

Introduction to high-performance computing

Frédéric Wautelet
CÉCI HPC training 2021

Outline

MATLAB

Accelerators/Co-processors

Python

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

18 Oct - Bernard Van Renterghem, "**Introduction to Linux and the command line**"

19 Oct - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"

19 Oct - Juan Cabrera, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"

19 Oct - Damien François, "**Introduction to scientific software development and deployment**"

20 Oct - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"

20 Oct - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"

21 Oct - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"

21 Oct - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"

21 Oct - Damien François, "**Introduction to parallel computing**"

26 Oct - Olivier Mattelaer, "**Introduction to C programming language**"

26 Oct - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"

27 Oct - Olivier Mattelaer, "**Introduction to code versioning**"

27 Oct - Bernard Van Renterghem, "**Debugging/profiling scientific code and scientific libraries**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part I)**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part II)**"

08 Nov - Jérôme de Favereau, "**Introduction to Python**"

08 Nov - Orian Louant, "**Parallel programming with OpenMP**"

09 Nov - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"

09 Nov - Ramon Winterhalter, "**An Introduction to Neural Networks**"

10 Nov - Damien François, "**Preparing, submitting and managing jobs with Slurm**"

10 Nov - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"

10 Nov - David Waroquiers, "**Using a workflow manager to handle large amounts of jobs**"

17 Nov - Damien François, "**Introduction to data storage and access**"

17 Nov - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"

17 Nov - Adeline Grard, "**Open Science and open research data**"

23 Nov - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"

23 Nov - Orian Louant, "**Directive Based Parallel programming on GPU**"

24 Nov - Damien François, "**Efficient use of MATLAB on the cluster**"

24 Nov - Ariel Lozano, "**Efficient use of Python on the clusters**"

Introduction to HPC

MATLAB on
the cluster

Accelerators/Co-processors

Python for HPC

Slurm workload manager

Share memory (OpenMP)

Message passing (MPI)

Checkpointing

Debugging and profiling

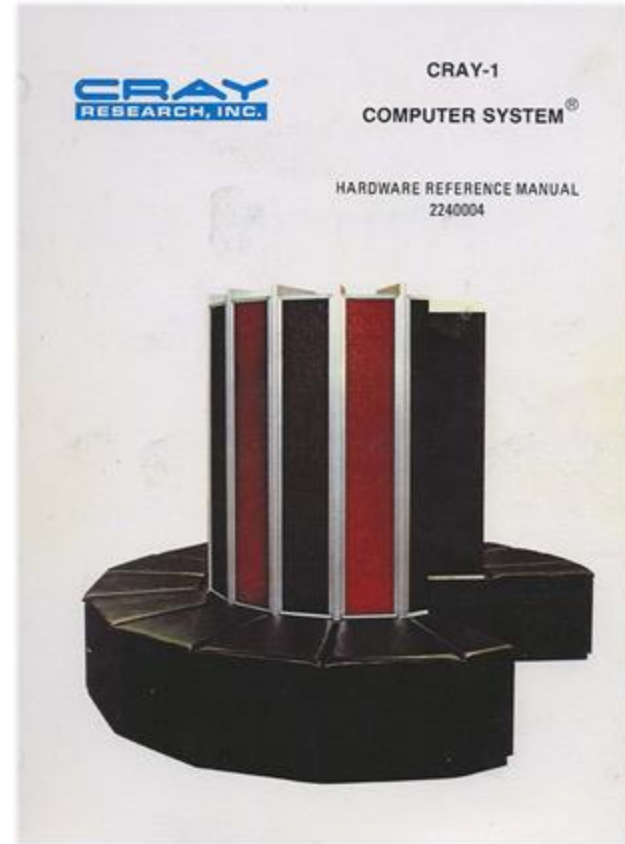
Compilers and libraries

Introduction to GNU/Linux and the command line

Introduction to HPC

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.

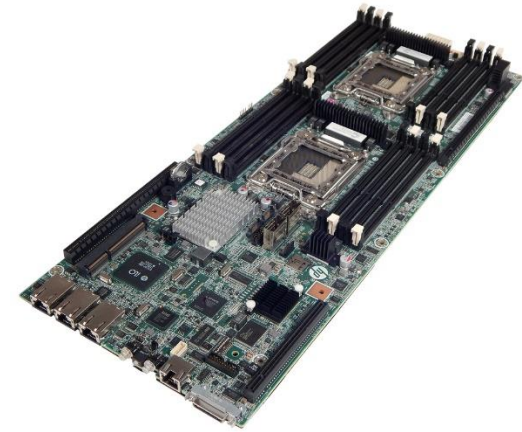


MareNostrum 4 (2017)

13.7 PFlops

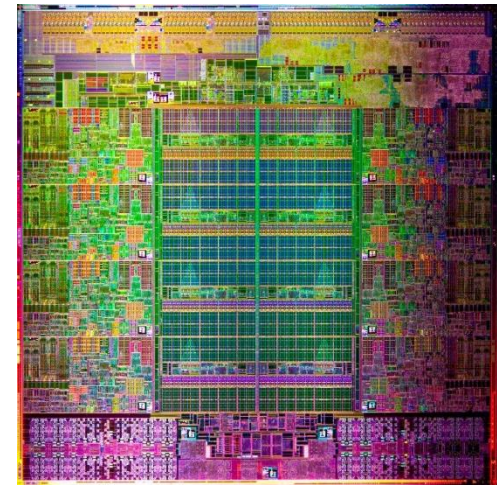
Nodes and Cores

- 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

Measure supercomputer power

- FLOPS
- floating-point operations per second

GigaFLOPS = one billion (10^9) floating-point operations per second

TeraFLOPS = one trillion (10^{12}) floating-point operations per second

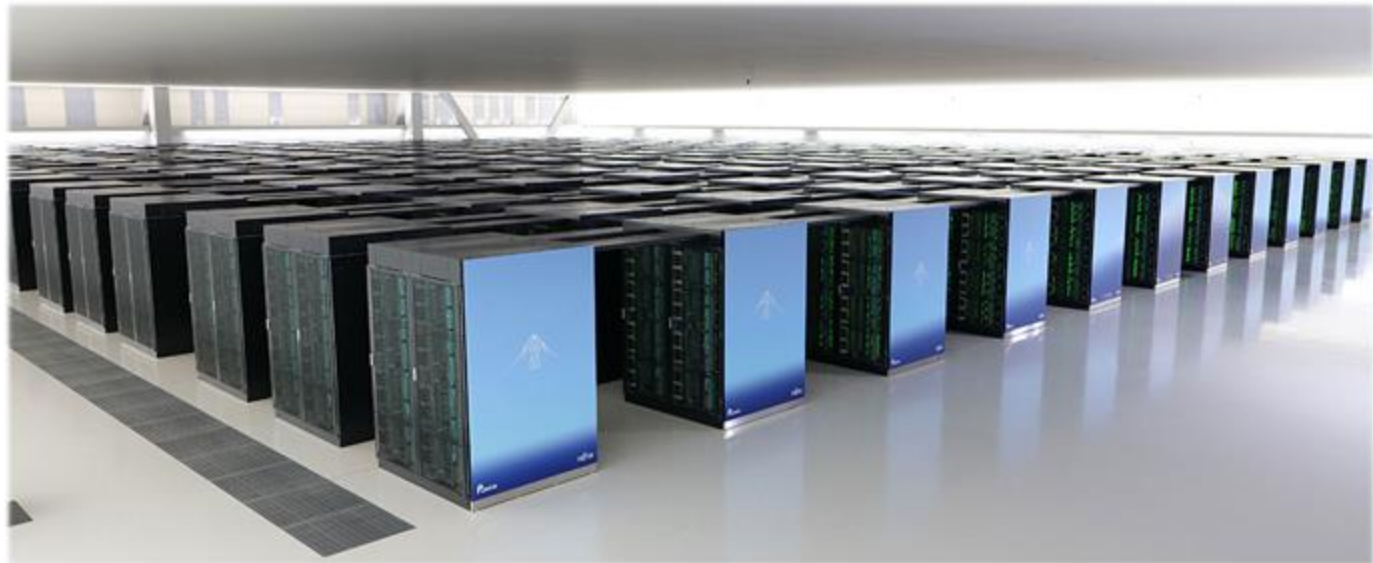
PetaFLOPS = one quadrillion (10^{15}) floating-point operations per second

ExaFLOPS = one quintillion (10^{18}) floating-point operations per second

TOP500



- Fugaku
 - RIKEN Center for Computational Science, Kobe, Japan
 - TOP500 #1 (June 2021)
 - ~7,600,000 cores
 - 440+ Pflop/s
 - ~30 MW



