



# UL HPC School 2018 (bis)

## Overview & Challenges of the UL HPC facility at the EuroHPC Horizon

High Performance Computing & Big Data Services

- hpc.uni.lu
- hpc@uni.lu
- @ULHPC



Prof. P. Bouvry, Dr. S. Varrette

V. Plugaru, S. Peter, H. Cartiaux & C. Parisot

University of Luxembourg (UL)

<https://hpc.uni.lu>



Nov 23<sup>th</sup>, 2018, Learning Hub 2.02



# Uni.lu HPC School 2018 (bis)

<https://hpc.uni.lu/hpc-school/>

- **8th edition** of this training...

- ↳ started in 2014

- ↳ This one is the **short** version

- ✓ 1-day event

- ✓ Parallel sessions, feat. basic tutorials

- **Requirement:**

- ↳ your favorite laptop with your favorite OS

- ✓ Linux / Mac OS preferred, but Windows accepted

- ↳ basic knowledge in Linux command line

- ↳ ability to take notes (Markdown etc.)



Online UL HPC Tutorials

<http://ulhpc-tutorials.rtfld.io/>



## Agenda - Friday Nov 23th, 2018

Time	Description (Learning Hub 2.02)	Speaker
9h00-10h00	<b>PS1a:</b> Getting Started on the UL HPC platform	C. Parisot
10h00-10h15	<b>break</b>	
10h15-11h30	Overview and Challenges of the UL HPC Facility at EuroHPC Horizon	S.Varrette
11h30-12h15	<b>PS1b:</b> Getting Started on the UL HPC platform - continued	C. Parisot
12h15-13h30	<b>LUNCH</b>	
13h30-14h45	<b>PS2:</b> HPC workflow with sequential jobs	H.Cartiaux
14h45-16h00	<b>PS3:</b> Advanced scheduling (SLURM, OAR)	V. Plugaru
16h00-16h15	<b>break</b>	
16h15-17h00	<b>PS4:</b> UL HPC Monitoring in practice	S. Peter
17h00-18h00	<b>PS5:</b> Parallel computations with OpenMP/MPI	S. Varrette
18h00-18h30	<b>PS6:</b> User environment and storage data management	S.Peter

**PS** = *Practical Session using your laptop*



# Summary

---

- 1 Introduction**
  - Preliminaries
  - [Parallel] Computing for Enhanced Research
  - Overview of the Main HPC Components
- 2 High Performance Computing (HPC) @ UL**
  - Overview
  - Platform Management
  - Back to last achievements & incoming developments
- 3 UL HPC in Practice: Toward an [Efficient] Win-Win Usage**
  - General Considerations
  - Environment & Typical Workflow Overview
  - Documentation & Reporting (problems or results)
- 4 HPC Strategy in Europe & Abroad**
- 5 Current and Future Developments in Luxembourg**
  - Trends in HPC
  - Incoming Milestones in Luxembourg
- 6 Conclusion & Perspectives**



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## Prerequisites: Metrics

● **HPC: High Performance Computing**

**BD: Big Data**

### Main HPC/BD Performance Metrics

- **Computing Capacity:** often measured in **flops** (or **flop/s**)
  - ↪ **Floating point operations per seconds** (often in DP)
  - ↪ **GFlops** =  $10^9$    **TFlops** =  $10^{12}$    **PFlops** =  $10^{15}$    **EFlops** =  $10^{18}$

# Prerequisites: Metrics

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## Main HPC/BD Performance Metrics

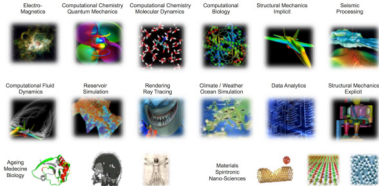
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- **Storage Capacity:** measured in multiples of **bytes** = 8 **bits**
  - ↪ **GB** =  $10^9$  bytes   **TB** =  $10^{12}$    **PB** =  $10^{15}$    **EB** =  $10^{18}$
  - ↪ **GiB** =  $1024^3$  bytes   **TiB** =  $1024^4$    **PiB** =  $1024^5$    **EiB** =  $1024^6$
- **Transfer rate** on a medium measured in **Mb/s** or **MB/s**
- **Other metrics:** Sequential vs Random **R/W speed, IOPS** ...





