

CÉCI Technical Talks

The CÉCI sysadmins
13th CÉCI Users Meeting



Vega
2112 cores

256 GB RAM

70 TiB storage

Decommissionned

Lemaitre 3
1984 cores

95 GB RAM

144 TB storage

Q2 2018

Dragon 2
592 cores

384 GB RAM

4 GPU

100 TB storage

Q1 2019

Hercules 2
1536 cores

2 TB RAM

16 GPU

60 TB storage

Q3 2019

NIC5
4672 cores

1 TB RAM

250 TB storage

Q4 2020

8656 cores total – 20 GPU



NIC5
4672 cores

1 TB RAM

250 TB storage

Q4 2020

Lemaitre 4
5120 cores

766 GB RAM

144 TB storage

Q1 2024

Lyra
1472 cores

384 GB RAM

46 GPU

3 PB storage

Q2 2024

Dragon 3
~1200 cores

512 GB RAM

120 TB storage

Q1 2025

Hercules 3
~2300 cores

3 TB RAM

16 GPU

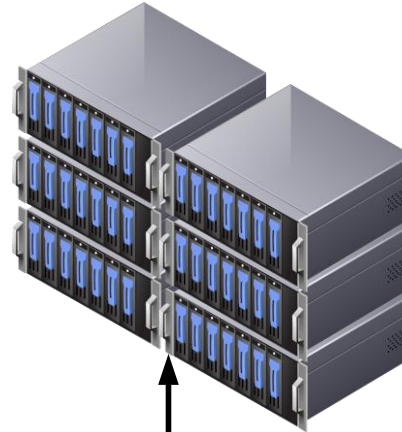
300 TB storage

Q1 2025

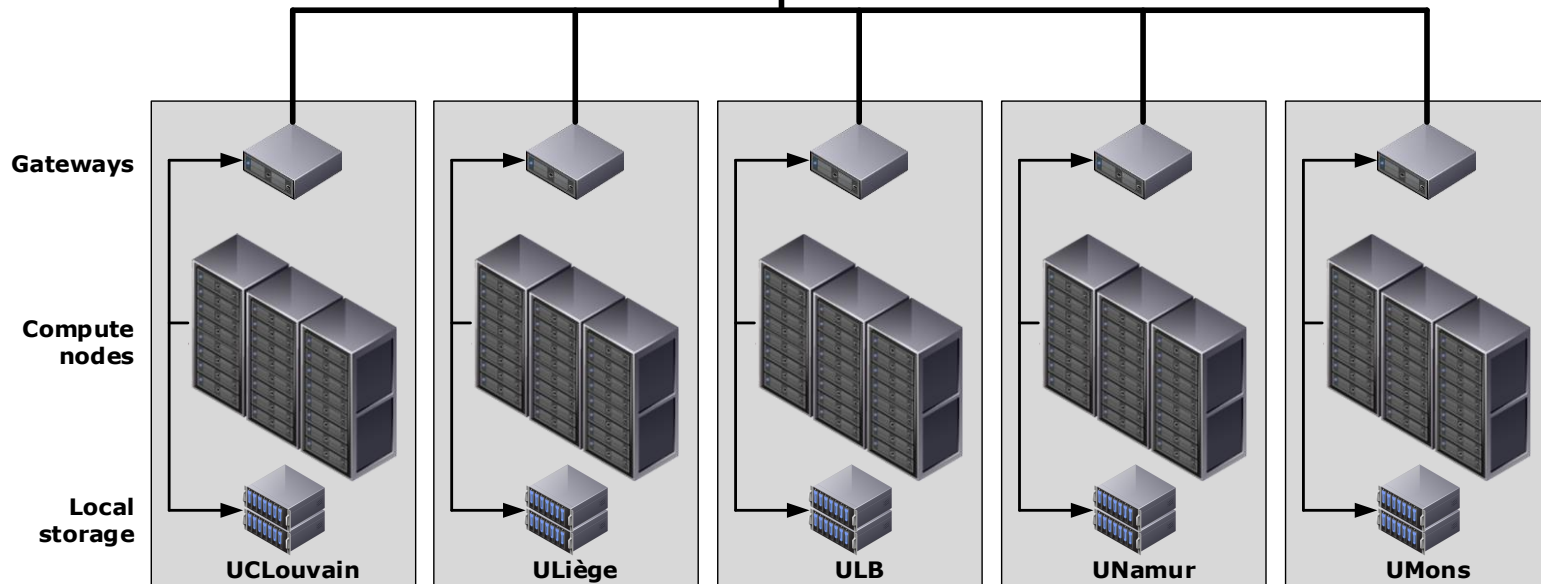
14,000+ cores total – 70+ GPU

CÉCI Common Storage

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




IBM
**Spectrum
Storage**





New CÉCI common storage

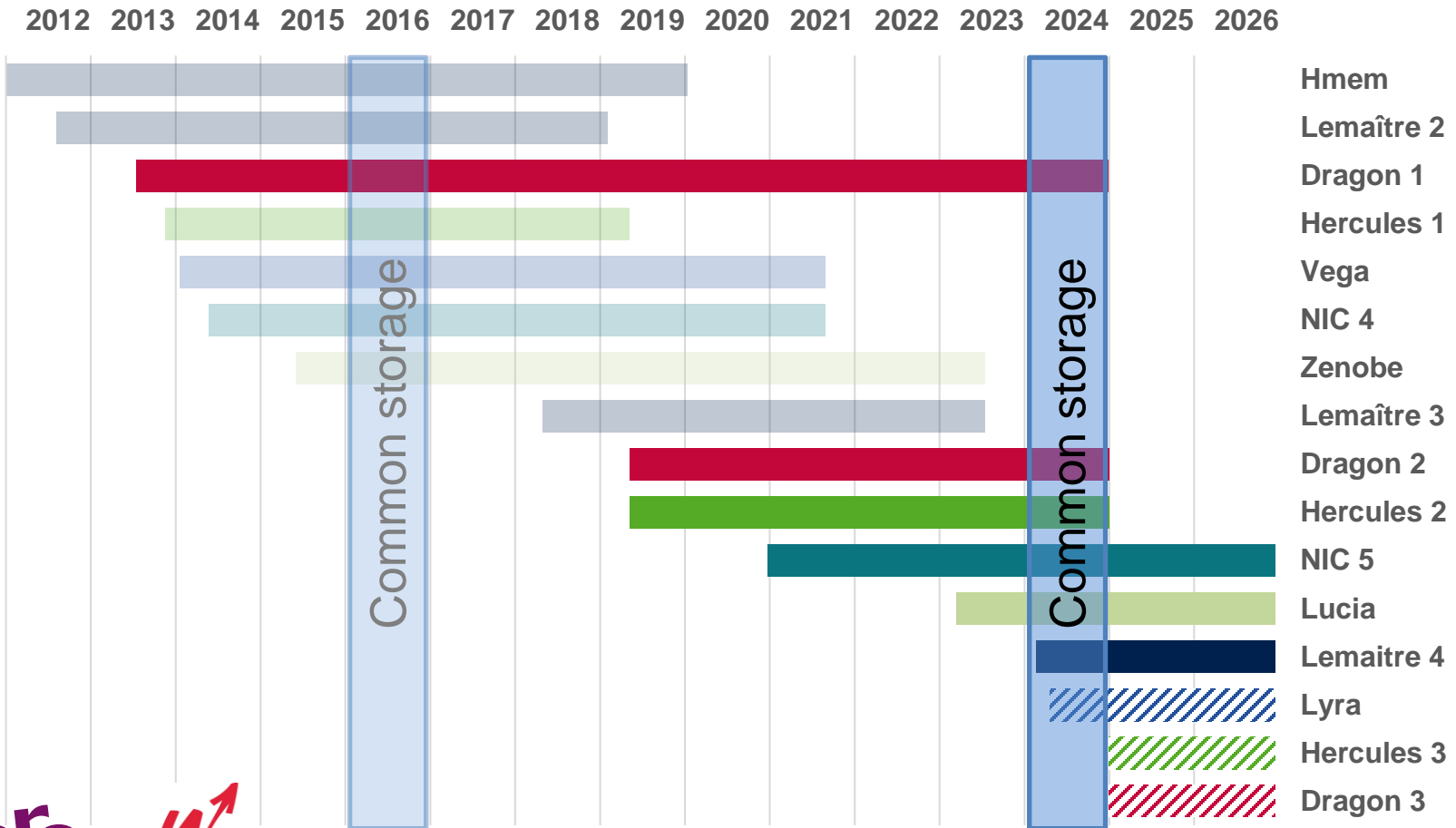
Current

- Installed in 2016
-  IBM **Spectrum Scale**
- 230 TB net storage on spinning rust
- Installed at UCLouvain and ULiège

New

- Expected Q3 2024
-  **Red Hat**  **ceph**
- **1 PB** net storage on NVMe SSD
- Fully distributed storage

CÉCI 2024 roadmap



Hercules 3



The CÉCI sysadmins
CÉCI day 2024

Hercules 2

1536 cores

up to 2 TiB memory

16 GPU

60 TB storage

10 GbE network

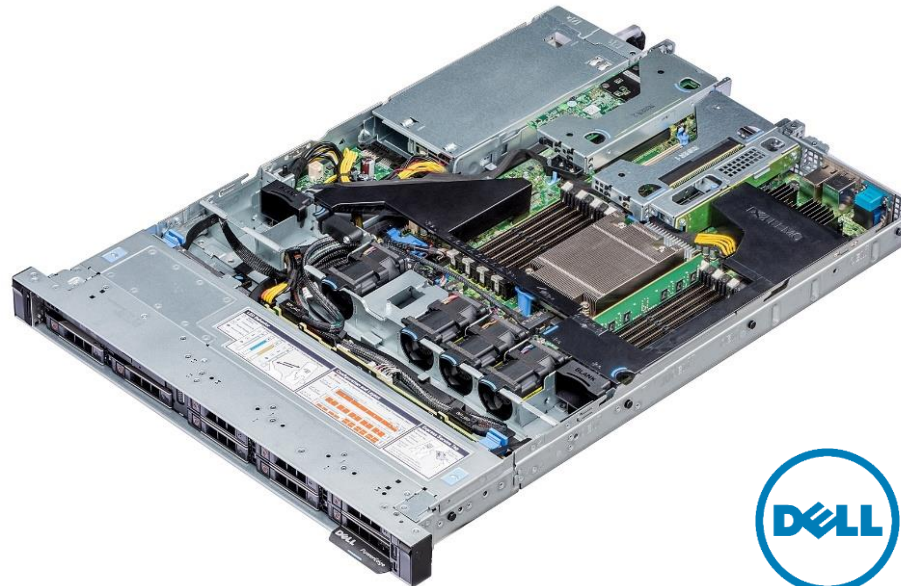


Hercules – CPU nodes

Hercules 2

#	Processor	Memory	Storage
30	2x 8-core Intel “Sandybridge”	64 – 128 GB	1 TB HDD
24	1x 32-core AMD EPYC Gen1 “Naples”	256 GB	5 TB HDD
4	1x 32-core AMD EPYC Gen1 “Naples”	512 GB	5 TB HDD
2	2x 32-core AMD EPYC Gen1 “Naples”	2 TB	8 TB HDD