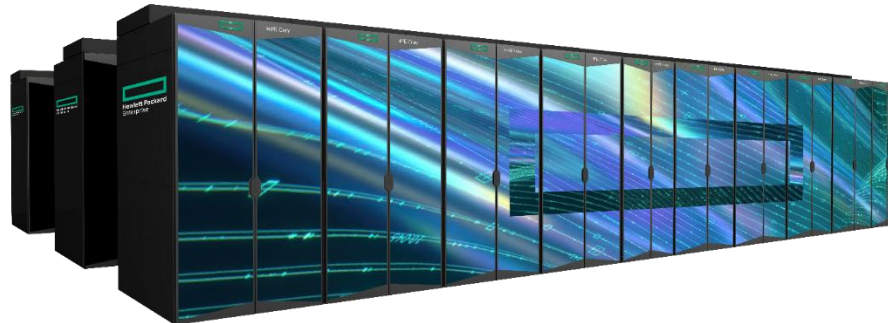
HPC to Exascale



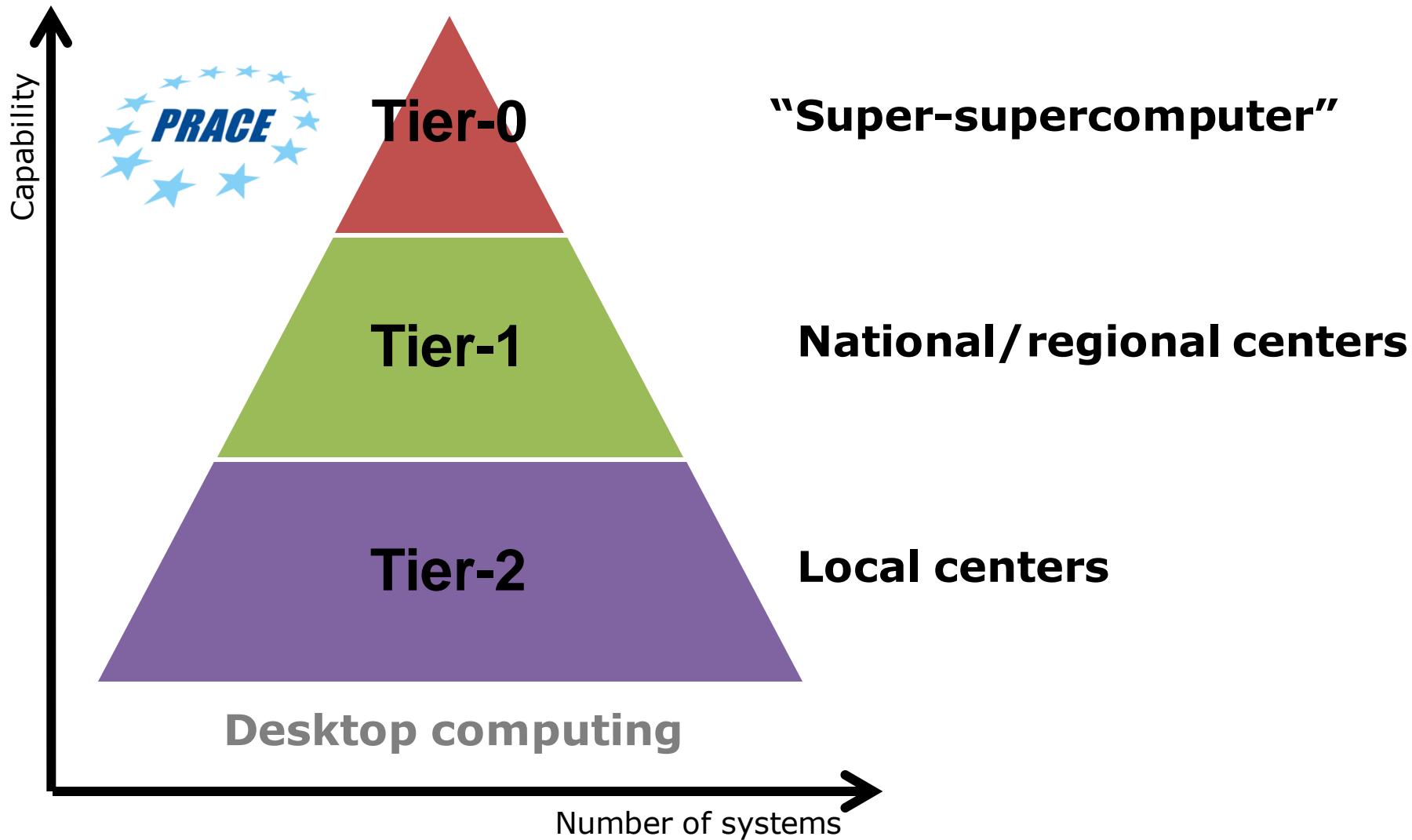
EuroHPC
Joint Undertaking

- Exascale
 - Eflop/s = 10^{18} flop/s
 - First European pre-Exascale system: Lumi
 - CSC, Kajaani, Finland
 - 200,000 cores, 500+ Pflop/s, ~120 PB storage
 - Belgian researchers eligible to apply for LUMI resources

L U M I



The European HPC ecosystem



PRACE



- Partnership for Advanced Computing in Europe
- 28 supercomputers in 26 countries
- Call for Proposals for Project Access



Tier-0

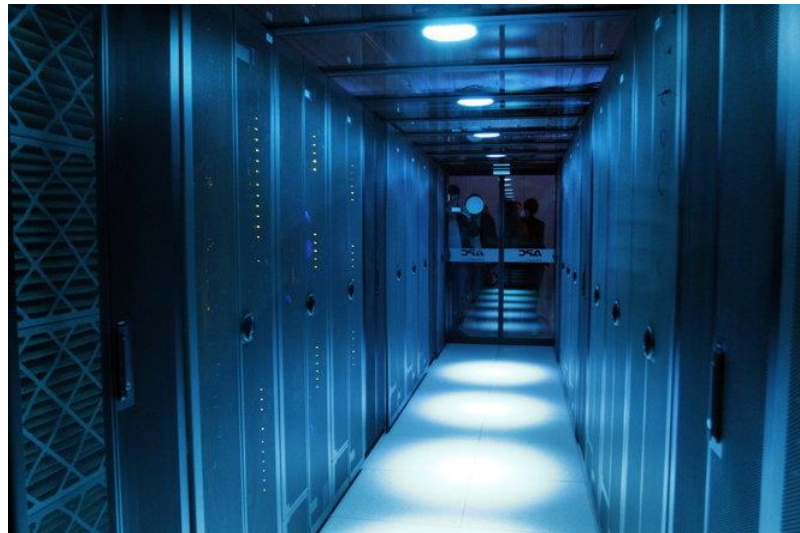


- JUWELS Booster Module
 - Forschungszentrum Juelich, Germany
 - TOP500 #8 (June 2021)
 - ~450,000 cores
 - 44 Pflop/s
 - 2 MW