# Why HPC and BD ?

**HPC: High Performance Computing**  
**BD: Big Data**



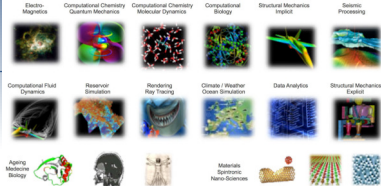
Andy Grant, Head of Big Data and HPC, Allos UK&I

## To out-compete you must out-compute

Increasing competition, heightened customer expectations and shortening product development cycles are forcing the pace of acceleration across all industries



# Why HPC and BD ?



**HPC: High Performance Computing**  
**BD: Big Data**

- Essential tools for **Science, Society and Industry**
  - ↳ **Data driven economy context**
  - ↳ All scientific disciplines are becoming computational today
    - ✓ require very high computing power, handle **huge** volumes of data
- **Industry, SMEs** increasingly relying on HPC
  - ↳ to invent innovative solutions
  - ↳ ... while reducing cost & decreasing time to market

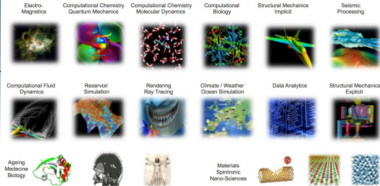
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- HPC = **global race** (strategic priority) - EU takes up the challenge:
  - ↳ PRACE / EuroHPC / IPCEI on HPC and Big Data (BD)

Applications



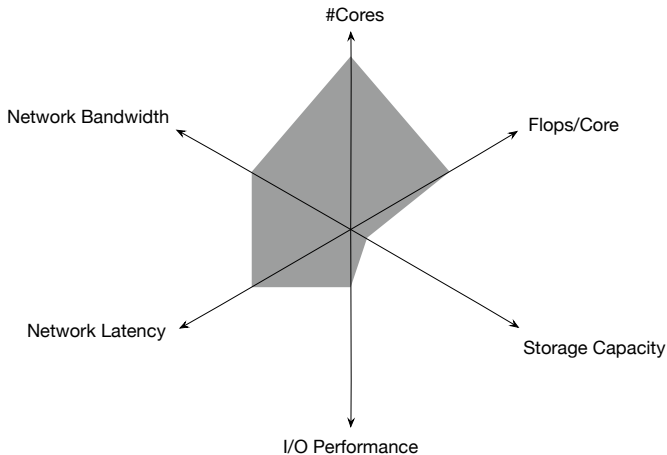
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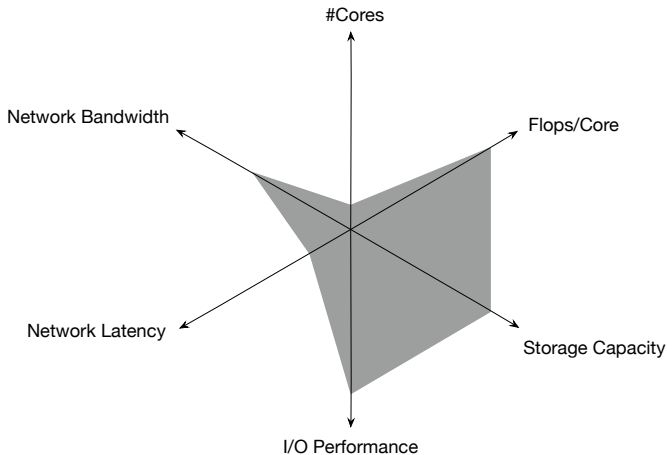
# Different HPC Needs per Domains

