](mailto:Sebastien.KOZLOWSKYJ@umons.ac.be))
- Other HPC resources
  - Biovia Materials Studio cluster
    - 144 cores total
    - 192 GB RAM per node
  - HTC cluster
    - 512 cores total
    - Up to 256 GB RAM per node





# Lemaitre 3 @ UCLouvain

- Massively parallel jobs
  - MPI
- I/O intensive jobs
- Short duration job
  - 2 days
- Fast parallel filesystem
  - \$GLOBALSCRATCH



# HPC @ UCLouvain

## CISM



- Local support
  - Institut de Calcul Intensif et de Stockage de Masse ([egs-cism@listes.uclouvain.be](mailto:egs-cism@listes.uclouvain.be))



Thomas Keutgen  
(Head)



Damien François



Olivier Mattelaer



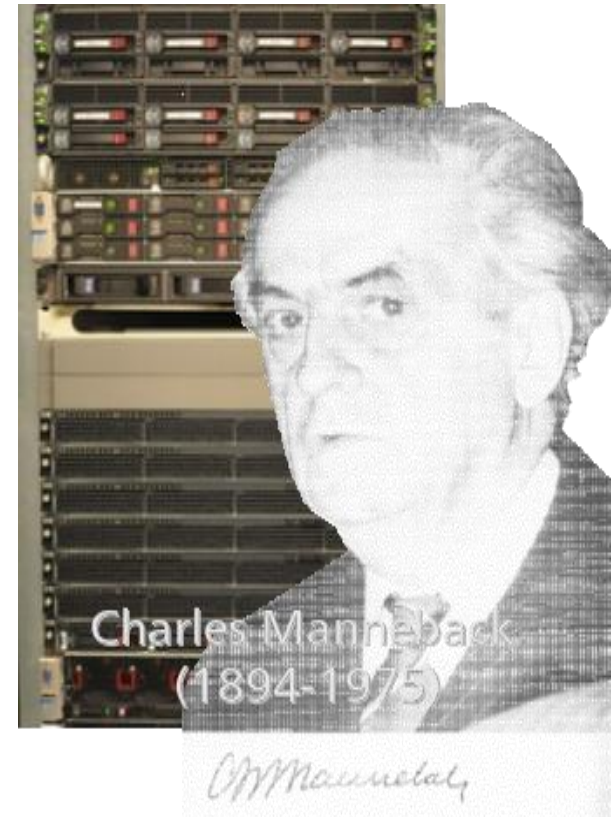
Bernard Van  
Renterghem



Patrick Vranckx

# HPC @ UCLouvain

- Other resources
  - Manneback HPC cluster
    - Heterogeneous hardware
    - +5700 cores
    - 82 Tflop/s
  - Mass storage
    - 317 TB storage total



# NIC5 @ ULiège

- Massively parallel jobs
  - MPI
- I/O intensive jobs
- Short duration job
  - 3 days
- Fast parallel filesystem
  - \$GLOBALSCRATCH
- Available Q4 2020



# HPC @ ULiège

- Local support
  - David COLIGNON  
([David.Colignon@uliege.be](mailto:David.Colignon@uliege.be))
- More info
  - <http://www.ulg.ac.be/nic4>



# Vega @ ULB

- Many single core jobs
  - High-Throughput Computing
- Fast parallel filesystem
  - `$GLOBALSCRATCH=$HOME`
- Retired Q4 2020



# Zenobe

- Massively parallel jobs
  - MPI
- I/O intensive jobs
- Very short duration job
  - 1 day



# How to get a CÉCI account?





## Consortium des Équipements de Calcul Intensif

8 clusters, 10k cores, 1 login, 1 home directory

### About

CÉCI is the 'Consortium des Équipements de Calcul Intensif', a consortium of high-performance computing centers of UCLouvain, ULB, ULiège, UMon, and UNamur. The CÉCI is supported by the F.R.S-FNRS and the Walloon Region. [Read more.](#)



### Quick links

- [Connecting from a Windows computer](#)
- [Connecting from a Linux/Unix or MacOS computer](#)
- [Slurm tutorial and quick start](#)
- [Slurm Frequently Asked Questions](#)
- [Tair-1 Zenobia quickstart](#)
- [Submission Script Generation Wizard](#)

### Quick search

Search site with Google...