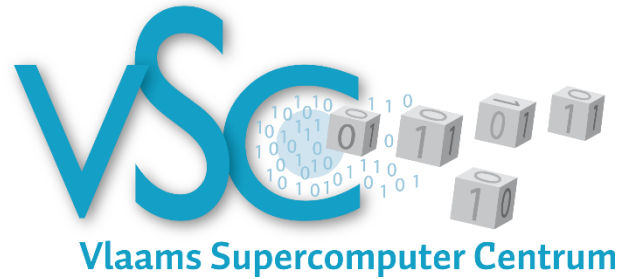
Tier-1

- 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€

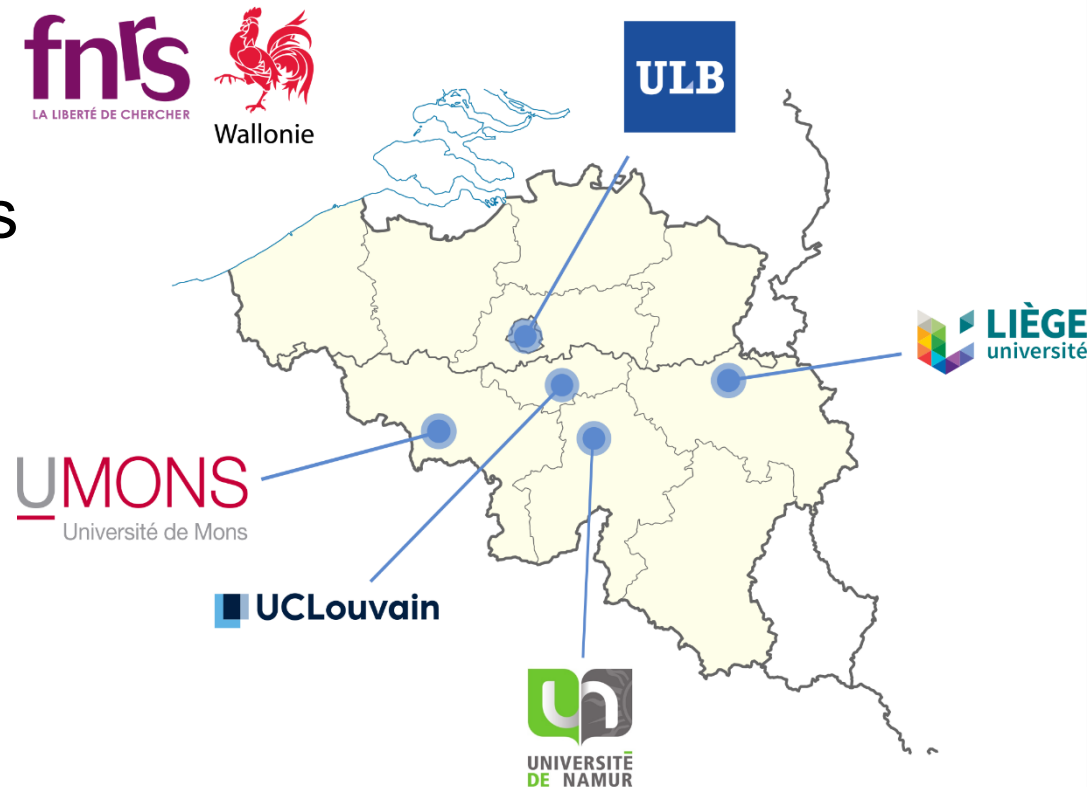


- Tier-2: CÉCI

- 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

Not available



Hercules 2
1536 cores
 Sandybridge
 Epyc

2 TB RAM

10 GbE

Q3 2019



Dragon 2
592 cores
 Skylake
 Tesla V100

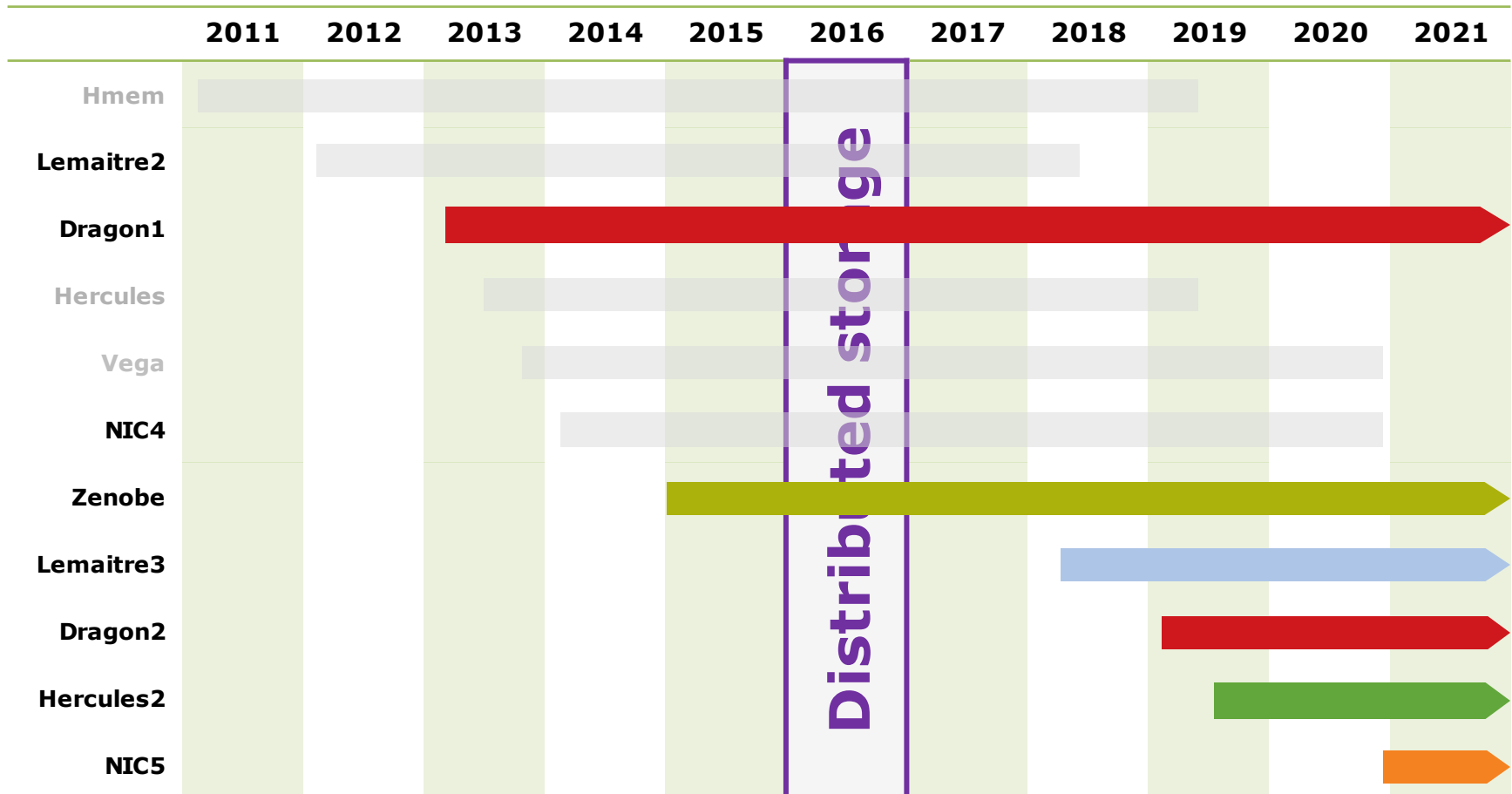
384 GB RAM

10 GbE

Q1 2019

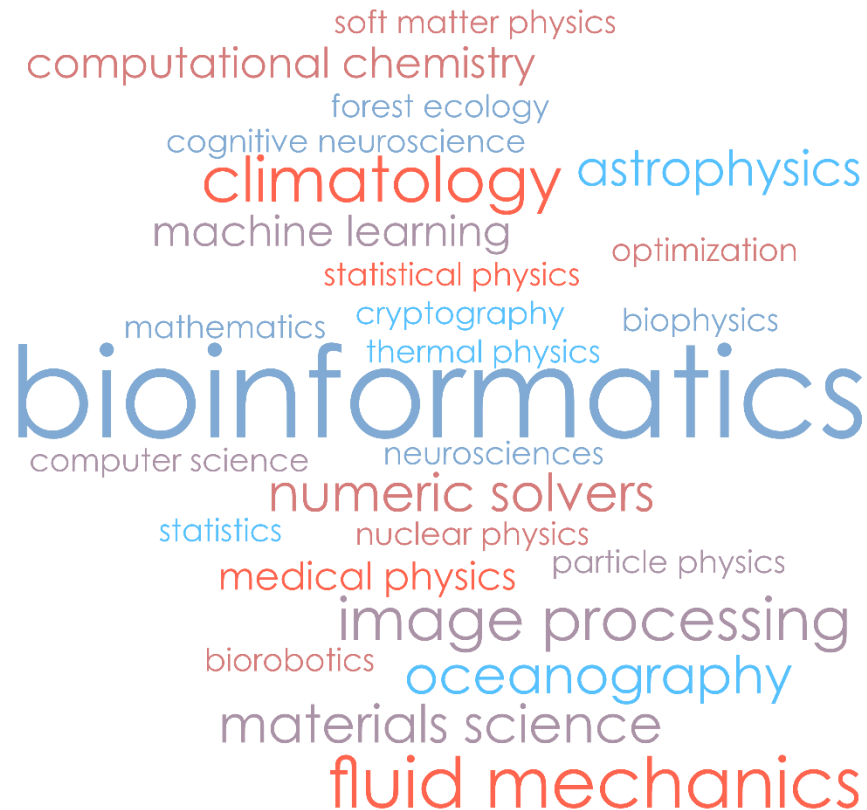
9248 cores total

The CÉCI upgrade



Users

- 400+ CÉCI actives users

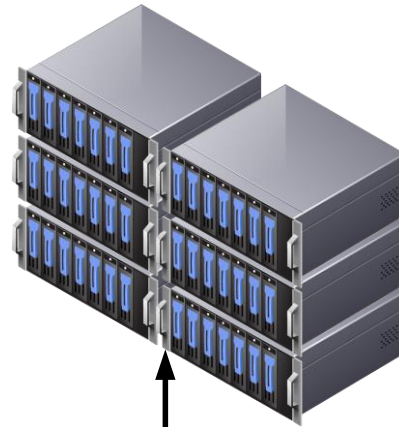


Fields of applications - CÉCI survey 2021

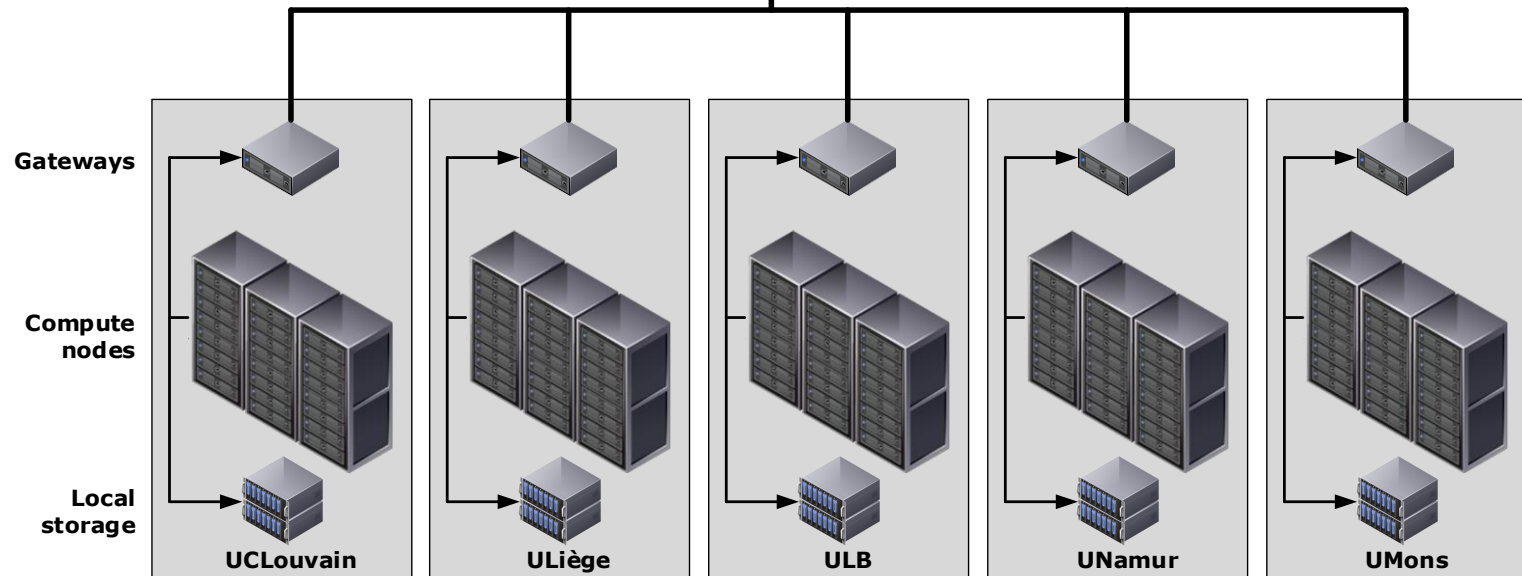
CÉCI distributed storage



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



IBM
Spectrum
Storage

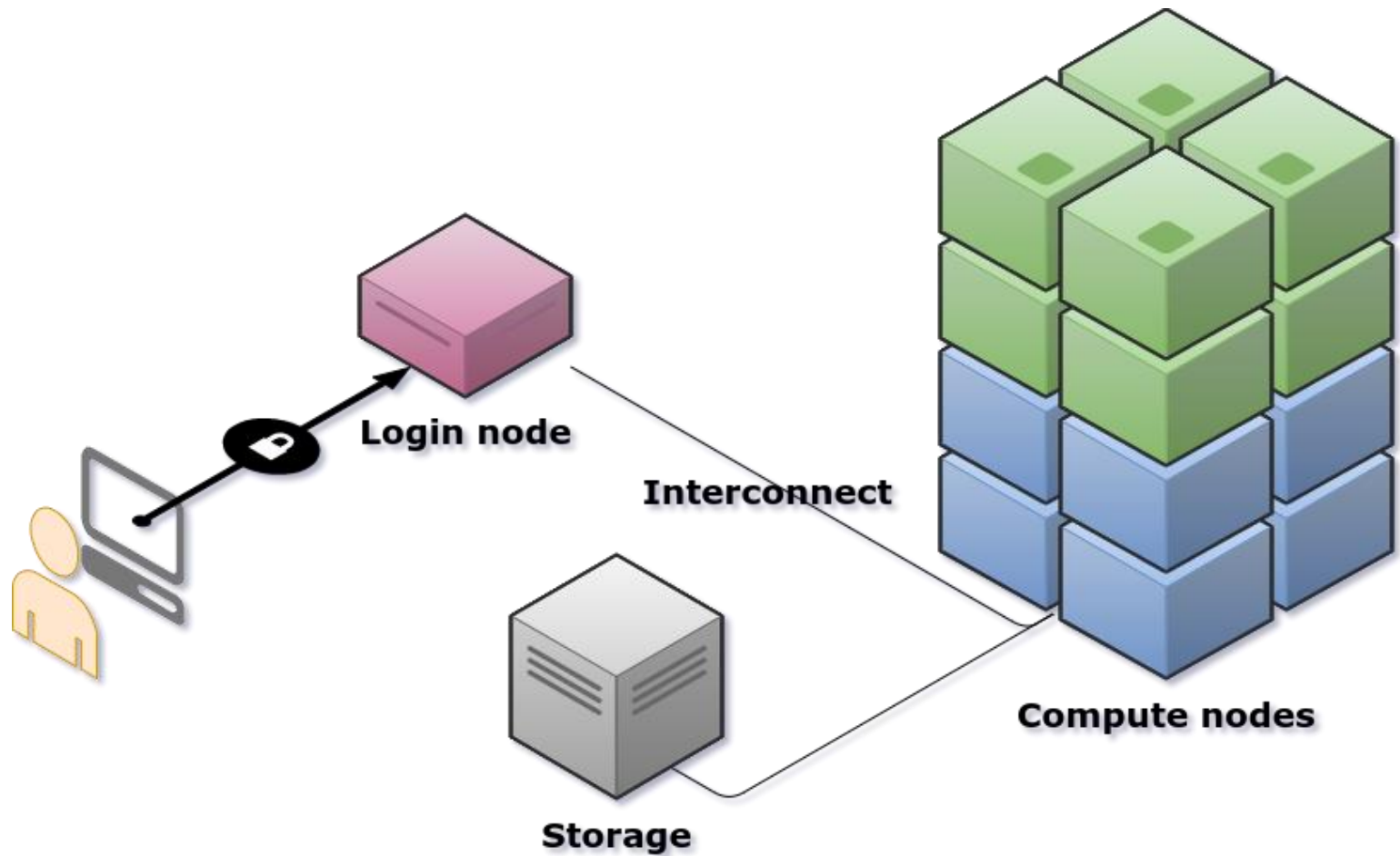


CÉCI distributed storage



- 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

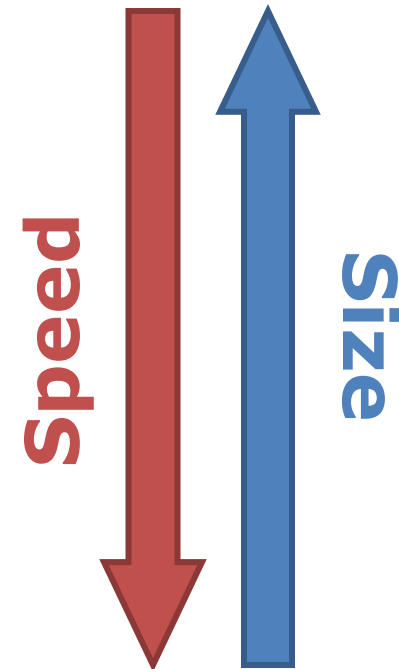


Login node

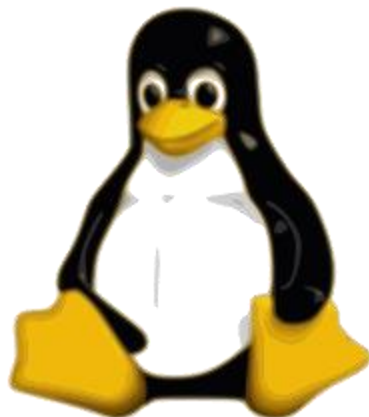
- Submit jobs to batch system
- Manage your files
- Interactive work at small scale
- CÉCI login nodes
 - hercules2.ptci.unamur.be
 - dragon2.umons.ac.be
 - lemaitre3.cism.ucl.ac.be
 - nic5segi.ulg.ac.be

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***
NIC5	ULiège	Rome 2.9 GHz	4672 (73 x 64)	256 GB..1 TB	HDR Ib	BeeGFS 520 TB	None	2 days	☐ MPI
Hercules2	UNamur	Naples 2 GHz SandyBridge 2.20 GHz	1024 (30 x 32 + 2 x 64) 512 (32 x 16)	64 GB..2 TB	10 GbE	NFS 20 TB	None	15 days	☐ serial / ☐ SMP
Dragon2	UMons	SkyLake 2.60 GHz	592 (17 x 32 + 2 x 24)	192..384 GB	10 GbE	RAID0 3.3 TB	4x Volta V100	21 days	☐ serial / ☐ SMP