In production
since 2012



Hercules – CPU nodes

Hercules 2

#	Processor	Memory	Storage
30	2x 8-core Intel "Sandybridge"	64 – 128 GB	1 TB HDD
26	1x 32-core AMD EPYC Gen1 "Naples"	256 GB	5 TB HDD
4	1x 32-core AMD EPYC Gen1 "Naples"	512 GB	5 TB HDD
2	2x 32-core AMD EPYC Gen1 "Naples"	2 TB	8 TB HDD

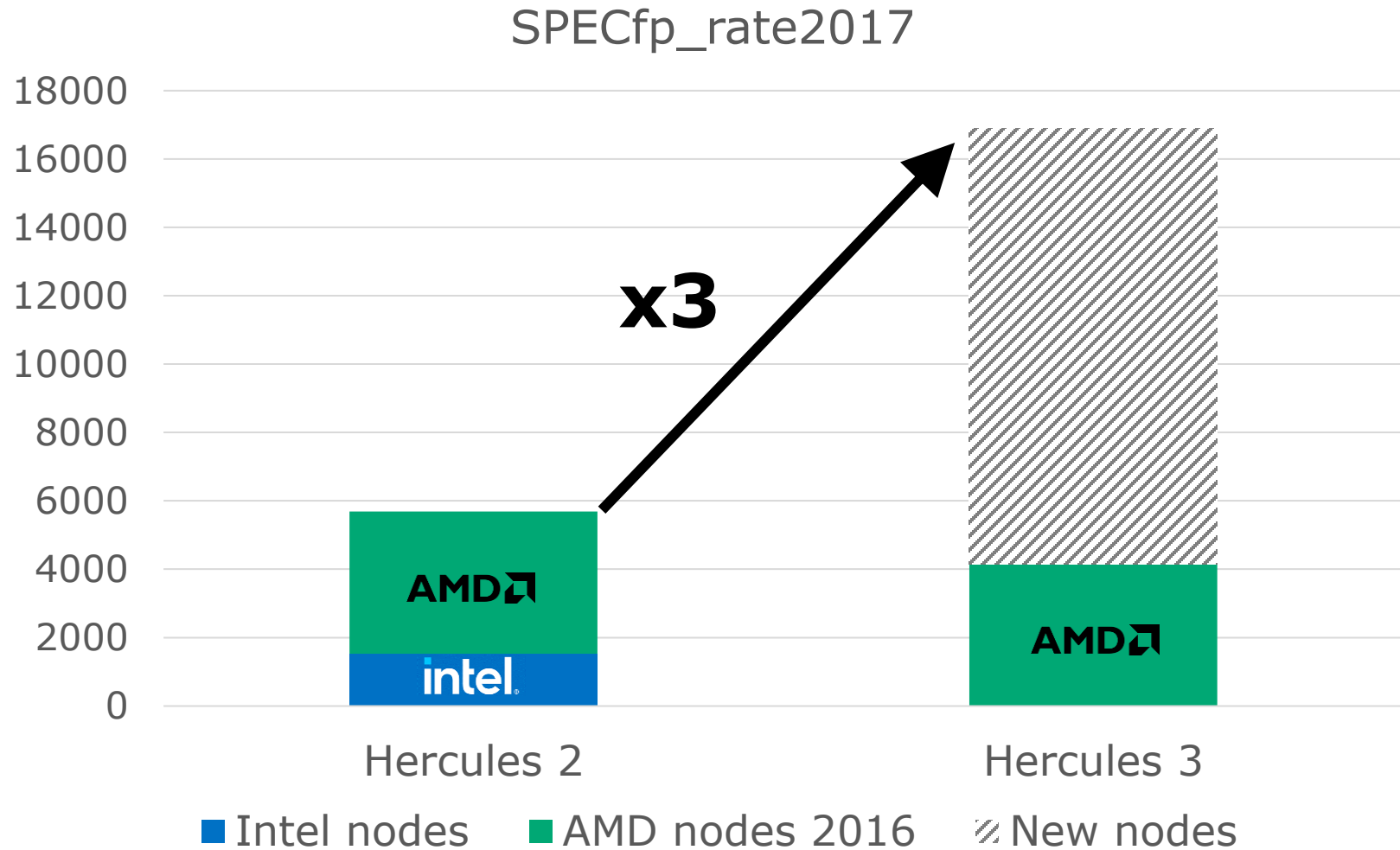
Hercules 3

#	Processor	Memory	Storage
26	1x 32-core AMD EPYC Gen1 "Naples"	256 GB	5 TB HDD
4	1x 32-core AMD EPYC Gen1 "Naples"	512 GB	5 TB HDD
2	2x 32-core AMD EPYC Gen1 "Naples"	2 TB	8 TB HDD
18	1x 48-core AMD EPYC Gen4 "Genoa"	384 GB	6 TB NVMe
4	1x 48-core AMD EPYC Gen4 "Genoa"	768 GB	6 TB NVMe
1	2x 48-core AMD EPYC Gen4 "Genoa"	3 TB	12 TB NVMe

32 nodes
from
Hercules 2

23 new
nodes

Total CPU performance



Hercules – GPU nodes

Hercules 2

#	Processor	Memory	Storage	#GPU	VRAM
1	1x 32-core AMD EPYC “Rome”	256 GB	7 TB HDD	4	11 – 24 GB
1	1x 32-core AMD EPYC “Rome”	256 GB	7 TB NVMe	4	48 GB
1	2x 32-core AMD EPYC “Milan”	512 GB	200 GB SSD	8	48 GB



Hercules – GPU nodes

Hercules 2

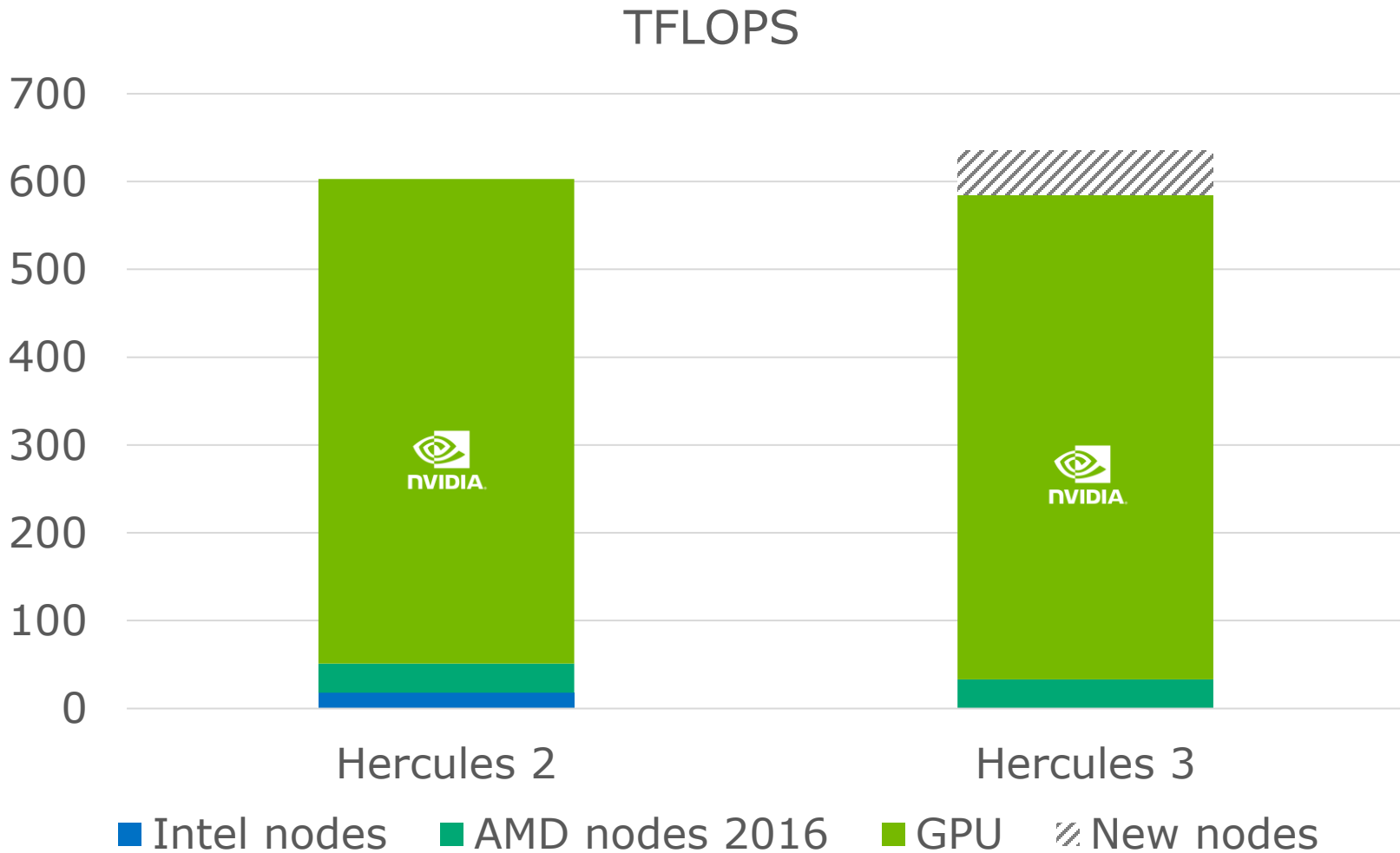
#	Processor	Memory	Storage	#GPU	VRAM
1	1x 32-core AMD EPYC “Rome”	256 GB	7 TB HDD	4	11 – 24 GB
1	1x 32-core AMD EPYC “Rome”	256 GB	7 TB NVMe	4	48 GB
1	2x 32-core AMD EPYC “Milan”	512 GB	200 GB SSD	8	48 GB



Hercules 3

#	Processor	Memory	Storage	#GPU	VRAM
1	1x 32-core AMD EPYC “Rome”	256 GB	14 TB HDD	4	11 – 24 GB
1	1x 32-core AMD EPYC “Rome”	256 GB	12 TB NVMe	4	48 GB
1	2x 32-core AMD EPYC “Milan”	512 GB	16 TB NVMe	8	48 GB