### Photo Gallery



### Save the date!

The next CÉCI scientific day will take place on Thursday April 25th in Brussels.  
[More information soon!](#)

### Latest News

MONDAY, 04 JUNE 2018

#### LEMAITRE3 installed at UCL

Lemaitre3 is now operational and replaces Lemaitre2, which will be decommissioned this Summer. It has 80 nodes (SkyLake 2.3 GHz, 24CPUs, 96GB RAM) interconnected with the Intel OmniPath Architecture and more than half a petabyte of scratch space.

TUESDAY, 08 MAY 2018

#### Dragon1 cluster featured in a Belnet article

The Dragon1 CÉCI cluster is highlighted in an interview from Belnet to Chantal Pointet, professor in Information and Communication Technology at the University of Mons.

Follow [this link](#) to read the complete note.

THURSDAY, 03 MAY 2018

#### Survey on Big Data and Machine Learning needs

We are conducting a survey about current and future High Performance Data Analysis (HPDA) works & needs, covering BigData, DeepLearning, MachineLearning, AI & co. Research groups already active in those fields are our primary center of interest. However, those moving or intending to move into those fields are welcome to fill the survey too. Our objective is to identify concrete hardware and software requirements for the future CÉCI Vega2 cluster which will be oriented towards HTC (High Throughput Computing) and HPDA.

You are therefore cordially invited to [follow this link](#) and fill the survey.

MONDAY, 26 MARCH 2018

#### 10th CÉCI Scientific Meeting

The next CÉCI scientific day will take place on May 4th in Namur.  
Details and registration [here](#).

FRIDAY, 16 MARCH 2018

#### PRACE Call for Proposal

PRACE has issued the 17th call for Proposals. Deadline: 2nd May 2018, 10:00 CEST; Stake: Single-year and Multi-year proposals starting 2nd October 2018; Resources: Joliot-Curie, Hazel Hen, JUWELS, Marconi, MareNostrum IV, Piz Daint and SuperMUC.

Let us know if you apply and participate!

# Create/Manage Account



The screenshot shows the top navigation bar of the CÉCI website with links for Clusters, News, Training, FAQ, Documentation, Support, and Contact. The main header area features the C.E.C.I logo and the text "Consortium des Équipements de Calcul Intensif". A red arrow points from the logo area to a modal dialog box titled "Create/Manage Account". The dialog box contains the text: "To create an account your computer must be connected to your university network." and an "Ok" button.

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TUESDAY, 05 MAY 2018

# I want to... create an account

## I want to...

[create an account](#)

You are about to request an account on the CÉCI clusters.

The first step is to enter your email address. You will receive an email with a link to an online form which you will have to fill and submit.

Once your request has been approved, you will receive proper information on how to access the CÉCI clusters.

[renew my account](#)

[join an existing project](#)

[reset my passphrase](#)

[retrieve my private key](#)

[change my email address](#)

[invite a guest or renew a guest account](#)

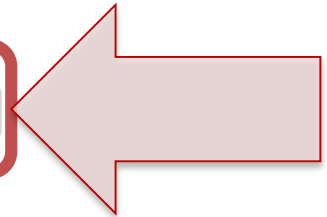
## create an account

**My email address:**

frederic.wautelet

@unamur.be

Send



# That's it

- Click on the link sent to you by email.
- Fill-in the form and hit the “Submit” button
- Get your SSH private key from your email
- Configure your SSH client
- Connect and profit!

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# SSH tools

- Windows
  - PuTTY
  - **MobaXterm**
  - X-Win32
  - OpenSSH on Windows (Windows 10)
- Linux/MacOS
  - ssh
  - scp

# MobaXterm



- Easy to use
- No installation needed
- Command line interface
- Allow use of graphical application remotely
- Files transfer

# Bash



- Shell is the interface between the user and the Linux system
- Interprets and run commands
- For Linux, “Bash” is the default
- Shell scripts



# Modules

- Modify user's environment
- Allow use of application with different versions
- Commands:
  - \$ module load/unload
  - \$ module list
  - \$ module available
  - \$ module spider