Lemaitre3	UCL	SkyLake 2.3 GHz Haswell 2.6 GHz	1920 (80 x 24) 112 (4 x 28)	95 GB 64 GB	Omnipath	FHGFS 580 TB	None	2 days 6 hours	☐ MPI
NIC4	ULiège	SandyBridge 2.0 GHz IvyBridge 2.0 GHz	2048 (120 x 16 + 8 x 16)	64 GB	QDR Ib	FHGFS 144 TB	None	3 days	☐ MPI
Dragon1	UMons	SandyBridge 2.60 GHz	416 (26 x 16)	128 GB	GbE	RAID0 1.1 TB	4x Tesla C2075	41 days	☐ serial / ☐ SMP
Vega*	ULB	Bulldozer 2.1 GHz	896 (14 x 64)	256 GB	QDR Ib	GPFS 70 TB	None	14 days	☐ serial / ☐ SMP / ☐ MPI
Hercules*	UNamur	SandyBridge 2.20 GHz	512 (32 x 16)	64..128 GB	GbE	NFS 20 TB	None	63 days	☐ serial / ☐ SMP
Lemaitre2*	UCL	Westmere 2.53 GHz	1380 (115 x 12)	48 GB	QDR Ib	Lustre 120 TB	3x Quadro Q4000	3 days	☐ MPI
Hmem*	UCL	MagnyCours 2.2 GHz	816 (17 x 48)	128..512 GB	QDR Ib	FHGFS 30 TB	None	15 days	☐ SMP

Hercules 2 @ UNamur


- High memory jobs
 - up to 2 TB
- Long duration jobs
 - 15 days
- GPU
 - 8 GPUs total
- No multi-node jobs



HPC @ UNamur

- Local support :
 - Plateforme Technologique en Calcul Intensif (PTCI)
 - Juan CABRERA
 - Frédéric WAUTELET
 - 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
- Long duration job
 - 21 days
- GPU
 - 4x  **nVIDIA**. Volta V100
- No multi-node jobs



HPC @ UMONS

- Local support
 - 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)



Thomas Keutgen
(Head)



Damien François



Olivier Mattelaer

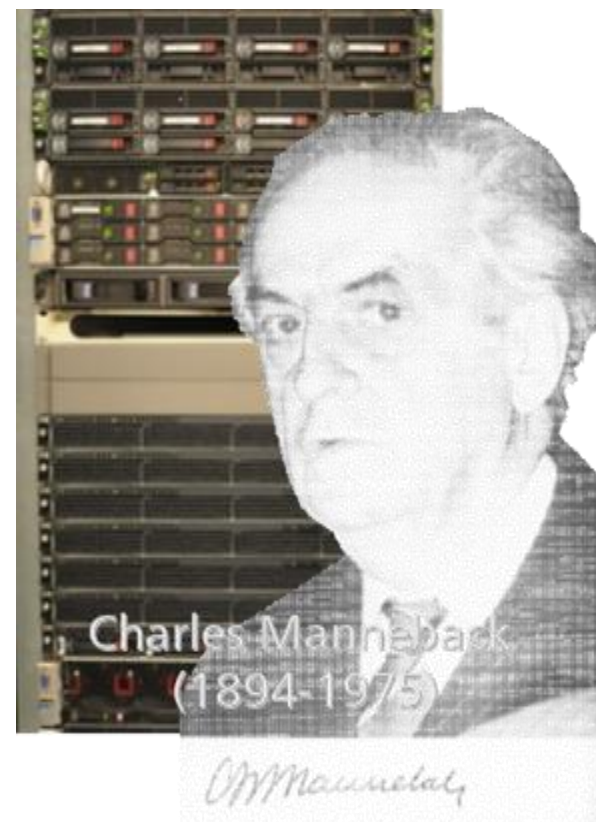


Bernard Van
Renterghem



Patrick Vranckx

- 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 jobs
 - 2 days
- Fast parallel filesystem
 - \$GLOBALSCRATCH



HPC @ ULiège

- Local support
 - David.Colignon@uliege.be
- More info
 - <http://www.ulg.ac.be/nic4>



Zenobe

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



How to get a CÉCI account?