CPU+GPU performance



Homedir storage

Hercules 2



HPE ProLiant XL420 Gen10

40 TB HDD
+3 TB SSD cache

Home directories

Quota: 1 TB/user

Hercules 3



5-nodes Ceph cluster

256 TB HDD
+64 TB NVMe cache

Home directories
Virtual Machines

Quota: **4 TB/user**

Globalscratch storage

Hercules 2



HPE StorageWorks D2700

20 TB HDD

Global scratch

Quota: 4 TB/user

Hercules 3



HPE ProLiant XL420 Gen10

60 TB HDD

+6 TB SSD cache

Global scratch

Databases

Quota: **8 TB/user**

From Hercules 2 to Hercules 3

Hercules 2

1536 cores

up to 2 TB memory

16 GPU

60 TB storage

10 GbE network

Hercules 3

2368 cores

up to **3 TB** memory

16 GPU

300 TB storage

25 GbE Network

Expected in production Q1 2025

Dragon 3

UMONS

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Dragon - Compute nodes

CPU nodes

#	Processor	Memory	Storage
15	2x 16-core Intel Xeon Gold 6142 "Skylake"	192 GB	3 TB HDD
2	2x 16-core Intel Xeon Gold 6142 "Skylake"	384 GB	3 TB HDD

GPU nodes

#	Processor	Memory	Storage	#GPU	VRAM
2	2x 12-core Intel Xeon Gold 6126 "Skylake"	192 GB	3 TB	2	16 GB

Dragon 2: 592 cores – 4 GPU

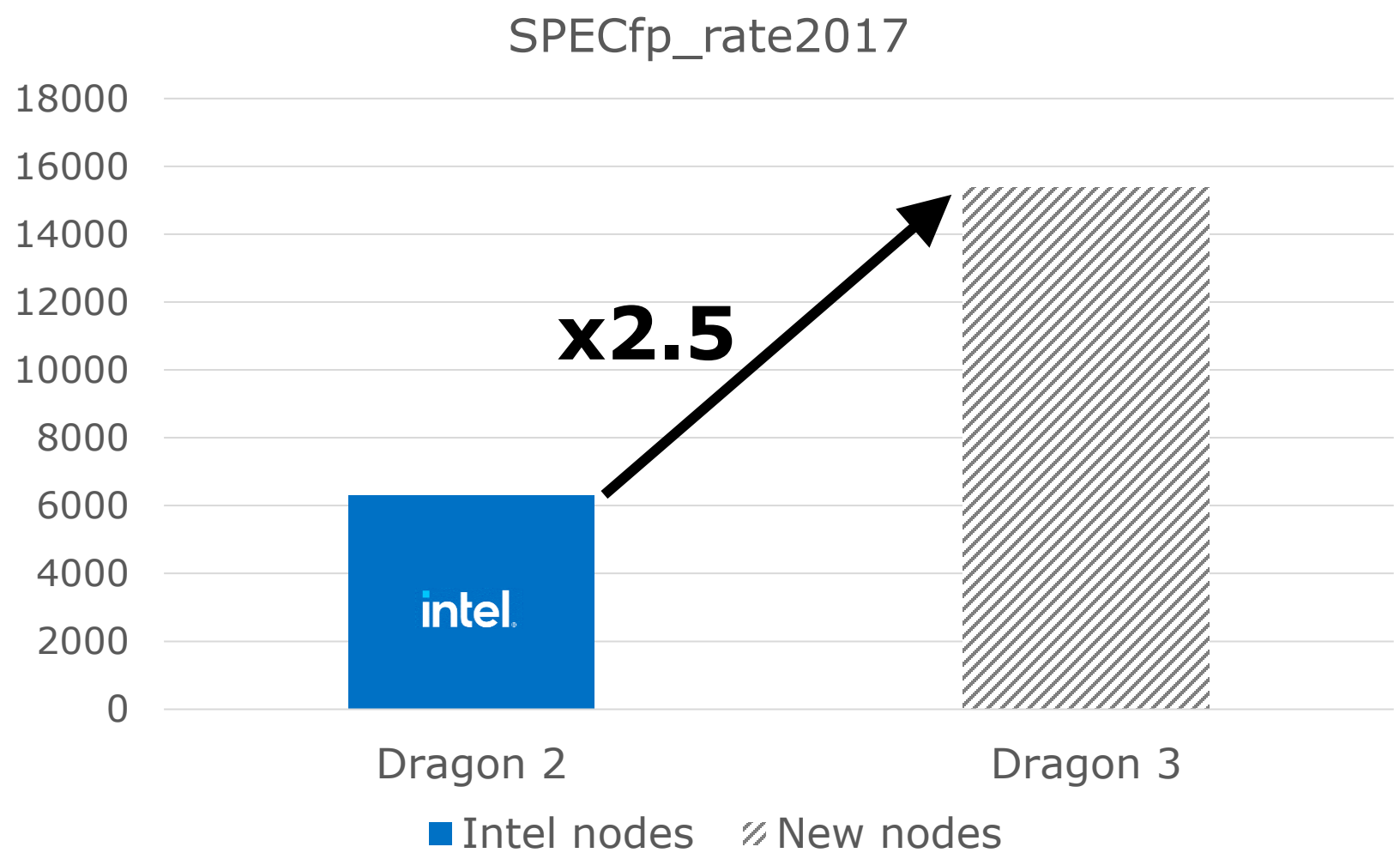


CPU nodes

#	Processor	Memory	Storage
20	2x 32-core Intel Xeon Gold 6548N "Emerald Rapids"	512 GB	6 TB NVMe

Dragon 3: 1280 cores – no GPU

Total CPU performance



From Dragon 2 to Dragon 3

Dragon 2

592 cores

up to 384 GB memory

4 GPU

40 TB storage

10 GbE Network

Dragon 3

1280 cores

up to **512 GB** memory

no GPU

120 TB storage

25 GbE Network

Expected in production Q1 2025

Lemaître 4



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Georges Lemaître

Father of the Big Bang Theory...



Burroughs E101, May 1959, Digital Laboratory of UCL (credit archives.uclouvain.be)

Previous Lemaître Clusters

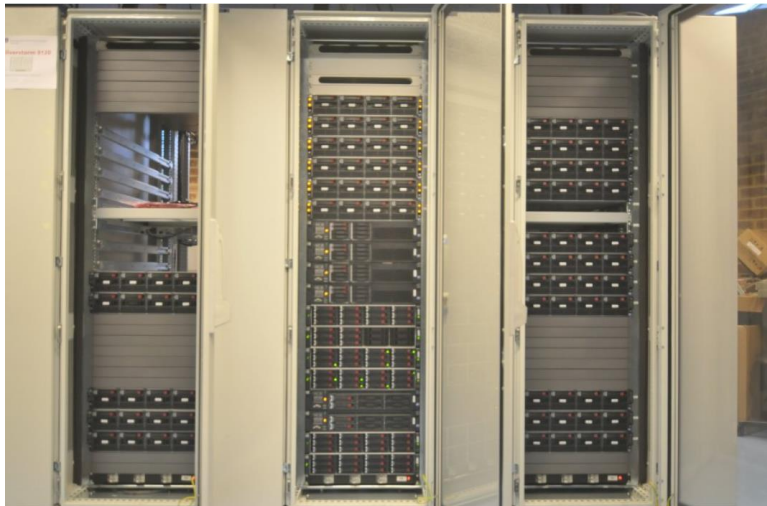
2005-2012 **Lemaitre 1** 256 Core, 1.3 TFlops, 120W/c



128 dual AMD Opteron 252/2.6Ghz 4GB RAM
10Gbps Infiniband
6TB /home, 1.2TB /scratch

Previous Lemaître Clusters

2005-2012 Lemaître 1 256 Core, 1.3 TFlops, 120W/c
 2012-2018 **Lemaître 2** 1334 Core, 13.6 TFlops, 22W/c



112 dual Intel 6 core
 Xeon/2.53Ghz 48GB RAM
 40Gbps QDR Infiniband
 40TB /home, 120TB /scratch

Previous Lemaître Clusters

2005-2012 Lemaître 1 256 Core, 1.3 TFlops, 120W/c
 2012-2018 Lemaître 2 1334 Core, 13.6 TFlops, 22W/c
 2018-2024 **Lemaître 3** 2032 Core, 75.4 Tflops, 13W/c



80 Intel
 2x12 core Skylake Gold 2.3Ghz
 96GB RAM
 56Gbps Omni-path
 35TB /home, 583TB /scratch

Current Lemaître Cluster

2005-2012	Lemaitre 1	256 Core,	1.3 TFlops,	120W/c
2012-2018	Lemaitre 2	1334 Core,	13.6 TFlops,	22W/c
2018-2024	Lemaitre 3	2032 Core,	75.4 TFlops,	13W/c
2024-	Lemaitre 4	5120 Core,	303 Tflops,	8W/c



40 Dual 64 Core AMD Epyc
Genoa 3.7GHz, 768GB RAM

100 Gbps Infiniband HDR
40TB /home, 318TB /scratch

Inside Lemaitre 4

The front-end, the working nodes, the file servers...



Inside Lemaitre 4

The working nodes



Inside Lemaitre 4

The AMD EPYC 9004 GENOA

	AMD EPYC 7001 'NAPLES'	AMD EPYC 7002 'ROME'	AMD EPYC 7003 'MILAN'	AMD EPYC 9004, 8004 'GENOA', 'SIENA'
				
Core Architecture	'Zen'	'Zen 2'	'Zen 3'	'Zen 4' and 'Zen 4c'
Cores	8 to 32	8 to 64	8 to 64	8 to 128
IPC Improvement Over Prior Generation	N/A	~24% ^{ROM-236}	~19% ^{MLN-003}	~14% ^{EPYC-038}
Max L3 Cache	Up to 64 MB	Up to 256 MB	Up to 256 MB	Up to 384 MB (EPYC 9004) Up to 128 MB (EPYC 8004)
Max L3 Cache with 3D V-Cache™ technology			768 MB	Up to 1152 MB
PCIe® Lanes	Up to 128 Gen 3	Up to 128 Gen 3	Up to 128 Gen 4	Up to 128 Gen 5 8 bonus lanes Gen 3
CPU Process Technology	14nm	7nm	7nm	5nm
I/O Die Process Technology	N/A	14nm	14nm	6nm
Power (Configurable TDP [cTDP])	120-200W	120-280W	155-280W	70-400W
Max Memory Capacity	2 TB DDR3-2400/2666	4 TB DDR4-3200	4 TB DDR4-3200	6 TB DDR5-4800