# module available



```
----- Meta Modules -----
dot      releases/elic-2017b  releases/2016b  releases/2018a  tis/2018.01 (S,L)
null     releases/2016a          releases/2017b (S,L,D)      releases/2018b  use.own

----- TIS: Toolchain Independent Software (2018.01) -----
EasyBuild/3.5.1  MCR/R2013a  MCR/R2015a  MCR/R2017a  crystal/17-v1.0.1  julia/0.6.3
Java/1.8.0_31    MCR/R2013b  MCR/R2015b  MCR/R2017b  crystal/17-v1.0.2 (D)  julia/1.0.0 (D)
Java/1.8.0_92    MCR/R2014a  MCR/R2016a  MCR/R2018a  (D)  freesurfer/6.0.0  xpress/xp850
Java/1.8.0_121  MCR/R2014b  MCR/R2016b  NCBI-BLAST-database/20170306  gurobi/gurobi800

----- Releases (2017b) -----
ABINIT/8.4.4-intel-2017b  Python/2.7.14-GCCcore-6.4.0-bare
ANTLR/2.7.7-intel-2017b  Python/3.6.3-foss-2017b
Boost/1.65.1-foss-2017b  Python/3.6.3-intel-2017b  (D)
Boost/1.66.0-intel-2017b  (D)  Qhull/2015.2-foss-2017b
CD0/1.9.2-intel-2017b  Qt/4.8.7-foss-2017b
CGAL/4.11-foss-2017b-Python-2.7.14  R/3.4.3-foss-2017b-X11-20171023
CP2K/5.1-intel-2017b  Ruby/2.5.0-intel-2017b
Doxygen/1.8.13-GCCcore-6.4.0  SCOTCH/6.0.4-foss-2017b
Eigen/3.3.4  SCOTCH/6.0.4-intel-2017b  (D)
FFTW/3.3.6-gompi-2017b  SQLite/3.20.1-GCCcore-6.4.0
FFTW/3.3.6-intel-2017b  (D)  SWIG/3.0.12-foss-2017b-Python-2.7.14
FLUENT/14.0  SWIG/3.0.12-foss-2017b-Python-3.6.3
FLUENT/18.2  (D)  SWIG/3.0.12-intel-2017b-Python-3.6.3  (D)
GCC/6.4.0-2.28  ScaLAPACK/2.0.2-gompi-2017b-OpenBLAS-0.2.20
GDAL/2.2.3-foss-2017b-Python-2.7.14  Singularity/2.5.2-foss-2017b
GDAL/2.2.3-foss-2017b-Python-3.6.3  (D)  UDUNITS/2.2.25-intel-2017b
GEOS/3.6.2-foss-2017b-Python-2.7.14  UDUNITS/2.2.26-intel-2017b  (D)
GEOS/3.6.2-foss-2017b-Python-3.6.3  X11/20171023-GCCcore-6.4.0
GEOS/3.6.2-intel-2017b-Python-3.6.3  (D)  YAXT/0.5.1-intel-2017b
GLib/2.53.5-GCCcore-6.4.0  foss/2017b
GMP/6.1.2-GCCcore-6.4.0  gc/7.6.0-GCCcore-6.4.0
GSL/2.4-GCCcore-6.4.0  gflags/2.2.1-intel-2017b
Guile/1.8.8-GCCcore-6.4.0  gompi/2017b
HDF5/1.8.19-intel-2017b  grib_api/1.24.0-intel-2017b

lines 1-36
```

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# Batch jobs

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# Interactive or batch

- Interactive
  - Short tasks
  - Tasks that require frequent user interaction
  - Graphically intensive tasks
- Batch
  - Longer running processes
  - Parallel processes
  - Running large numbers of short jobs simultaneously
  - Submitted to a job scheduler

# Job scheduler



- Dispatch the batch jobs on compute nodes
- Parameters
  - Memory
  - Processor type
  - Execution time
  - Number of processors
  - Software license tokens
- Slurm workload manager

# Submit a batch job



- Connect to a login node

```
$ ssh hercules.ptci.unamur.be
```

# Job scripts



- Define resources to be reserved for your job:
  - CPU time
  - memory
  - platform
  - number of CPUs
  - List instructions to be executed
- Bash shell script



# Job scripts

- run.sh

```
#!/bin/bash
#SBATCH --job-name=hello
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=1
#SBATCH --time=1:00:00
#SBATCH --mem-per-cpu=1000

echo "Hello World!"
```

# Submitting jobs



- Submit the job script

```
$ sbatch run.sh
Submitted batch job 3513668
```

- Return the job id

- Job is running

```
$ squeue -u $USER
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST
3513667	cpu	hello	fwautele	R	0:12	1	n065

- Job is finished

```
$ squeue -u $USER
$
```

# Batch jobs



- Check output file

```
$ ls -altr
...
-rw-rw-r-- 1 fwautele fwautele          13 Feb 26 11:16 slurm-3513668.out
```

- Hello world!