[CÉCI](#) [Clusters](#) [News](#) [Training](#) [FAQ](#) [Documentation](#) [Support](#) [Contact](#) [Create/Manage 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, UMONS, 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 UNIX/Linux or MacOS computer](#)
- [Sturm tutorial and quick start](#)
- [Sturm Frequently Asked Questions](#)
- [Tier-1 Zenobe quickstart](#)
- [Submission Script Generation Wizard](#)

Quick search

Photo Gallery



Save the date!

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

Latest News

LEMATRE3 installed at UCL
Monday, 04 June 2018
Lemaître3 is now operational and replaces Lemaître2, 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.

Dragon1 cluster featured in a Belnet article
Tuesday, 05 May 2018
The Dragon1 CÉCI cluster is highlighted in an interview from Belnet to Chantal Poiret, professor in Information and Communication Technology at the University of Mons. Follow [this link](#) to read the complete note.

Survey on Big Data and Machine Learning needs
Thursday, 03 May 2018
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.

10th CÉCI Scientific Meeting
Monday, 26 March 2018
The next CÉCI scientific day will take place on May 4th in Namur. Details and registration [here](#).

PRACE Call for Proposal
Friday, 16 March 2018
PRACE has issued the 17th [call for Proposals](#). Deadline: 2nd May 2018, 10:00 CET. 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!

[RSS](#) [© CÉCI](#) [Contact](#)

Create/Manage Account



The screenshot shows the top navigation bar of the CÉCI website. The navigation bar is blue with white text. On the left, it says 'CÉCI' followed by links for 'Clusters', 'News', 'Training', 'FAQ', 'Documentation', 'Support', and 'Contact'. On the right, there is a link 'Create/Manage Account' which is highlighted with a red box. A red arrow points from the main content area towards this link. Below the navigation bar, there is a large banner with the C.E.C.I. logo on the left and the text 'Consortium des Équipements de Calcul Intensif' on the right. Below this text, it says '6 clusters, 101 cores, 1 login, 1 home'.

About

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



Quick links



Save the date!

The next CÉCI scientific day will take place on Thursday April 25th in Brussels.

More information soon!

Latest News

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.

MONDAY, 04 JUNE 2018

Dragon1 cluster featured in a Belnet article

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

TUESDAY, 08 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!

Introduction to Linux and the command line

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

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	
Doxxygen/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

lines 1-36

18 Oct - Bernard Van Renterghem, "**Introduction to Linux and the command line**"

19 Oct - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"

19 Oct - Juan Cabrera, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"

19 Oct - Damien François, "**Introduction to scientific software development and deployment**"

20 Oct - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"

20 Oct - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"

21 Oct - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"

21 Oct - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"

21 Oct - Damien François, "**Introduction to parallel computing**"

26 Oct - Olivier Mattelaer, "**Introduction to C programming language**"

26 Oct - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"

27 Oct - Olivier Mattelaer, "**Introduction to code versioning**"

27 Oct - Bernard Van Renterghem, "**Debugging/profiling scientific code and scientific libraries**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part I)**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part II)**"