Inside Lemaitre 4

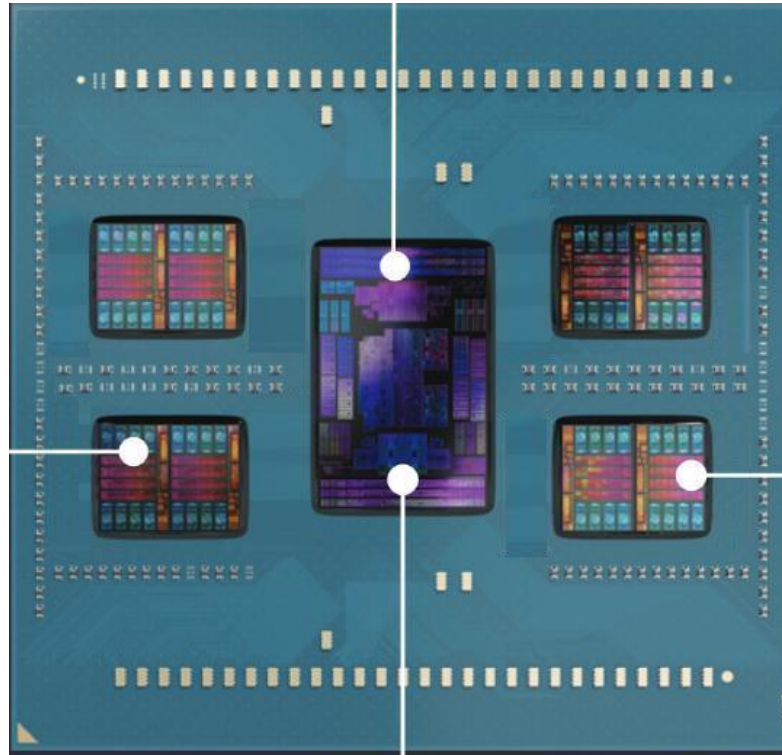
The AMD EPYC 9534 GENOA

8 zen4 cores
with 1MB L2 cache

=

a Core Complex CCX,
with 32MB L3 cache

Z4	L2	32MB L3 Cache	L2	Z4
Z4	L2		L2	Z4
Z4	L2		L2	Z4
Z4	L2		L2	Z4



Two CCX

=

A CPU Die CCD

4 CCD + 1 I/O Die

=

EPYC 9534

I/O die : 12 Mem DDR5, PCIe, Infinity Fabric 36Gb/s, SATA Controllers,...

Inside Lemaitre 4

The AMD EPYC 9534 GENOA

- 12 Channel DDR5 Mem (2x 12x 32GB = 768 GB per node)
- AVX512 support, on a 256-bit data path
(Since 2017 on Intel Skylake SP)
- +123% SPECrate 2017_fp_base on previous AMD Zen3 Milan
- 2.45GHz normal frequency, 3.7GHz in Turbo mode
- NUMA architecture !

Lemaitre 4 I/O considerations

Cluster	FS	IOzone MB/s	Mdtest
Lemaitre3	/home	811	28377
Lemaitre4	/home	1718 (x2)	123659 (x4)
Lemaitre3	/scratch	3466	16937
Lemaitre4	/scratch	2224 (-64%)	158745 (x9)

- **iozone** (write throughput, 256KB block on one node)
- **Mdtest** IOR (iops, write/s of 100 process on 10 nodes)
- /home Lemaitre3 : 23 SAS 2TB in ZFS Raid6
- /home Lemaitre4 : 9 SATA 7.68TB **SSD** in RAID6
- /scratch Lemaitre3 Beegfs with 4 file servers
- /scratch Lemaitre4 Beegfs with 1 file server

Lemaitre 3 decommissioning

PRELEMINARY PROPOSAL, feedback welcome by email...

- **May 1st** : no new user account
 - some working nodes are removed

- **July 1st** : no more running jobs
 - cleaning of the /scratch
 - /home in readonly

- **September 1st** : stop with a R/O /home copy on lemaitre4

Lemaitre 4 Welcome!

```

Welcome to

      /_(-//)(// // (- //

Massively parallel CISM-CECI cluster

40 nodes: 2 x AMD EPYC 9534 64-Core processors (128 HT) 768GB RAM
non-blocking 100Gbps Infiniband network
318T BeeGFS global scratch

contact, support: egs-cism@listes.uclouvain.be
-----
4422/10240 CPUs available (load 56%) - 77 jobs running, 0 pending.

* Job info for user bvr: 0 job running, 0 pending.
* Diskquotas for user bvr
Filesystem      used      limit      files      limit
$HOME           53K       100G       10
$GLOBALSCRATCH  0.0kB    unlimited  0    unlimited
$CECIHOME       365.4MB   100.0GB    690    100000
$CECITRSF       0.0kB     1.0TB     1    unlimited
* Account expiration: 2033-05-12

Don't know where to start?
--> http://www.cec-hpc.be/install_software.html
--> http://www.cec-hpc.be/slurm_tutorial.html
[bvr@lm4-f001 ~]$

```

Vega



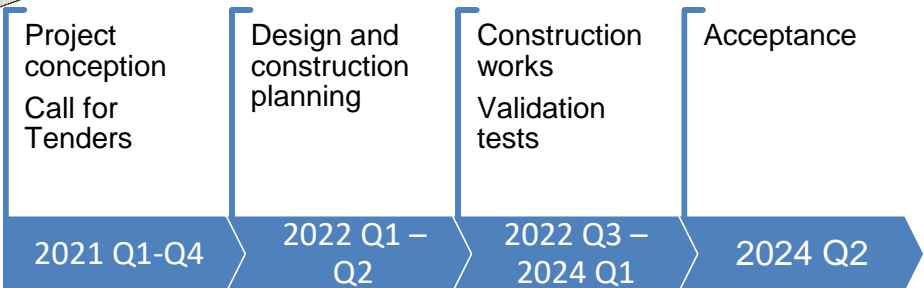
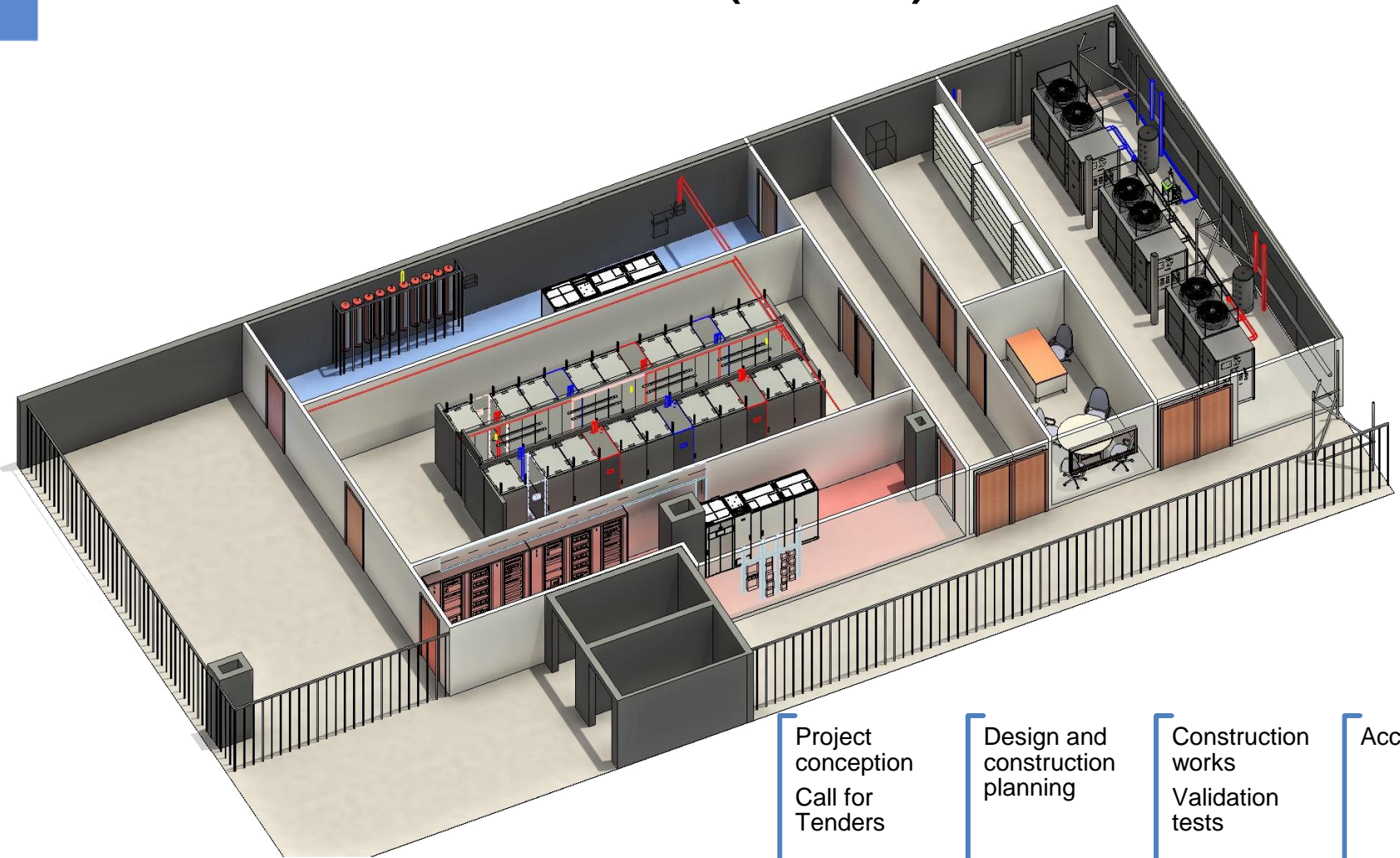
ULB

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ULB – New CECI Cluster

- Vega Cluster decommissioned in Oct 2020
- ULB Solbosch DC not appropriate to host new cluster
- 2020 Q3 the ULB approved a long-awaited project for building a new DC

ULB – New DC (A6K)



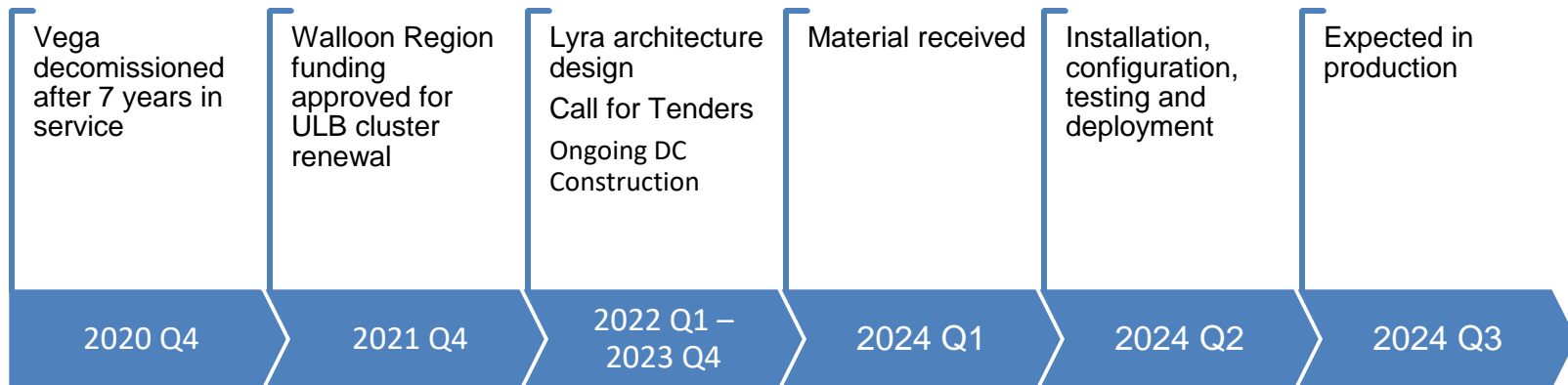
ULB – New DC (A6K)