## Material Science & Engineering



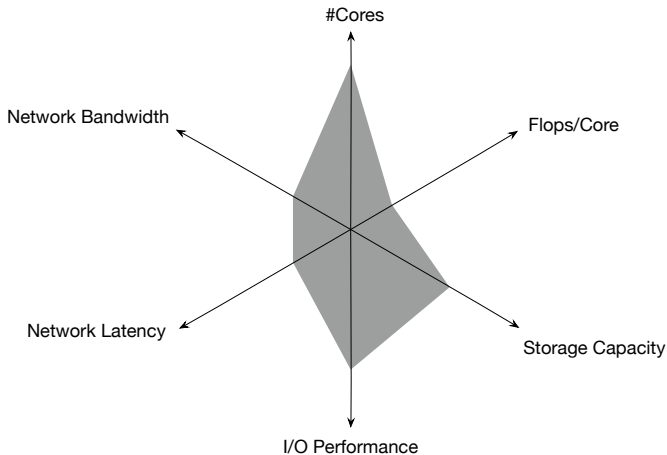
# Different HPC Needs per Domains

## Biomedical Industry / Life Sciences



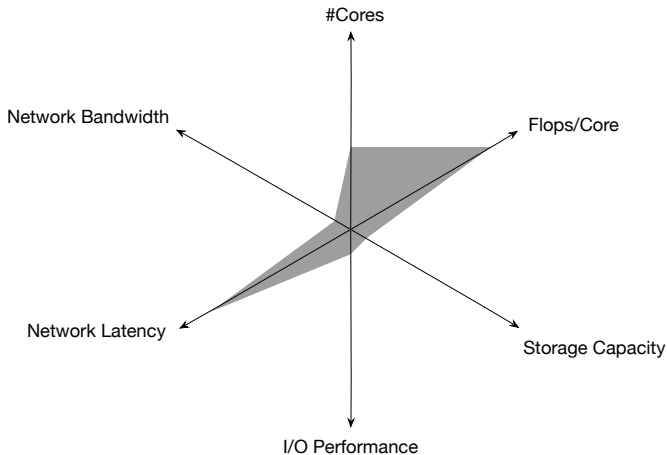
# Different HPC Needs per Domains

## Deep Learning / Cognitive Computing



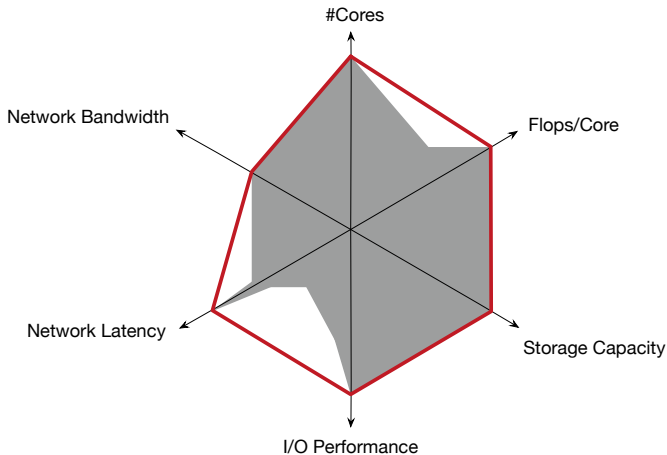
# Different HPC Needs per Domains

IoT, FinTech



# Different HPC Needs per Domains

**ALL Research Computing Domains**







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# Computing for Researchers: Laptop

- **Regular PC / Local Laptop / Workstation**
  - ↳ **Native OS** (Windows, Linux, Mac etc.)



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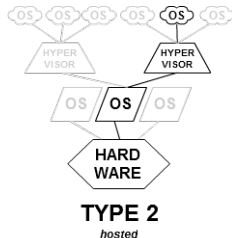
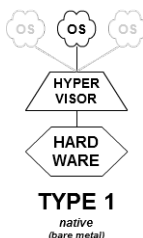
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- **Virtualized OS (VM) through an hypervisor**

↳ *Hypervisor*: core virtualization engine / environment

- ✓ Ex: *Xen*, *VMWare ESXi*, *KVM*, *VirtualBox*
- ✓ Non-negligible Performance loss:  $\geq 20\%$



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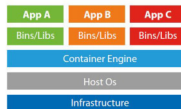
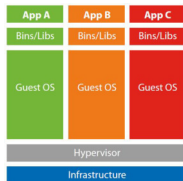
↳ *Hypervisor*: core virtualization engine / environment

- ✓ Ex: *Xen*, *VMWare ESXi*, *KVM*, *VirtualBox*
- ✓ Non-negligible Performance loss:  $\geq 20\%$

- **Container-based Virtualization**

↳ similar to VMs ...

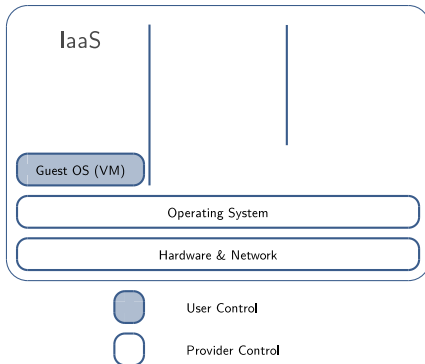
- ✓ **yet** containers **share** the system kernel of the host with others
- ✓ Ex: *Docker*, *Singularity*, *Shifter*



# Computing for Researchers: Cloud

## • Cloud Computing

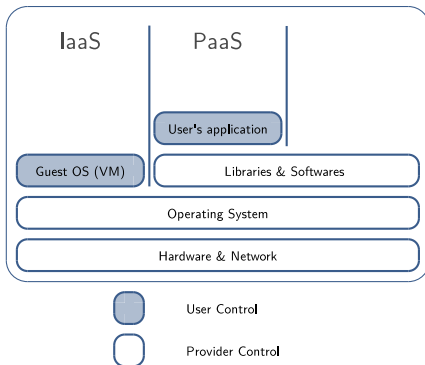
- ↪ access to shared (*generally virtualized*) resources
- ↪ pay-per-use approach
- ↪ **Infrastructure** as a Service (IaaS)