```
$ cat slurm-3513668.out
Hello World!
```

# Safeguards



- Slurm will automatically cancel jobs:
  - When the memory reserved is exceeded
  - When time is over
- Slurm constraint job in the number of core requested

# Delete a job



- scancel

```
$ scancel 2243523
```

- You can only delete your own jobs... (hopefully)

# Monitoring jobs



- squeue

```
$ squeue
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST (REASON)
2619747	cpu	PYV3_FBI	jquertin	R	16:15:37	1	n076
2619745	cpu	PYV3_DHB	jquertin	R	4-14:36:35	1	n020
2620638	cpu	PYV3_FA_	jquertin	R	43:33	1	n025
2618213	cpu	PYV3_SDP	jquertin	R	9-19:40:43	1	n054
2620635	cpu	PYV3-CC2	jquertin	R	56:59	1	n020
2620632	cpu	PYV3-CC2	jquertin	R	59:22	1	n014
2620633	cpu	PYV3-CC2	jquertin	R	59:22	1	n014
2620630	cpu	PYV3-CC2	jquertin	R	59:52	1	n054
2620631	cpu	PYV3-CC2	jquertin	R	59:52	1	n064
2620627	cpu	PYV3-CC2	jquertin	R	1:01:24	1	n064
2620628	cpu	PYV3-CC2	jquertin	R	1:01:24	1	n064
2620622	cpu	PYV3-CC2	jquertin	R	1:18:17	1	n076

# scriptgen

- Slurm Script Generation Wizard

<http://www.cec-hpc.be/scriptgen.html>

<p><b>1. Describe your job</b></p> <p>Email address: <input type="text" value="user@example.com"/></p> <p>Job name: <input type="text" value="Some name"/></p> <p>Project: <input type="text" value="Some project"/></p> <p><b>Parallelization paradigm(s)</b></p> <p><input type="checkbox"/> Embarrassingly parallel / Job array</p> <p><input checked="" type="checkbox"/> Shared memory / OpenMP</p> <p><input type="checkbox"/> Message passing / MPI</p> <p><b>Job resources</b></p> <p>Duration : <input type="text" value="0"/> days, <input type="text" value="1"/> hour, <input type="text" value="0"/> minutes.</p> <p>Number of threads : <input type="text" value="2"/></p> <p>Memory per thread: <input type="text" value="32"/> <input type="text" value="GB"/></p> <p><b>Filesystem</b></p> <p>Filesystem: <input type="text" value="\$HOME"/></p> <p>Total CPUs: 2   Total Memory: 65536 MB   Total CPU.Hours: 2</p>	<p><b>2. Choose a cluster</b></p> <p><input type="radio"/> Vega</p> <p><input type="radio"/> Lemaitre3</p> <p><input checked="" type="radio"/> Hercules</p> <p><input type="radio"/> Dragon1</p> <p><input type="radio"/> HMEM</p> <p>NIC4</p> <p>Lemaitre2</p> <p>Zenobe*</p>	<p><b>3. Copy-paste your script</b></p> <pre>#!/bin/bash # Submission script for Hercules #SBATCH --time=01:00:00 # hh:mm:ss # #SBATCH --ntasks=1 #SBATCH --cpus-per-task=2 #SBATCH --mem-per-cpu=32768 # 32GB #SBATCH --partition=cpu  export OMP_NUM_THREADS=2 export MKL_NUM_THREADS=2</pre>
---	--	---

# Array jobs



- Run several instances of the same program with different inputs
- Same allocation options
  - Memory size
  - Time limit
  - ...



# --array options

```
# SBATCH --array=0-31
```

```
# SBATCH --array=1,3,5,7
```

```
# SBATCH --array=1-7:2
```

```
# SBATCH --array=1-15%4
```