- 18 racks 48U
- 250 kW of IT equipment
- Redundant power supply
- 2 power line sources with UPS
- Free cooling ~9 months/year
- PoP Belnet with redundant links
- Power Usage Effectiveness PUE \approx 1.2



ULB – New CECI cluster (Lyra)

- Walloon Region funding approved 2021 Q4
 - CECI cluster oriented for ML, AI, Big Data
 - All compute nodes will have GPUs



ULB – New CECI cluster (Lyra)



- 23x Servers:
 - 2x 32 core Epyc 9354 3.25GHz
 - 384GB RAM
 - 2x Nvidia RTX 6000 ADA
 - 6x 22TB HDD
 - 4x 2TB NVMe
 - 25GbE
- Totals
 - Cores: 1472
 - RAM: 8832 GB
 - Raw HDD: 3036 TB
 - Raw flash: 176 TB
 - GPUs: 46

ULB – New CECI cluster (Lyra)

Planned Hyperconverged architecture

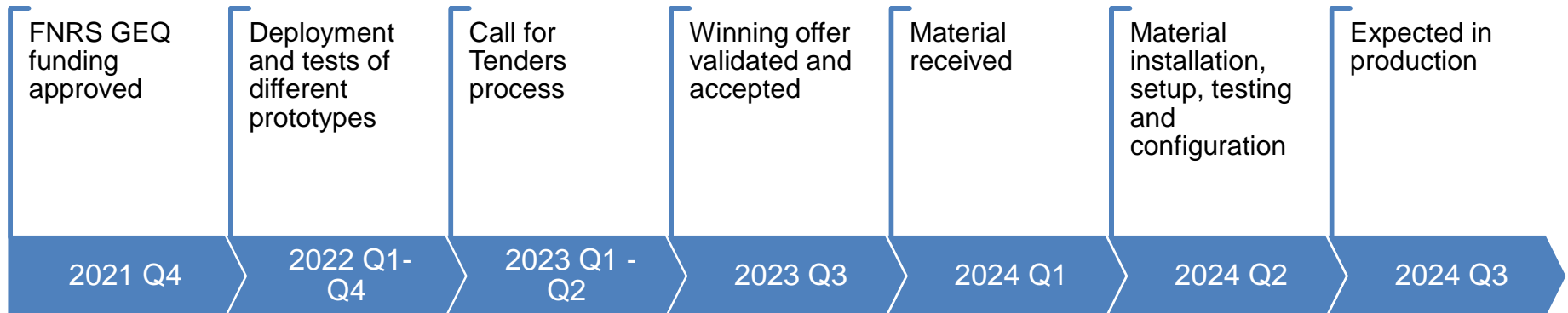
- Everything will be virtualized
- 3x servers:
 - Run all management services and login nodes
 - Login nodes will have GPUs !
 - Compute nodes for debug partition
 - CEPH cluster for Home and Software (~100TB net)
- 20x servers:
 - 40x VMs as compute nodes
 - 28 Cores
 - 160GB RAM
 - 1x RTX A6000 ADA GPU
 - 2TB LOCALSCRATCH
 - Total dedicated to compute: 1120 cores / 6400 GB RAM
 - CEPH cluster for GLOBALSCRATCH (~880 TB net)

New CÉCI Common Storage

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New CECI Common Storage

- Current common storage on production since 2017 Q2
- CECI submission to the 2021 FNRS GEQ call:
 - Storage solution, distributed and accessible by all CECI clusters
 - 1PB net minimum



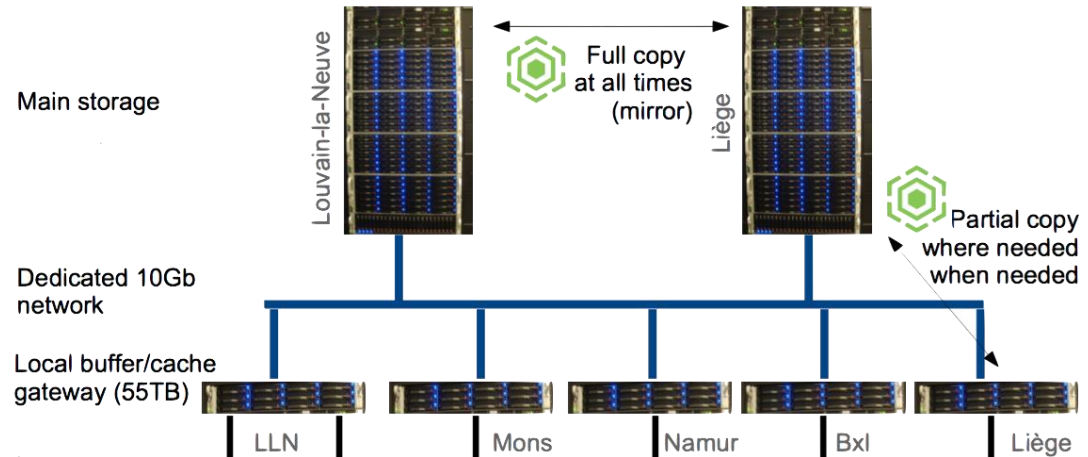
New CECI Common Storage



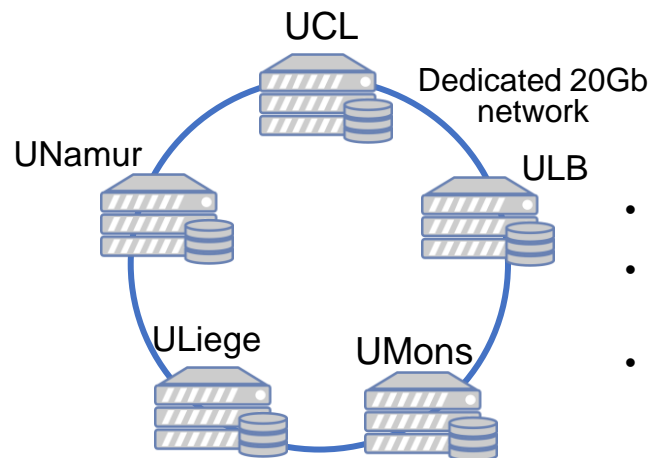
- Per site 4x storage servers:
 - 2x 16 core Epyc 9121 3GHz
 - 192GB RAM
 - 24x 7.68TB NVMe
 - 10GbE
- 20 Gbps Belnet multisite link
- Distributed CEPH cluster

New CECI Common Storage

Current
GPFS
storage



New
CEPH
storage



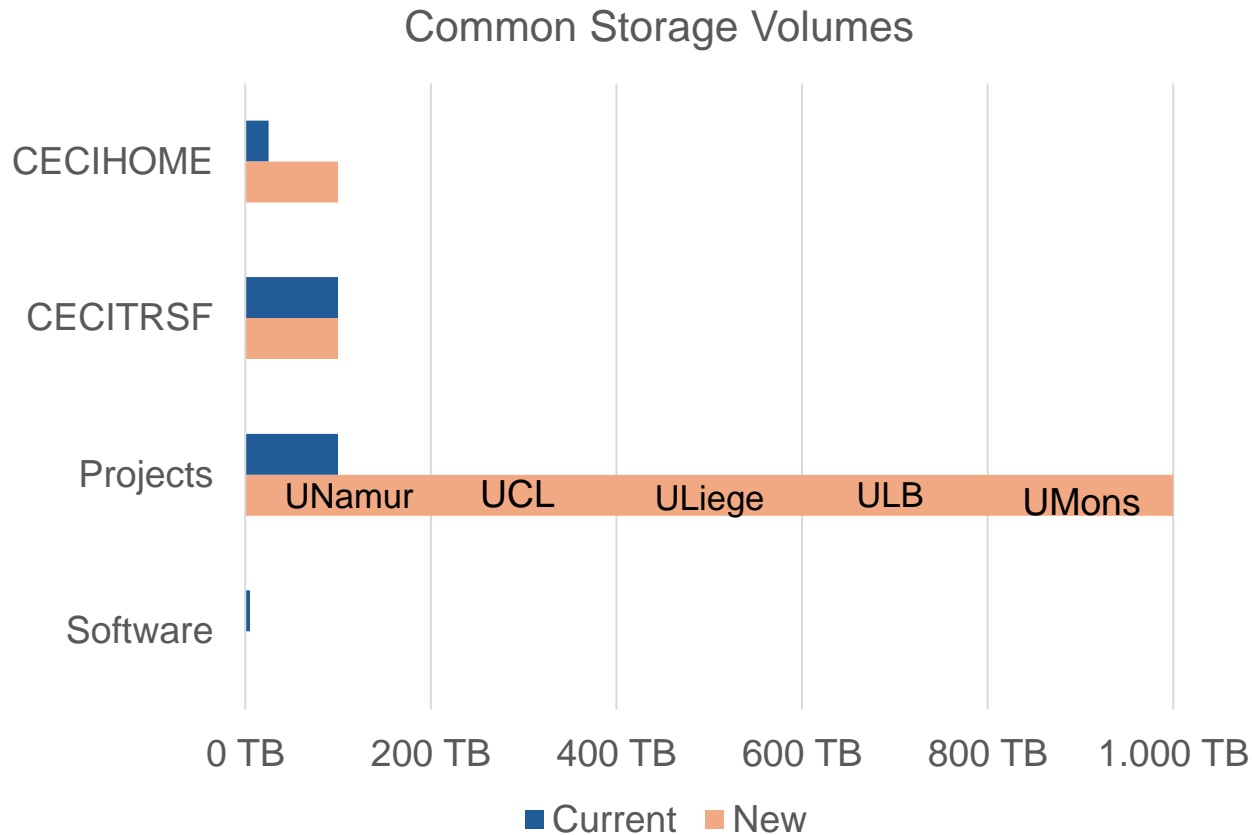
CEPH cluster

- Each site has identical equipment
- Global cephfs filesystem with 3x replication
- With this setup **~1200 TB** net