# Computing for Researchers: Cloud

## ● Cloud Computing

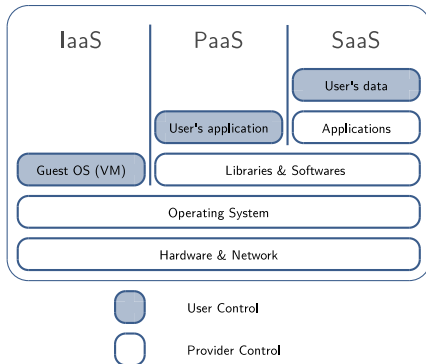
- ↪ access to shared (*generally virtualized*) resources
- ↪ pay-per-use approach
- ↪ **Platform** as a Service (**PaaS**)



# Computing for Researchers: Cloud

## • Cloud Computing

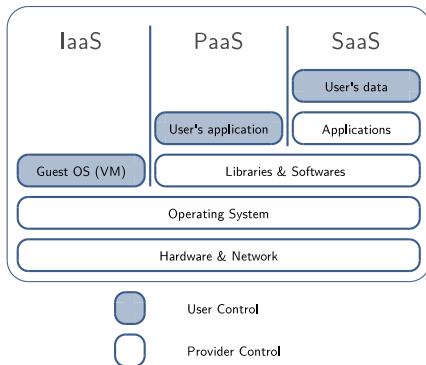
- ↪ access to shared (*generally virtualized*) resources
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- ↪ **Software as a Service (SaaS)**



# Computing for Researchers: Cloud

## • Cloud Computing

- ↪ access to shared (*generally virtualized*) resources
- ↪ pay-per-use approach
- ↪ **XXX** as a Service (<X>aaS)







# Computing for Researchers: HPC

- High Performance Computing (HPC) platforms
  - ↳ For **Speedup**, **Scalability** and **Faster Time to Solution**





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**YET...**

**PC  $\neq$  Cloud  $\neq$  HPC**

# Computing for Researchers: HPC



- High Performance Computing (HPC) platforms
  - ↳ For **Speedup**, **Scalability** and **Faster Time to Solution**

**YET...**

**PC  $\neq$  Cloud  $\neq$  HPC**

- HPC  $\simeq$  Formula 1
  - ↳ relies on ultra efficient hardware / interconnect (IB EDR...)
  - ↳ ... when Cloud has to stay standard ([10] GbE etc...)
- **Does not mean the 3 approaches cannot work together**



# Jobs, Tasks & Local Execution



```
$> ./myprog
```



# Jobs, Tasks & Local Execution



\$> ./myprog



# Jobs, Tasks & Local Execution



```
$> ./myprog  
$> ./myprog -n 10
```



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# Jobs, Tasks & Local Execution



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# Jobs, Tasks & Local Execution



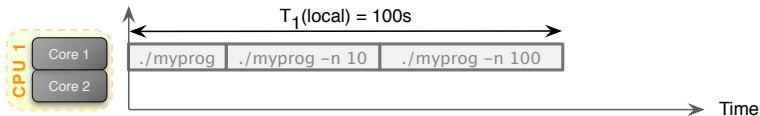
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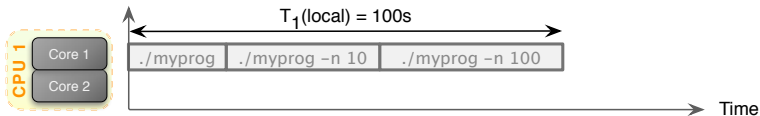
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Job(s)

3

Task(s)

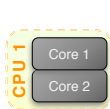
3



# Jobs, Tasks & Local Execution



```
# launcher  
./myprog  
./myprog -n 10  
./myprog -n 100
```



# Jobs, Tasks & Local Execution



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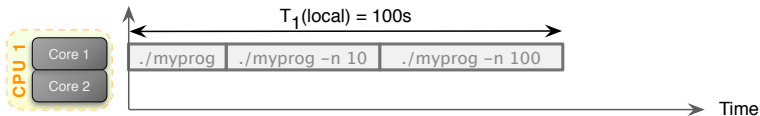
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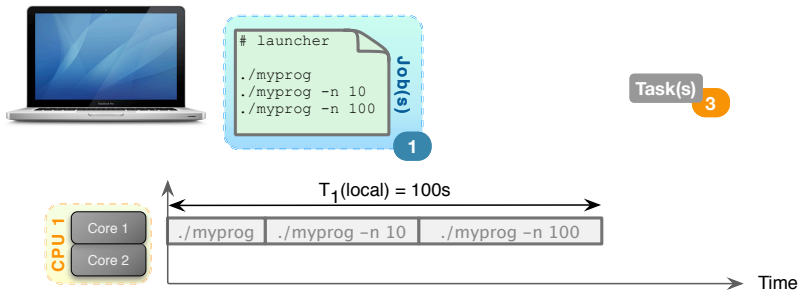