# Example



```
$ sbatch --array=0-3 run.sh  
Submitted batch job 3512681
```

```
$ squeue -u fwautele
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST
3512681_0	cpu	run.sh	fwautele	R	0:12	1	n064
3512681_1	cpu	run.sh	fwautele	R	0:12	1	n077
3512681_2	cpu	run.sh	fwautele	R	0:12	1	n047
3512681_3	cpu	run.sh	fwautele	R	0:12	1	n047

# Job Dependencies

- A job can be dependent upon other job(s) status
- Dependency type:
  - after
    - after the specified jobs have started
  - afterany
    - after the specified jobs have terminated
  - afternotok
    - after the specified jobs have failed
  - afterok
    - after the specified jobs have terminated successfully

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# Job type

- Sequential job
  - A single core on one node
- Threaded jobs
  - Several cores on one node
  - OpenMP
- MPI jobs
  - Several cores on several nodes
  - OpenMPI, MPICH, ...

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# Scripting languages

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# Available modules



- Python/2.7.14-foss-2017b
- Python/2.7.14-foss-2018a
- Python/2.7.14-GCCcore-6.4.0-bare
- Python/2.7.14-intel-2017b
- Python/2.7.15-foss-2018b
- Python/2.7.15-GCCcore-7.3.0-bare
- Python/2.7.15-intel-2018b
- Python/2.7.16-GCCcore-8.3.0
- Python/2.7.18-GCCcore-9.3.0
- Python/3.6.3-foss-2017b
- Python/3.6.3-foss-2018a
- Python/3.6.3-intel-2017b
- Python/3.6.4-foss-2018a
- Python/3.6.4-intel-2018a
- Python/3.6.6-foss-2018b
- Python/3.7.4-GCCcore-8.3.0
- Python/3.8.2-GCCcore-9.3.0

# Installing languages extensions



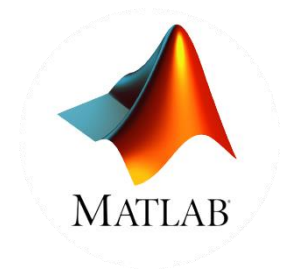
- Install with PIP
  - PIP is the easiest and recommended way to install Python packages

```
$ pip install --user example
```

- Install from source
  - If package not available on PIP
  - Steps:
    - Download the source and unpack it
    - Change to the source directory
    - `python setup.py install --prefix=$HOME/.local`

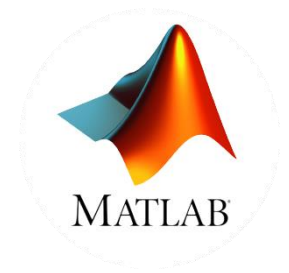
```
$ python setup.py install --prefix=$HOME/.local
```

# MATLAB



- On Hercules
  - matlab/R2015a
  - matlab/R2014b
  - matlab/R2013a

# Batch jobs



- “m-file” (hello.m)

```
disp('Hello, World!');
```

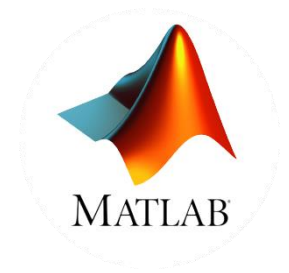
- Job script (run.sh)

```
#!/bin/bash
#SBATCH --job-name=hello
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=1
#SBATCH --time=1:00:00
#SBATCH --mem-per-cpu=1000
#SBATCH --licenses=matlab:1

module load legacy
module load matlab/R2015a

matlab hello.m
```

# Batch jobs



- Submit your job

```
$ sbatch run.sh  
Submitted batch job 3513667
```

- Job is running

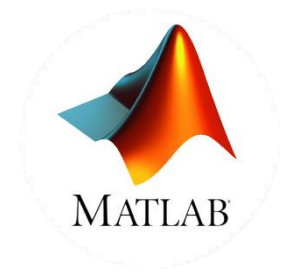
```
$ squeue -u $USER
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST
3513667	cpu	hello	fwautele	R	0:12	1	n065

- Job is finished

```
$ squeue -u $USER  
$
```

# Batch jobs



- Check output file

```
$ ls -altr
...
-rw-rw-r-- 1 fwautele fwautele          771 Feb 26 10:23 slurm-3513667.out
```

- Hello world!

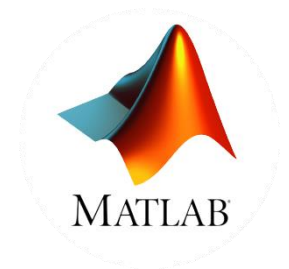
```
$ cat slurm-3513667.out
```

```
      < M A T L A B (R) >
Copyright 1984-2015 The MathWorks, Inc.
R2015a (8.5.0.197613) 64-bit (glnxa64)
      February 12, 2015
```

```
To get started, type one of these: helpwin, helpdesk, or demo.
For product information, visit www.mathworks.com.
```