New CECI Common Storage

Planned volumes distribution

- Current storage: 230TB
- New storage: 1200TB



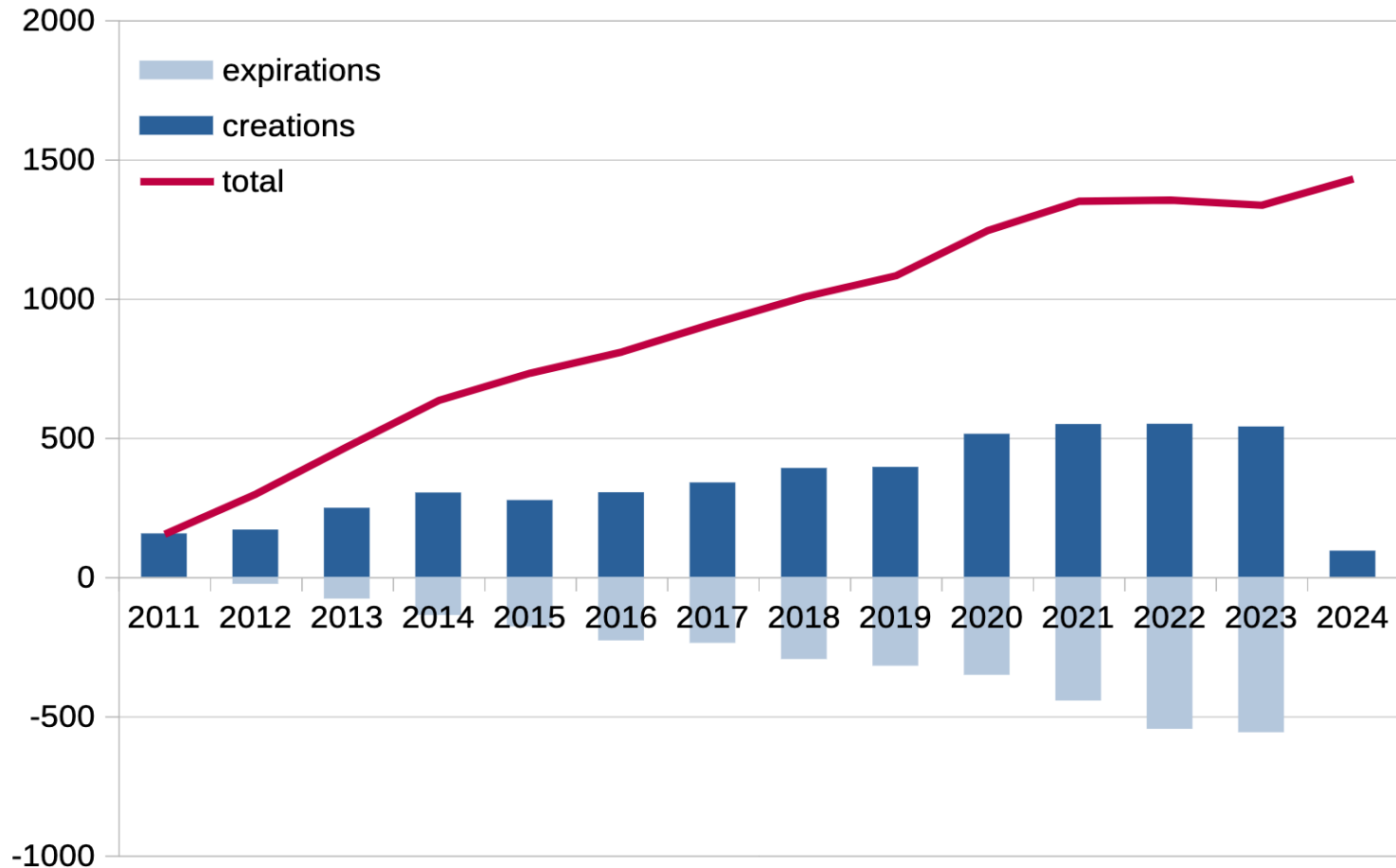
Help us help you!

The CÉCI sysadmins
13th CÉCI Users Meeting

Help "you": the CÉCI users



4900+ Accounts created since 2011



Help "us": the CÉCI sysadmins

UCLouvain: **CISM** (4.4)
ULiège: **nicadm** (1)
UNamur: **PTCI** (1.5)
UMons: **CMN** (1)
ULB: **HPC team** (2)
CÉCI: Logisticien (1.5)

~11.5

Help "us": the CÉCI sysadmins

**WE'RE
HIRING!**

<https://www.ceci-hpc.be>

Help "us": the CÉCI sysadmins

UCLouvain: **CISM** (4.4)
ULiège: **nicadm** (1)
UNamur: **PTCI** (1.5)
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ULB: **HPC team** (2)
CÉCI: Logisticien (1.5)

~11.5

Our goals

 provide as much uptime as possible

 accommodate a wide spectrum of jobs

 maximize resource utilization

 minimize turnaround for your jobs

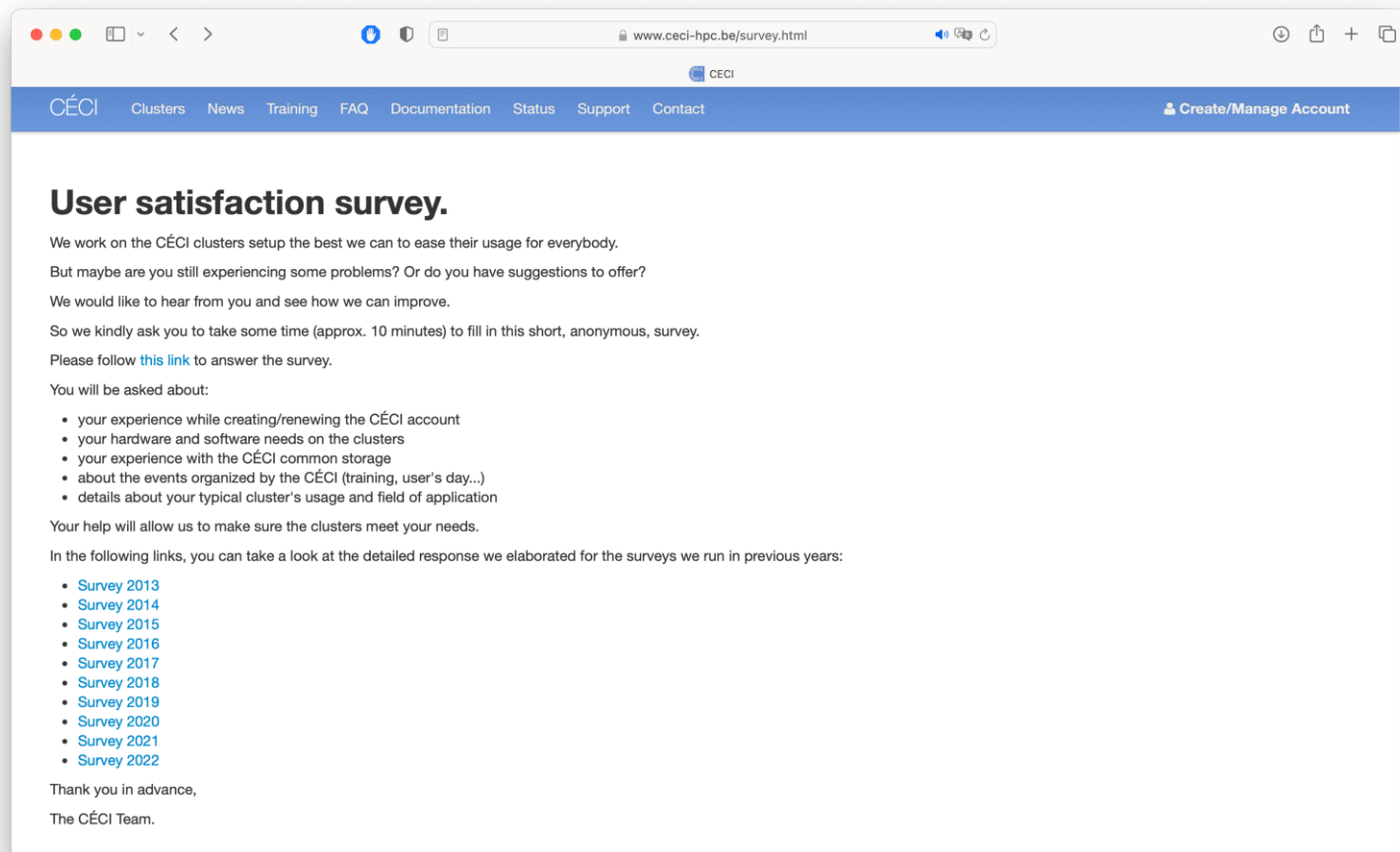


Our messages today

- we can only act on your problems if you report them
- how you request help really impacts the possible time to response
- there are certain tasks you can do by yourself
- wasting resources has an impact on the planet and on other's research
- certain workflows can lead to problems on HPC clusters

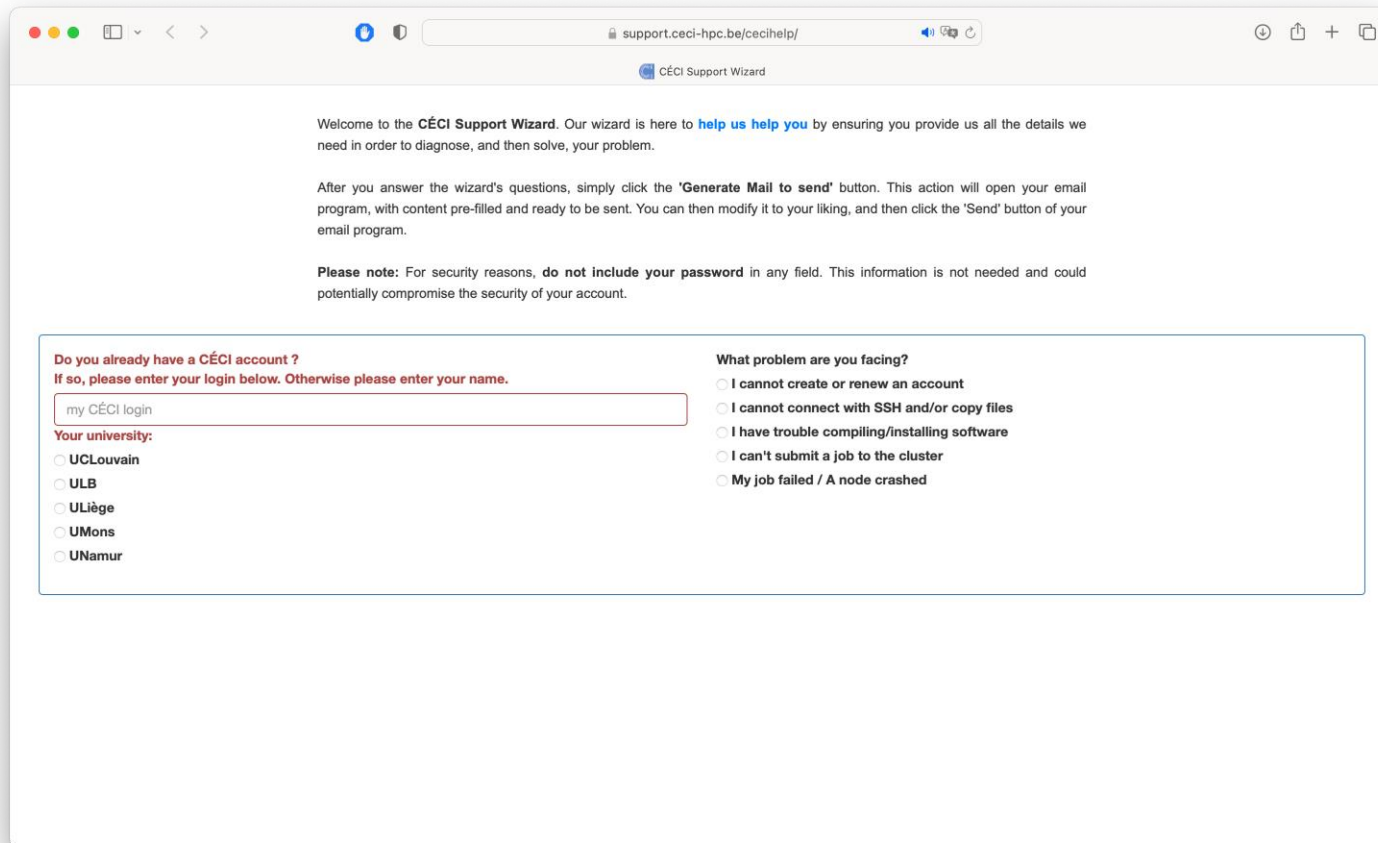
We can only act on your problems if you report them