08 Nov - Jérôme de Favereau, "**Introduction to Python**"

08 Nov - Orian Louant, "**Parallel programming with OpenMP**"

09 Nov - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"

09 Nov - Ramon Winterhalter, "**An Introduction to Neural Networks**"

10 Nov - Damien François, "**Preparing, submitting and managing jobs with Slurm**"

10 Nov - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"

10 Nov - David Waroquiers, "**Using a workflow manager to handle large amounts of jobs**"

17 Nov - Damien François, "**Introduction to data storage and access**"

17 Nov - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"

17 Nov - Adeline Grard, "**Open Science and open research data**"

23 Nov - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"

23 Nov - Orian Louant, "**Directive Based Parallel programming on GPU**"

24 Nov - Damien François, "**Efficient use of MATLAB on the cluster**"

24 Nov - Ariel Lozano, "**Efficient use of Python on the clusters**"

Batch jobs

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

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>

1. Describe your job Email address: <input type="text" value="user@example.com"/> Job name: <input type="text" value="Some name"/> Project: <input type="text" value="Some project"/> Parallelization paradigm(s) <input type="checkbox"/> Embarrassingly parallel / Job array <input checked="" type="checkbox"/> Shared memory / OpenMP <input type="checkbox"/> Message passing / MPI Job resources Duration : <input type="text" value="0"/> days, <input type="text" value="1"/> hour, <input type="text" value="0"/> minutes. Number of threads : <input type="text" value="2"/> Memory per thread: <input type="text" value="32"/> GB Filesystem Filesystem: <input type="text" value="\$HOME"/> Total CPUs: 2 Total Memory: 65536 MB Total CPU.Hours: 2	2. Choose a cluster <input type="radio"/> Vega <input type="radio"/> Lemaitre3 <input checked="" type="radio"/> Hercules <input type="radio"/> Dragon1 <input type="radio"/> HMEM NIC4 Lemaitre2 Zenobe*	3. Copy-paste your script <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
```

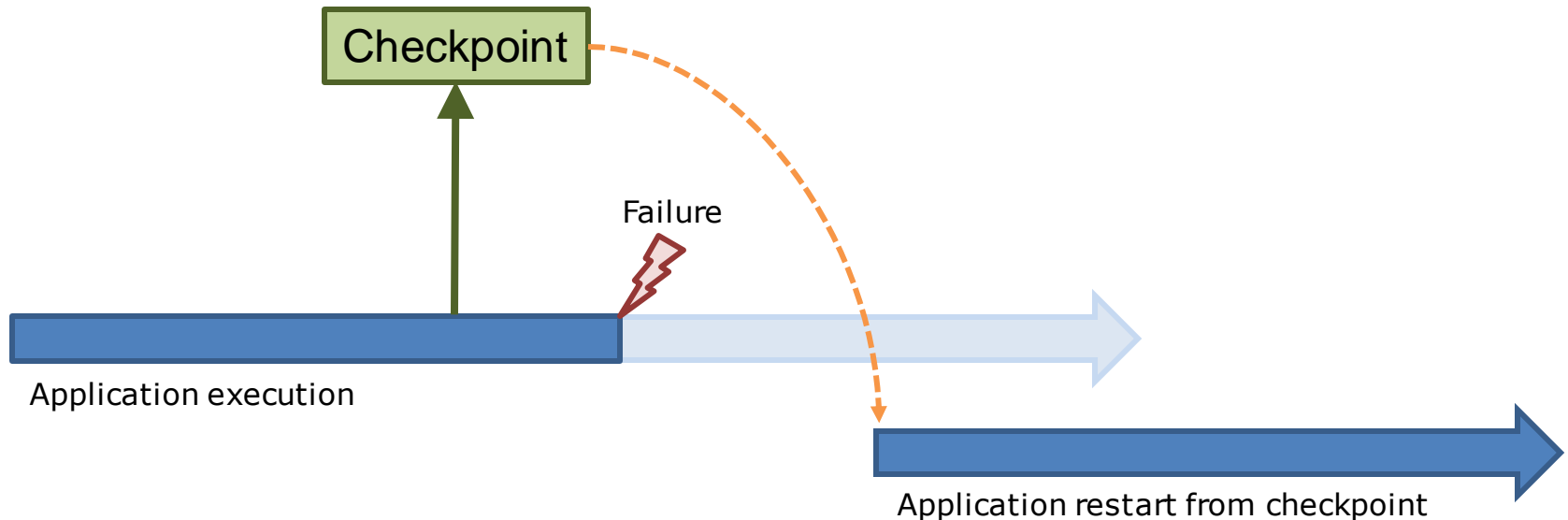
JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST
3512681_0	cpu	run.sh	fwautele	R	0:12	1	n064
3512681_1	cpu	run.sh	fwautele	R	0:12	1	n077
3512681_2	cpu	run.sh	fwautele	R	0:12	1	n047
3512681_3	cpu	run.sh	fwautele	R	0:12	1	n047

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

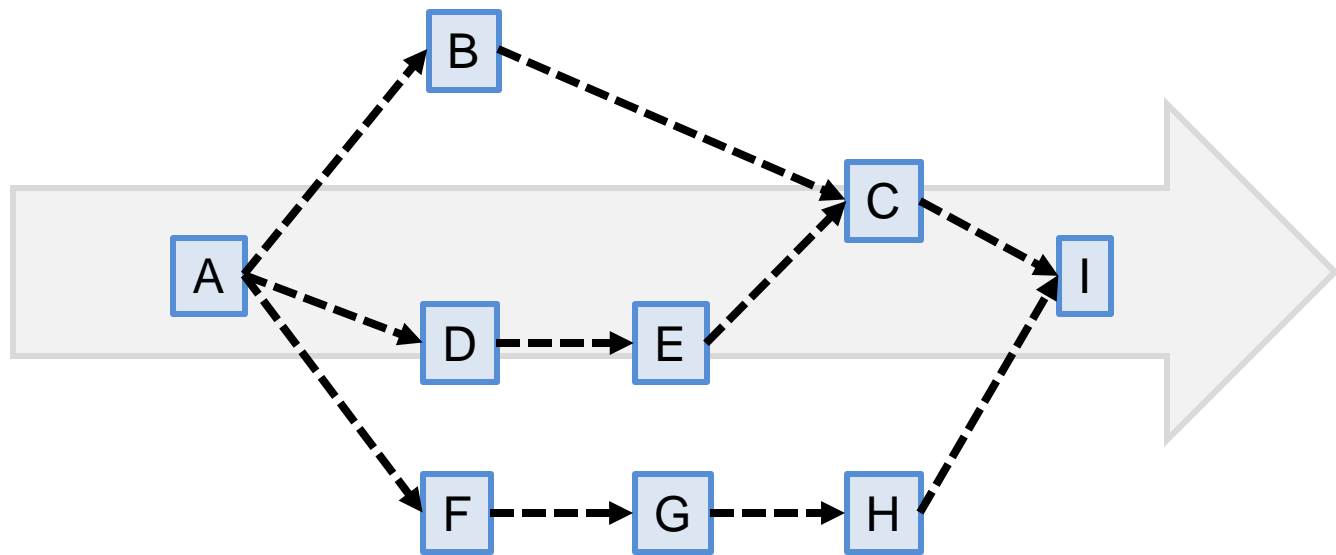
Checkpointing

- To overcome job time limitation
- Allow rollback-recovery for long-running applications
- Enable job migration



Workflow manager

- Automates execution of software flows on HPC clusters



18 Oct - Bernard Van Renterghem, "Introduction to Linux and the command line"

19 Oct - Olivier Mattelaer, "Connecting with SSH from Windows: Introduction and advanced topics"

19 Oct - Juan Cabrera, "Connecting with SSH from Linux or Mac: Introduction and advanced topics"

19 Oct - Damien François, "Introduction to scientific software development and deployment"

20 Oct - Bernard Van Renterghem, "Introduction to modules and software on a CÉCI cluster"

20 Oct - Bernard Van Renterghem, "Introduction to compilers and compiling, and optimized libraries"

21 Oct - Pierre-Yves Barriat, "Introduction to structured programming with Fortran"

21 Oct - Damien François, "Introduction to scripting and interpreted languages (Python, R, Octave)"

21 Oct - Damien François, "Introduction to parallel computing"

26 Oct - Olivier Mattelaer, "Introduction to C programming language"

26 Oct - Olivier Mattelaer, "Introduction to Object-Oriented programming with C++"

27 Oct - Olivier Mattelaer, "Introduction to code versioning"

27 Oct - Bernard Van Renterghem, "Debugging/profiling scientific code and scientific libraries"

28 Oct - Orian Louant, "Parallel programming with MPI (Part I)"

28 Oct - Orian Louant, "Parallel programming with MPI (Part II)"

08 Nov - Jérôme de Favereau, "Introduction to Python"

08 Nov - Orian Louant, "Parallel programming with OpenMP"

09 Nov - Olivier Mattelaer, "Parallel programming on GPU with CUDA"

09 Nov - Ramon Winterhalter, "An Introduction to Neural Networks"

10 Nov - Damien François, "Preparing, submitting and managing jobs with Slurm"

10 Nov - Olivier Mattelaer, "Using a Checkpoint/restart program to overcome time limits"

10 Nov - David Waroquiers, "Using a workflow manager to handle large amounts of jobs"

17 Nov - Damien François, "Introduction to data storage and access"

17 Nov - Ariel Lozano, "How to use efficiently the different storage solutions provided with the CECI clusters"

17 Nov - Adeline Grard, "Open Science and open research data"

23 Nov - Olivier Mattelaer, "Packaging software in portable containers with Singularity"

23 Nov - Orian Louant, "Directive Based Parallel programming on GPU"

24 Nov - Damien François, "Efficient use of MATLAB on the cluster"

24 Nov - Ariel Lozano, "Efficient use of Python on the clusters"

Parallel computing

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

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, ...

18 Oct - Bernard Van Renterghem, "**Introduction to Linux and the command line**"

19 Oct - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"

19 Oct - Juan Cabrera, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"

19 Oct - Damien François, "**Introduction to scientific software development and deployment**"

20 Oct - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"

20 Oct - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"

21 Oct - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"

21 Oct - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"

21 Oct - Damien François, "**Introduction to parallel computing**"

26 Oct - Olivier Mattelaer, "**Introduction to C programming language**"

26 Oct - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"

27 Oct - Olivier Mattelaer, "**Introduction to code versioning**"

27 Oct - Bernard Van Renterghem, "**Debugging/profiling scientific code and scientific libraries**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part I)**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part II)**"

08 Nov - Jérôme de Favereau, "**Introduction to Python**"

08 Nov - Orian Louant, "**Parallel programming with OpenMP**"

09 Nov - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"

09 Nov - Ramon Winterhalder, "**An Introduction to Neural Networks**"

10 Nov - Damien François, "**Preparing, submitting and managing jobs with Slurm**"

10 Nov - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"

10 Nov - David Waroquiers, "**Using a workflow manager to handle large amounts of jobs**"

17 Nov - Damien François, "**Introduction to data storage and access**"

17 Nov - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"

17 Nov - Adeline Grard, "**Open Science and open research data**"

23 Nov - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"

23 Nov - Orian Louant, "**Directive Based Parallel programming on GPU**"

24 Nov - Damien François, "**Efficient use of MATLAB on the cluster**"

24 Nov - Ariel Lozano, "**Efficient use of Python on the clusters**"

Scripting languages

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

Available modules



- Python 2
 - Python/2.7.16-GCCcore-8.3.0
 - Python/2.7.18-GCCcore-9.3.0
 - Python/2.7.18-GCCcore-10.2.0
- Python 3
 - Python/3.7.4-GCCcore-8.3.0
 - Python/3.8.2-GCCcore-9.3.0
 - Python/3.8.6-GCCcore-10.2.0

Installing languages extensions



- Install with PIP

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

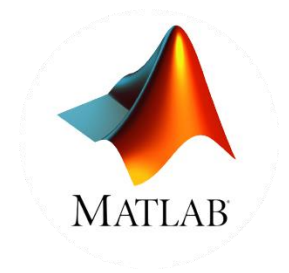
```
$ pip install --user example
```

- Install from source

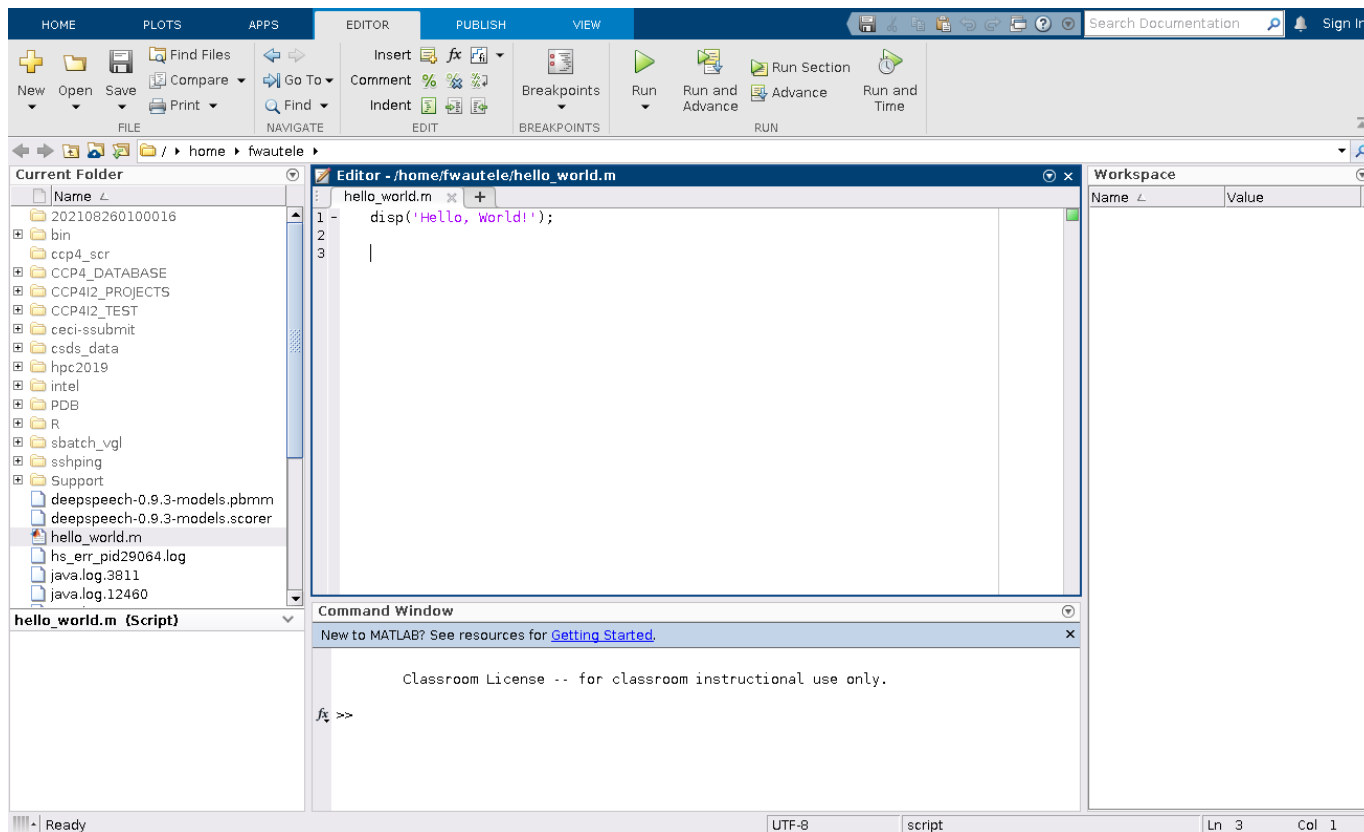
- If package not available on PIP
- Steps:
 - Download the source and unpack it
 - Change to the source directory
 - `python setup.py install --prefix=$HOME/.local`

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

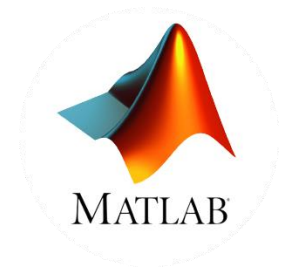
MATLAB



- On Hercules
 - MATLAB/2020b.5



Batch jobs



- “m-file” (hello_world.m)

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

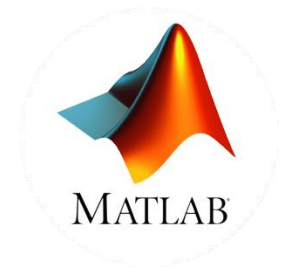
- Job script (run.sh)