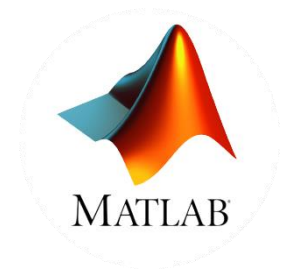
```
>> Hello, World!
```

# Parallel MATLAB



- Several function and toolboxes has multiprocessor support
- A multiprocessor MATLAB job will consume only one license token
- Parallel Computing Toolbox

# Multiprocessor support



- Job on 4 cpus

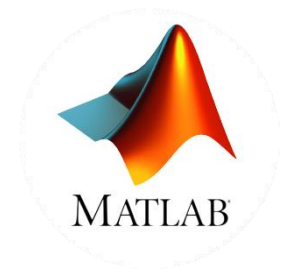
```
#!/bin/bash
#SBATCH --job-name=smp
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4
#SBATCH --ntasks-per-node=1
#SBATCH --time=1:00:00
#SBATCH --mem-per-cpu=1000
#SBATCH --licenses=matlab:1

module load legacy
module load matlab/R2015a

matlab smp.m
```



# MATLAB Compiler



- Allow to run MATLAB precompiled script
- Generate standalone executables
- MATLAB executables do not consume MATLAB licenses tokens
- The compilation can be done on an login node
- Not all MATLAB functionalities can be compiled

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# Objectives

- Building from source is preferred in an HPC environment
- Allow users to install applications
  - Link with numerical libraries
  - Built with optimized compiler
- Special case
  - Python
  - R
  - Perl

# Compilers available

- GNU Compiler Collection (GCC)
- Intel Parallel Studio XE Cluster Edition
- The Portland Group PGI Accelerator CDK

# GNU Compiler Collection (GCC)

- Open Source (GPL)
- Pretty good performance
- Compiler suite
  - gcc: C compiler
  - g++: C++ compiler
  - gfortran: Fortran compiler
- module load foss

# Intel Parallel Studio XE Cluster Edition



- Commercial
- High performance compiler
- Compiler suite
  - icc: C compiler
  - icpc: C++ compiler
  - ifort: Fortran compiler
- `module load intel`

# PGI



- The Portland Group PGI Accelerator CDK
- Commercial (NVIDIA)
- Offloading on GPU
- Compiler suite
  - pgcc: C compiler
  - pgCC: C++ compiler
  - pgf77: Fortran 77 compiler
  - pgf90: Fortran 90 compiler
- module load PGI



# Optimized libraries

- Do not reinvent the wheel
- Use multicore-tuned libraries.
- Use optimized libraries
  - Boost
  - FFTW
  - GMP
  - GSL
  - HDF5
  - ...

# Compiler Toolchains

- Compiler toolchain =
  - Compiler
  - + MPI library
  - + BLAS/LAPACK library
    - linear algebra routines
  - + FFT library
    - Fast Fourier Transforms
- Examples
  - foss/2019b
  - intel/2019b

# Compiler Toolchains

- Open Source compiler toolchain
  - foss/2019b
    - GCC 8.3.0
    - OpenMPI 3.1.4
    - OpenBLAS 0.3.7
    - LAPACK 3.7.0
    - ScaLAPACK 2.0.2
    - FFTW 3.3.8

# Compiler Toolchains

- Intel Parallel Studio XE Cluster Edition 2019
  - A toochain: intel/2019b
    - icc 19.0.5 (C compiler)
    - icpc 19.0.5 (C++ compiler)
    - ifort 19.0.5 (Fortran compiler)
    - impi 2018.5.222 (Intel MPI)
    - MKL 2019.5.281 (Math Kernel Library)

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# Debugging and profiling

MATLAB on  
the cluster

Accelerators/Co-processors

Python for HPC

Slurm workload manager

Share memory (OpenMP)

Message passing (MPI)

Checkpointing

**Debugging and profiling**

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# Profiling = finding hotspots

- Hotspot = Where in an application or system there is a significant amount of activity
  - Where: address in memory → line of source code
  - Significant: activity that occurs infrequently probably does not have much impact on system performance
  - Activity: time spent or other internal processor event

# Intel Vtune™ Amplifier

- What is the VTune™ Performance Analyzer?
  - Helps you identify and characterize performance issues by:
    - Collecting performance data
    - Organizing and displaying the data from system-wide down to source code or processor instruction
    - Identifying potential performance issues and suggesting improvements
  - Able to analyse serial, OpenMP and MPI application



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# Miscellaneous

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**Thanks you for your attention**  
and happy computing