- Via the annual satisfaction survey <https://www.ceci-hpc.be/survey.html>



We can only act on your problems if you report them

- Via the Support Wizard <https://support.cec-hpc.be/cecihelp/>



The screenshot shows a web browser window with the URL support.cec-hpc.be/cecihelp/. The page title is "CÉCI Support Wizard".

Welcome to the **CÉCI Support Wizard**. Our wizard is here to **help us help you** by ensuring you provide us all the details we need in order to diagnose, and then solve, your problem.

After you answer the wizard's questions, simply click the **'Generate Mail to send'** button. This action will open your email program, with content pre-filled and ready to be sent. You can then modify it to your liking, and then click the **'Send'** button of your email program.

Please note: For security reasons, **do not include your password** in any field. This information is not needed and could potentially compromise the security of your account.

Do you already have a CÉCI account ?
If so, please enter your login below. Otherwise please enter your name.

Your university:

- UCLouvain
- ULB
- ULiège
- UMons
- UNamur

What problem are you facing?

- I cannot create or renew an account
- I cannot connect with SSH and/or copy files
- I have trouble compiling/installing software
- I can't submit a job to the cluster
- My job failed / A node crashed

How you request help impacts the possible time to response

1. Start with **Due Diligence**

- Read the error message, try to find words you understand
- Check <http://www.ceci-hpc.be/status.html>

2. Use the **Correct Channel**: (support wizard unless stated otherwise)

3. State the **General Goal**; explain your intentions

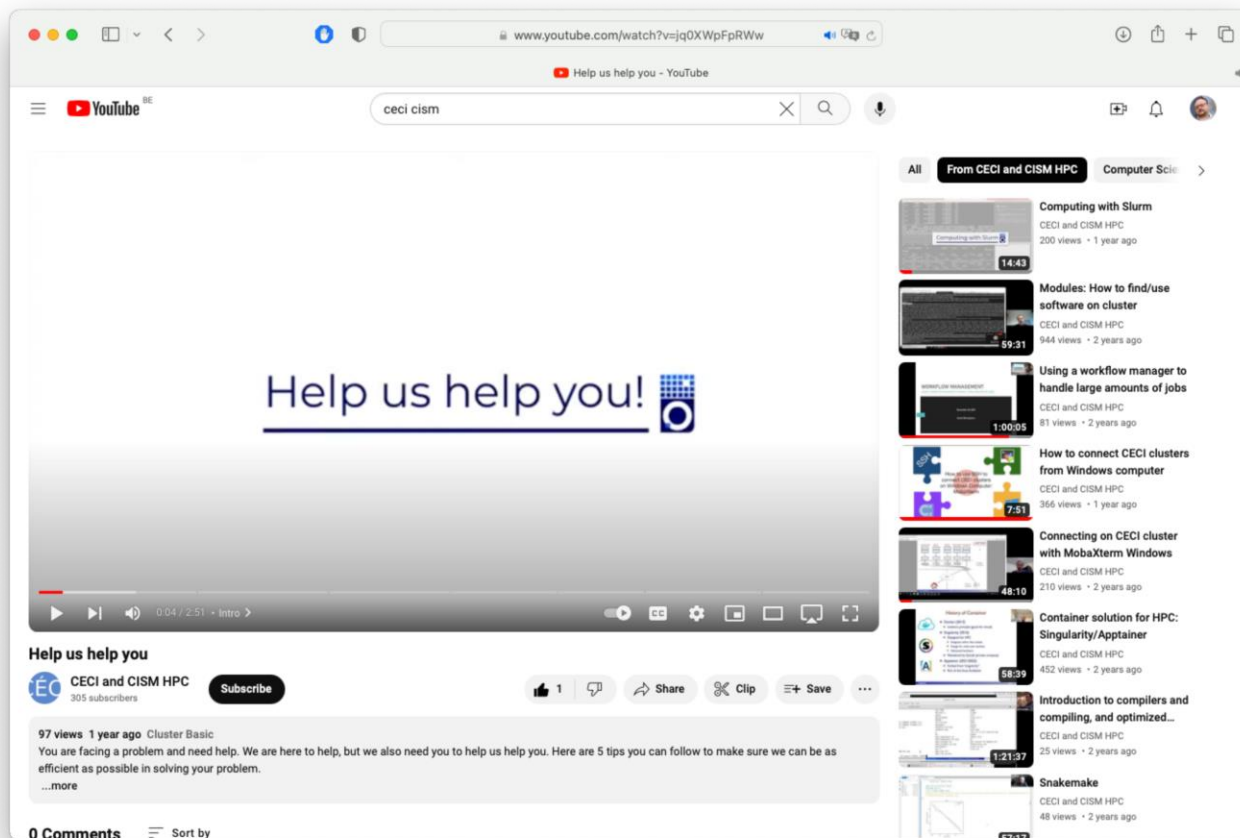
4. Provide **Important Information**

- *Who*: what is your login?
- *What*: what job ID, what file, what modules?
- *When*: on which date, at what time?
- *Where*: which cluster, which directory?
- *Why*: what is the problem?

5. Give the **Exact Error** message you are facing

How you request help impacts the possible time to response

More info: <http://www.ceci-hpc.be/helpushelpyou.html>



The screenshot shows a YouTube video player interface. The video title is "Help us help you!" and the channel is "CECI and CISM HPC" with 305 subscribers. The video description reads: "97 views 1 year ago Cluster Basic You are facing a problem and need help. We are here to help, but we also need you to help us help you. Here are 5 tips you can follow to make sure we can be as efficient as possible in solving your problem. ...more". The video player shows a progress bar at 0:04 / 2:51. To the right of the video player is a list of recommended videos from the same channel, including "Computing with Slurm", "Modules: How to find/use software on cluster", "Using a workflow manager to handle large amounts of jobs", "How to connect CECI clusters from Windows computer", "Connecting on CECI cluster with MobaXterm Windows", "Container solution for HPC: Singularity/Apptainer", "Introduction to compilers and compiling, and optimized...", and "Snakemake".

There are certain tasks you can do by yourself

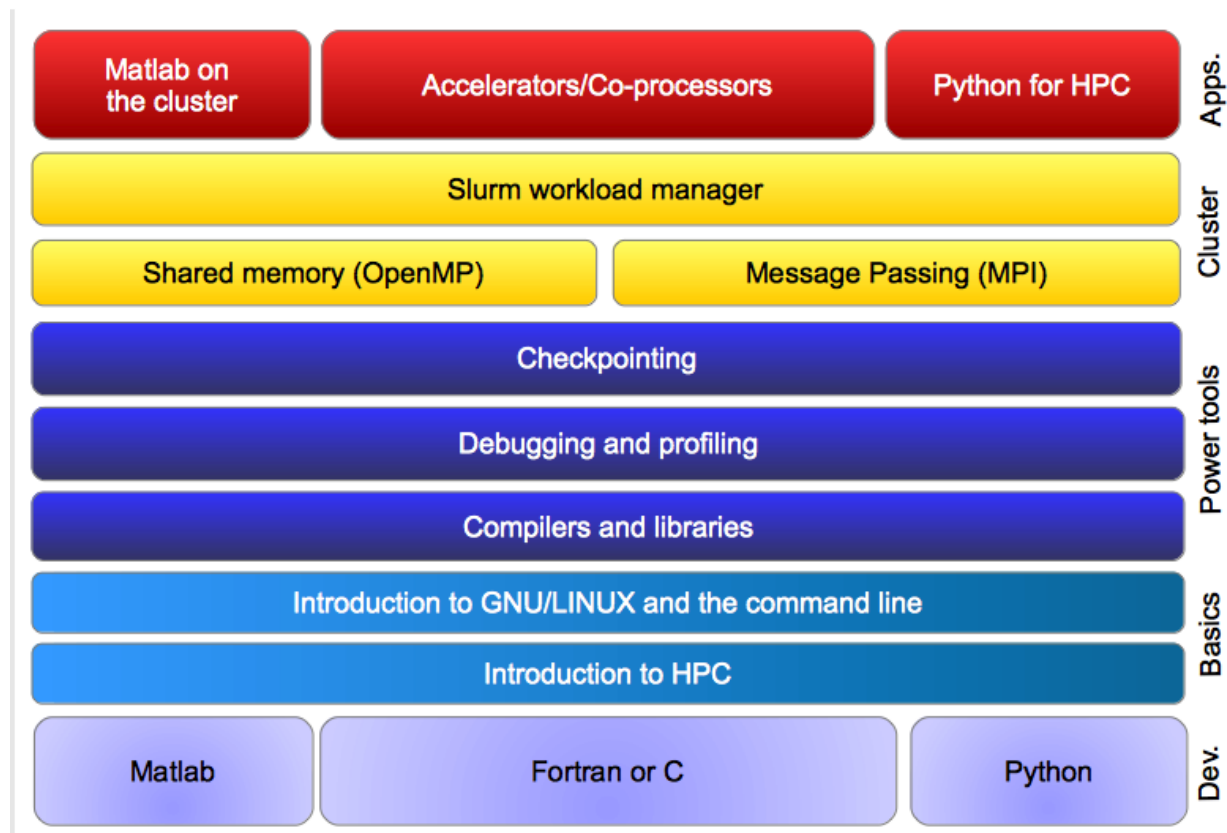
- installing software (modules included)
- changing permissions back after an error
- sharing files among users
- changing group ownership (not user ownership)
- joining a tier-1 project
- learning Linux
- ...