```
#!/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

ml load MATLAB/2020b.5

matlab -batch hello_world
```

Batch jobs



- Submit your job

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

- Job is running

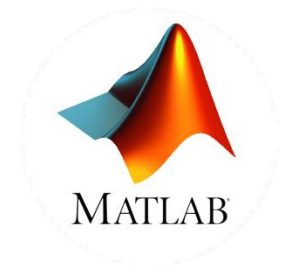
```
$ squeue -u $USER
```

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

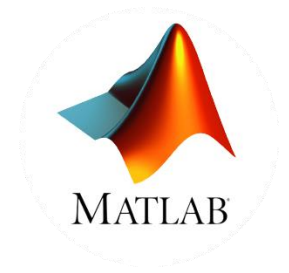
```
$ ls -altr
...
-rw-rw-r--  1 fwautele fwautele          771 Feb 26 10:23 slurm-3513667.out
```

- Hello world!

```
$ cat slurm-3513667.out
Opening log file:  /home/fwautele/java.log.22568

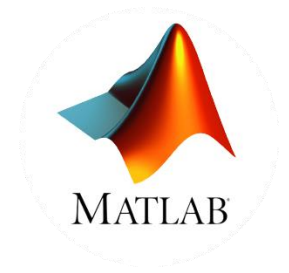
Hello, World!
```

Parallel MATLAB



- Several functions and toolboxes has multiprocessor support
- A multiprocessor MATLAB job will consume only one license token
- Parallel Computing Toolbox
- More infos on <https://www.mathworks.com>

Multiprocessor support



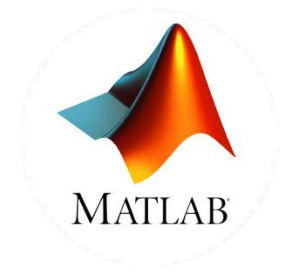
- Job on 4 cpus

```
#!/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

ml load MATLAB/2020b.5

matlab -batch smp
```

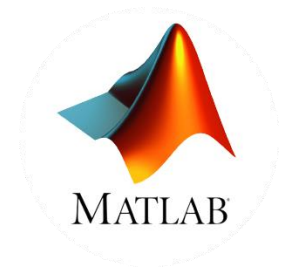

MATLAB Compiler



- Allow to run MATLAB precompiled script
- MATLAB executables do not consume MATLAB licenses tokens
- The compilation can be done on an login node
- Not all MATLAB functionalities can be compiled
- Running compiled MATLAB code requires loading the “MATLAB Compiler Runtime” (MCR).

```
$ ml load MCR/R2020b.5
```

MATLAB



- Run compiled MATLAB application

1. Compile your code using the MATLAB compiler

```
$ ml load MATLAB/2020b.5  
$ mcc -m -v -R '-singleCompThread,-nodisplay,-nodesktop,-  
nojvm' hello_world.m
```

2. Load the corresponding MATLAB Runtime (MCR)

```
$ ml load MCR/R2020b.5
```

3. Run the compiled MATLAB application

```
$ ./hello_world
```

- <https://nl.mathworks.com/help/sl3d/matlab-compiler-support.html>

18 Oct - Bernard Van Renterghem, "**Introduction to Linux and the command line**"

19 Oct - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"

19 Oct - Juan Cabrera, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"

19 Oct - Damien François, "**Introduction to scientific software development and deployment**"

20 Oct - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"

20 Oct - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"

21 Oct - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"

21 Oct - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"

21 Oct - Damien François, "**Introduction to parallel computing**"

26 Oct - Olivier Mattelaer, "**Introduction to C programming language**"

26 Oct - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"

27 Oct - Olivier Mattelaer, "**Introduction to code versioning**"

27 Oct - Bernard Van Renterghem, "**Debugging/profiling scientific code and scientific libraries**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part I)**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part II)**"

08 Nov - Jérôme de Favereau, "**Introduction to Python**"

08 Nov - Orian Louant, "**Parallel programming with OpenMP**"

09 Nov - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"

09 Nov - Ramon Winterhalder, "**An Introduction to Neural Networks**"

10 Nov - Damien François, "**Preparing, submitting and managing jobs with Slurm**"

10 Nov - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"

10 Nov - David Waroquiers, "**Using a workflow manager to handle large amounts of jobs**"

17 Nov - Damien François, "**Introduction to data storage and access**"

17 Nov - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"

17 Nov - Adeline Grard, "**Open Science and open research data**"

23 Nov - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"

23 Nov - Orian Louant, "**Directive Based Parallel programming on GPU**"

24 Nov - Damien François, "**Efficient use of MATLAB on the cluster**"

24 Nov - Ariel Lozano, "**Efficient use of Python on the clusters**"

Compilers and libraries

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

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/2020b
 - intel/2020b

Compiler Toolchains

- Open Source compiler toolchain
 - foss/2020b
 - GCC 10.2.0
 - OpenMPI 4.0.5
 - OpenBLAS 0.3.12
 - LAPACK 3.7.0
 - ScaLAPACK 2.1.0
 - FFTW 3.3.8

Compiler Toolchains

- Intel Parallel Studio XE Cluster Edition 2020
 - A toochain: intel/2020b
 - icc 2020.4.304 (C compiler)
 - icpc 2020.4.304 (C++ compiler)
 - ifort 2020.4.304 (Fortran compiler)
 - impi 2019.9.304 (Intel MPI)
 - MKL 2020.4.304 (Math Kernel Library)

18 Oct - Bernard Van Renterghem, "**Introduction to Linux and the command line**"

19 Oct - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"

19 Oct - Juan Cabrera, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"

19 Oct - Damien François, "**Introduction to scientific software development and deployment**"

20 Oct - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"

20 Oct - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"

21 Oct - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"

21 Oct - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"

21 Oct - Damien François, "**Introduction to parallel computing**"

26 Oct - Olivier Mattelaer, "**Introduction to C programming language**"

26 Oct - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"

27 Oct - Olivier Mattelaer, "**Introduction to code versioning**"

27 Oct - Bernard Van Renterghem, "**Debugging/profiling scientific code and scientific libraries**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part I)**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part II)**"

08 Nov - Jérôme de Favereau, "**Introduction to Python**"

08 Nov - Orian Louant, "**Parallel programming with OpenMP**"

09 Nov - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"

09 Nov - Ramon Winterhalder, "**An Introduction to Neural Networks**"

10 Nov - Damien François, "**Preparing, submitting and managing jobs with Slurm**"

10 Nov - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"

10 Nov - David Waroquiers, "**Using a workflow manager to handle large amounts of jobs**"

17 Nov - Damien François, "**Introduction to data storage and access**"

17 Nov - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"

17 Nov - Adeline Grard, "**Open Science and open research data**"

23 Nov - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"

23 Nov - Orian Louant, "**Directive Based Parallel programming on GPU**"

24 Nov - Damien François, "**Efficient use of MATLAB on the cluster**"

24 Nov - Ariel Lozano, "**Efficient use of Python on the clusters**"

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

Compilers and libraries

Introduction to GNU/Linux and the command line

Introduction to HPC

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

```
$ ml load VTune
```

18 Oct - Bernard Van Renterghem, "**Introduction to Linux and the command line**"

19 Oct - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"

19 Oct - Juan Cabrera, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"

19 Oct - Damien François, "**Introduction to scientific software development and deployment**"

20 Oct - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"

20 Oct - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"

21 Oct - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"

21 Oct - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"

21 Oct - Damien François, "**Introduction to parallel computing**"

26 Oct - Olivier Mattelaer, "**Introduction to C programming language**"

26 Oct - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"

27 Oct - Olivier Mattelaer, "**Introduction to code versioning**"

27 Oct - Bernard Van Renterghem, "**Debugging/profiling scientific code and scientific libraries**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part I)**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part II)**"

08 Nov - Jérôme de Favereau, "**Introduction to Python**"

08 Nov - Orian Louant, "**Parallel programming with OpenMP**"

09 Nov - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"

09 Nov - Ramon Winterhalder, "**An Introduction to Neural Networks**"

10 Nov - Damien François, "**Preparing, submitting and managing jobs with Slurm**"

10 Nov - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"

10 Nov - David Waroquiers, "**Using a workflow manager to handle large amounts of jobs**"

17 Nov - Damien François, "**Introduction to data storage and access**"

17 Nov - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"

17 Nov - Adeline Grard, "**Open Science and open research data**"

23 Nov - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"

23 Nov - Orian Louant, "**Directive Based Parallel programming on GPU**"

24 Nov - Damien François, "**Efficient use of MATLAB on the cluster**"

24 Nov - Ariel Lozano, "**Efficient use of Python on the clusters**"

Accelerators

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

Accelerators

- Hardware component with a specialized microprocessor
- Mostly General Purpose Graphical Processing Units (GPGPUs)
- Offer excellent floating point performance per Watt
- Parts of computation “offloaded” to accelerator

GPGPUs resources at CÉCI

Cluster	Model	Cores	Memory	Float performance (FP32)	Double performance (FP64)
Dragon2	4 x NVIDIA Tesla V100	5120	16GB	14 TFLOPS	<u>7 TFLOPS</u>
Hercules2	4 x NVIDIA RTX A6000	10752	48GB	<u>40 TFLOPS</u>	1 TFLOPS

18 Oct - Bernard Van Renterghem, "**Introduction to Linux and the command line**"

19 Oct - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"

19 Oct - Juan Cabrera, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"

19 Oct - Damien François, "**Introduction to scientific software development and deployment**"

20 Oct - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"

20 Oct - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"

21 Oct - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"

21 Oct - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"

21 Oct - Damien François, "**Introduction to parallel computing**"

26 Oct - Olivier Mattelaer, "**Introduction to C programming language**"

26 Oct - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"

27 Oct - Olivier Mattelaer, "**Introduction to code versioning**"

27 Oct - Bernard Van Renterghem, "**Debugging/profiling scientific code and scientific libraries**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part I)**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part II)**"

08 Nov - Jérôme de Favereau, "**Introduction to Python**"

08 Nov - Orian Louant, "**Parallel programming with OpenMP**"

09 Nov - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"

09 Nov - Ramon Winterhalter, "**An Introduction to Neural Networks**"

10 Nov - Damien François, "**Preparing, submitting and managing jobs with Slurm**"

10 Nov - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"

10 Nov - David Waroquiers, "**Using a workflow manager to handle large amounts of jobs**"

17 Nov - Damien François, "**Introduction to data storage and access**"

17 Nov - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"

17 Nov - Adeline Grard, "**Open Science and open research data**"

23 Nov - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"

23 Nov - Orian Louant, "**Directive Based Parallel programming on GPU**"

24 Nov - Damien François, "**Efficient use of MATLAB on the cluster**"

24 Nov - Ariel Lozano, "**Efficient use of Python on the clusters**"

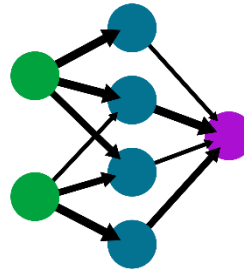
And also...



Source versioning



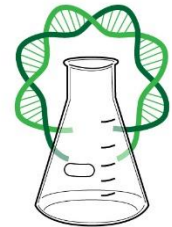
Data storage



Neural networks



Singularity



Open Science

18 Oct - Bernard Van Renterghem, "**Introduction to Linux and the command line**"

19 Oct - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"

19 Oct - Juan Cabrera, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"

19 Oct - Damien François, "**Introduction to scientific software development and deployment**"

20 Oct - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"

20 Oct - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"

21 Oct - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"

21 Oct - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"

21 Oct - Damien François, "**Introduction to parallel computing**"

26 Oct - Olivier Mattelaer, "**Introduction to C programming language**"

26 Oct - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"

27 Oct - Olivier Mattelaer, "**Introduction to code versioning**"

27 Oct - Bernard Van Renterghem, "**Debugging/profiling scientific code and scientific libraries**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part I)**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part II)**"

08 Nov - Jérôme de Favereau, "**Introduction to Python**"

08 Nov - Orian Louant, "**Parallel programming with OpenMP**"

09 Nov - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"

09 Nov - Ramon Winterhalter, "**An Introduction to Neural Networks**"

10 Nov - Damien François, "**Preparing, submitting and managing jobs with Slurm**"

10 Nov - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"

10 Nov - David Waroquiers, "**Using a workflow manager to handle large amounts of jobs**"

17 Nov - Damien François, "**Introduction to data storage and access**"

17 Nov - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"

17 Nov - Adeline Grard, "**Open Science and open research data**"

23 Nov - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"

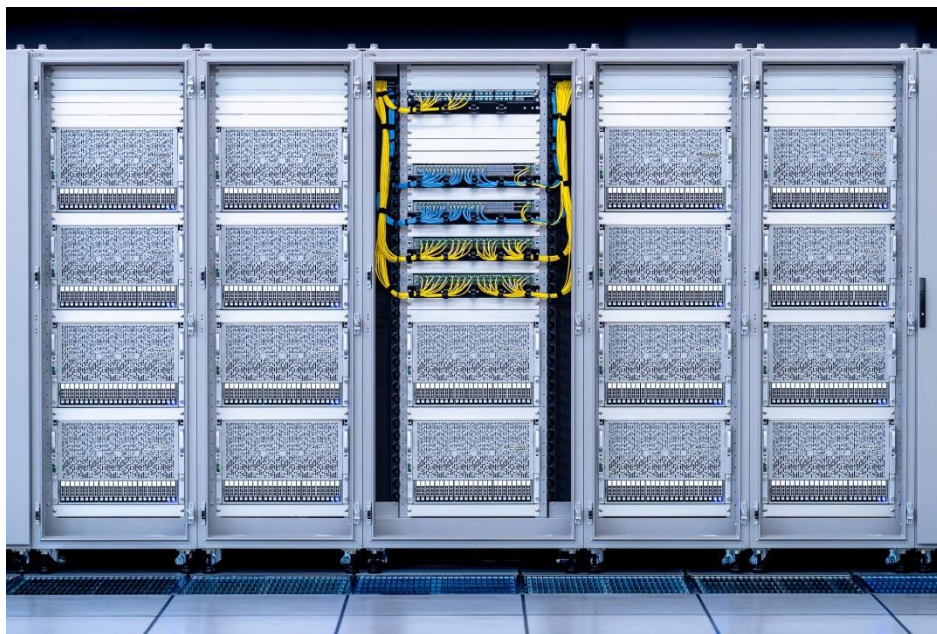
23 Nov - Orian Louant, "**Directive Based Parallel programming on GPU**"

24 Nov - Damien François, "**Efficient use of MATLAB on the cluster**"

24 Nov - Ariel Lozano, "**Efficient use of Python on the clusters**"

Green HPC

- Green500
 - Rank supercomputers in terms of energy efficiency
 - Performance per Watt (GFLOPS/W)
 - <https://www.top500.org/lists/green500>



MN-3, Preferred Networks, Japan

A green supercomputer: LUMI

- 200,000 cores
- Negative carbon footprint
- 100% renewable energy
- Wasted heat can be used by 20% of the houses of the surrounding city



Carbon footprint of your computation

- <http://www.green-algorithms.org>

Green Algorithms

How green are your computations?

Details about your algorithm

To understand how each parameter impacts your carbon footprint, check out the formula below and the [methods article](#).

Runtime (HH:MM)


Type of cores

Number of cores


Model

Memory available (in GB)


Select the platform used for the computations




303.10 g CO2e
Carbon footprint




2.28 kWh
Energy needed



0.33 tree-months
Carbon sequestration



1.73 km
in a passenger car



1 %
of a flight Paris-London

Share your results with [this link!](#)



Thanks you for your attention
and happy computing

18 Oct - Bernard Van Renterghem, "**Introduction to Linux and the command line**"

19 Oct - Olivier Mattelaer, "**Connecting with SSH from Windows: Introduction and advanced topics**"

19 Oct - Juan Cabrera, "**Connecting with SSH from Linux or Mac: Introduction and advanced topics**"

19 Oct - Damien François, "**Introduction to scientific software development and deployment**"

20 Oct - Bernard Van Renterghem, "**Introduction to modules and software on a CÉCI cluster**"

20 Oct - Bernard Van Renterghem, "**Introduction to compilers and compiling, and optimized libraries**"

21 Oct - Pierre-Yves Barriat, "**Introduction to structured programming with Fortran**"

21 Oct - Damien François, "**Introduction to scripting and interpreted languages (Python, R, Octave)**"

21 Oct - Damien François, "**Introduction to parallel computing**"

26 Oct - Olivier Mattelaer, "**Introduction to C programming language**"

26 Oct - Olivier Mattelaer, "**Introduction to Object-Oriented programming with C++**"

27 Oct - Olivier Mattelaer, "**Introduction to code versioning**"

27 Oct - Bernard Van Renterghem, "**Debugging/profiling scientific code and scientific libraries**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part I)**"

28 Oct - Orian Louant, "**Parallel programming with MPI (Part II)**"

08 Nov - Jérôme de Favereau, "**Introduction to Python**"

08 Nov - Orian Louant, "**Parallel programming with OpenMP**"

09 Nov - Olivier Mattelaer, "**Parallel programming on GPU with CUDA**"

09 Nov - Ramon Winterhalder, "**An Introduction to Neural Networks**"

10 Nov - Damien François, "**Preparing, submitting and managing jobs with Slurm**"

10 Nov - Olivier Mattelaer, "**Using a Checkpoint/restart program to overcome time limits**"

10 Nov - David Waroquiers, "**Using a workflow manager to handle large amounts of jobs**"

17 Nov - Damien François, "**Introduction to data storage and access**"

17 Nov - Ariel Lozano, "**How to use efficiently the different storage solutions provided with the CECI clusters**"

17 Nov - Adeline Grard, "**Open Science and open research data**"

23 Nov - Olivier Mattelaer, "**Packaging software in portable containers with Singularity**"

23 Nov - Orian Louant, "**Directive Based Parallel programming on GPU**"

24 Nov - Damien François, "**Efficient use of MATLAB on the cluster**"

24 Nov - Ariel Lozano, "**Efficient use of Python on the clusters**"