Lemaitre3: module load
gameshell

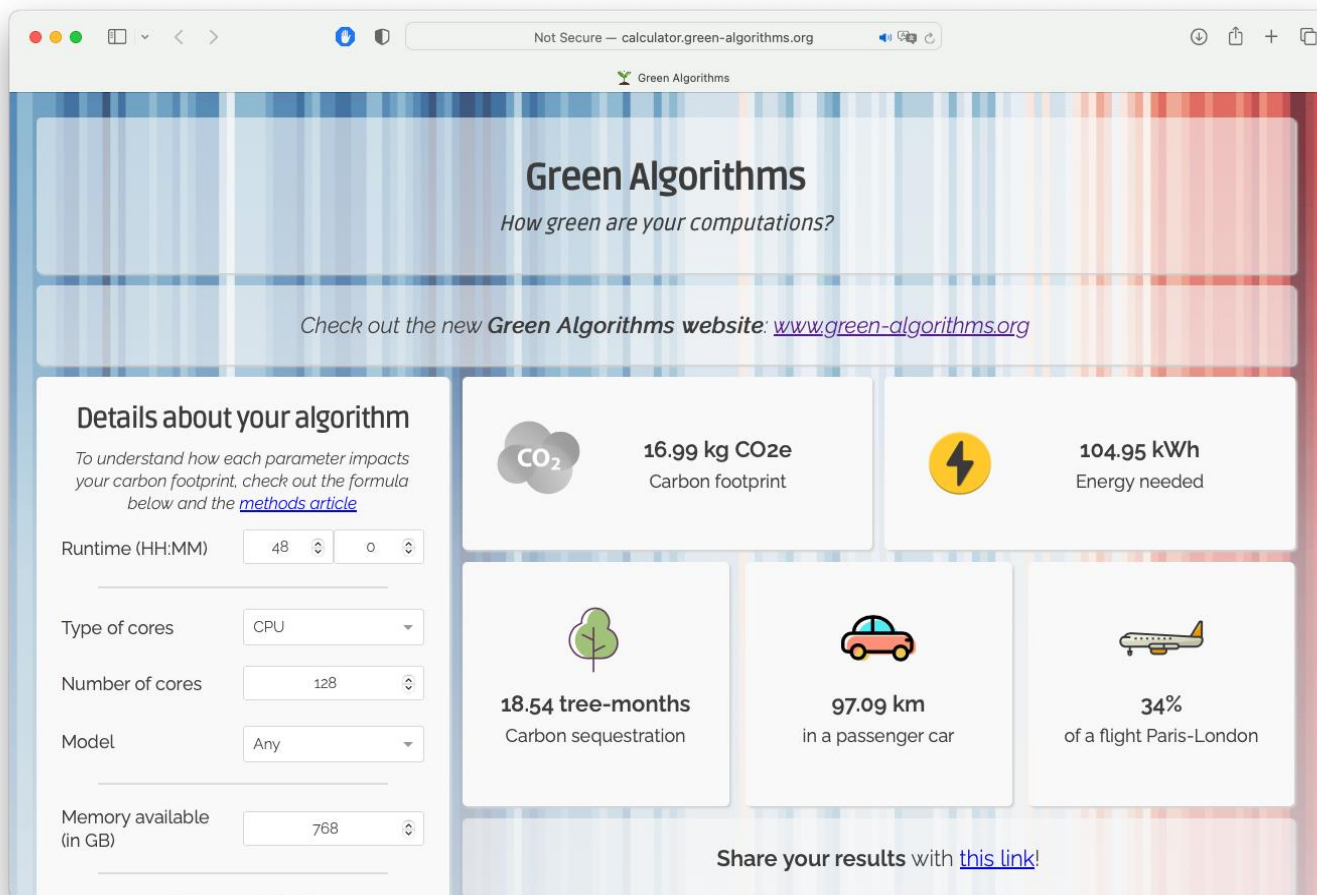
There are certain tasks you can do by yourself

<https://www.cec-hpc.be/training.html> | <https://www.cism.ucl.ac.be/videos>



Wasting resources has an impact on the planet

More info: <http://calculator.green-algorithms.org>



Wasting resources has an impact on the planet

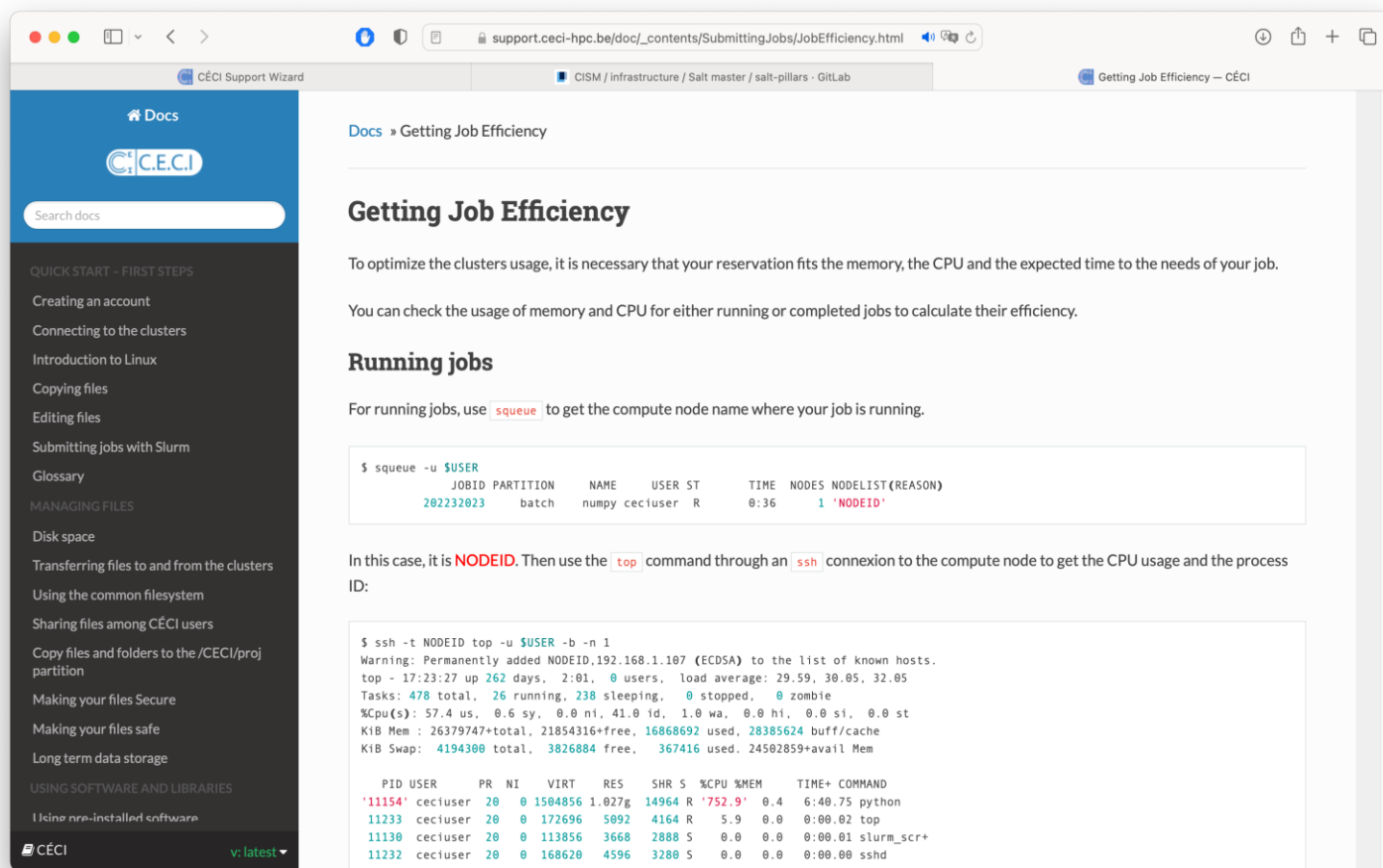
- jobs whose output is discarded because of misconfiguration
- jobs whose output is unsaved due to file manipulation error
- jobs whose results are lost because of hardware failure
- jobs not using the resources requested because of misconfiguration
- interactive jobs sitting idle
- jobs under-using resources due to bad scaling

are negatively impacting the climate and your colleagues' research

$$P(\text{idle}) \approx \frac{1}{2} P(\text{running})$$

Wasting resources has an impact on the planet

So be considerate of the resources you ask for and use them.
https://www.ceci-hpc.be/job_efficiency



Docs » Getting Job Efficiency

Getting Job Efficiency

To optimize the clusters usage, it is necessary that your reservation fits the memory, the CPU and the expected time to the needs of your job.

You can check the usage of memory and CPU for either running or completed jobs to calculate their efficiency.

Running jobs

For running jobs, use `squeue` to get the compute node name where your job is running.

```
$ squeue -u $USER
JOBID PARTITION   NAME     USER ST   TIME  NODES NODELIST(REASON)
202232023  batch         numpy ceciuser  R    0:36      1 'NODEID'
```

In this case, it is **NODEID**. Then use the `top` command through an `ssh` connexion to the compute node to get the CPU usage and the process ID:

```
$ ssh -t NODEID top -u $USER -b -n 1
Warning: Permanently added NODEID,192.168.1.107 (ECDSA) to the list of known hosts.
top - 17:23:27 up 262 days, 2:01, 0 users, load average: 29.59, 30.05, 32.05
Tasks: 478 total, 26 running, 238 sleeping, 0 stopped, 0 zombie
%Cpu(s): 57.4 us, 0.6 sy, 0.0 ni, 41.0 id, 1.0 wa, 0.0 hi, 0.0 si, 0.0 st
KiB Mem : 26379747+total, 21854316+free, 16868692 used, 28385624 buff/cache
KiB Swap: 4194300 total, 3826884 free, 367416 used, 24502859+avail Mem

  PID USER      PR  NI   VIRT   RES   SHR  S  %CPU  %MEM     TIME+ COMMAND
11154' ceciuser  20   0 1504856 1.027g 14964 R  752.9' 0.4   6:40.75 python
11233 ceciuser  20   0 172696  5092  4164 R   5.9  0.0   0:00.02 top
11130 ceciuser  20   0 113856  3668  2888 S   0.0  0.0   0:00.01 slurm_scr+
11232 ceciuser  20   0 168620  4596  3280 S   0.0  0.0   0:00.00 sshd
```

Certain workflows create problems on HPC clusters

- Running anything CPU-intensive on the head node
- Issuing too many requests to the scheduler
- Not testing first on a small scale
- Excessive and/or “bad” I/O on a parallel/network filesystem
- Storing a large number of small files
- Not double checking the email options

are example of user behavior that impacts other users' experience

So please

Help us help you!