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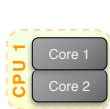
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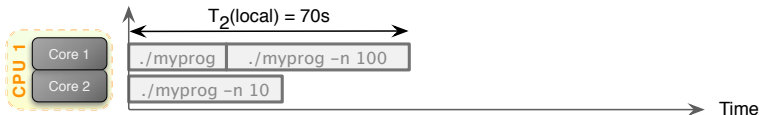
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# launcher2  
"Run in //:"  
./myprog  
./myprog -n 10  
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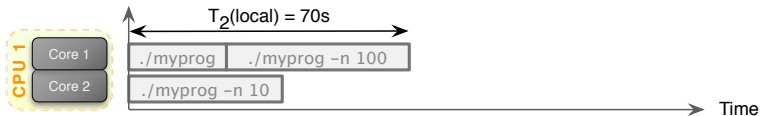
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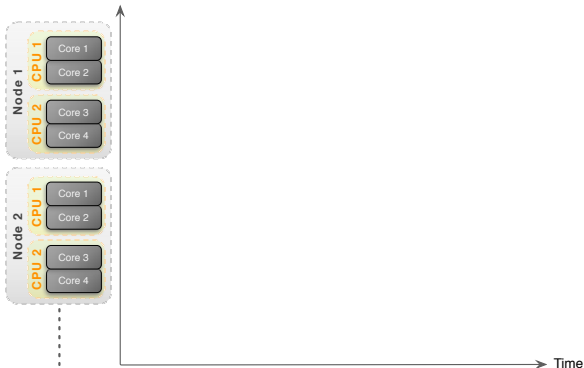
Task(s) 3



# Jobs, Tasks & HPC Execution



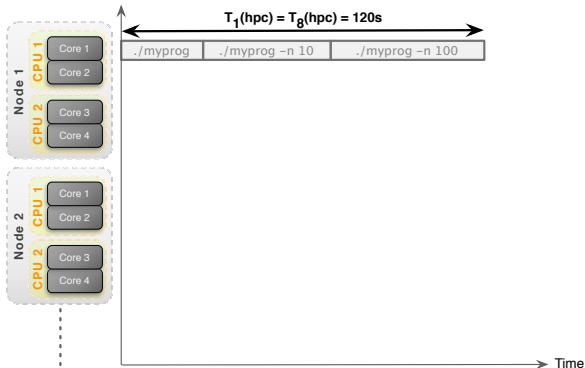
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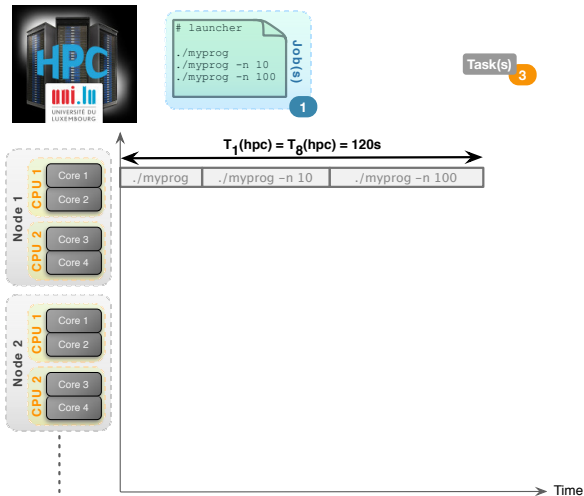
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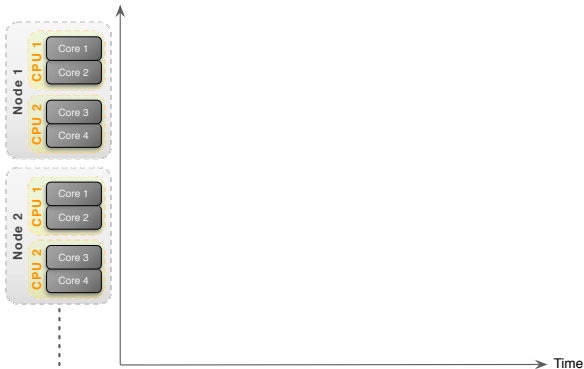




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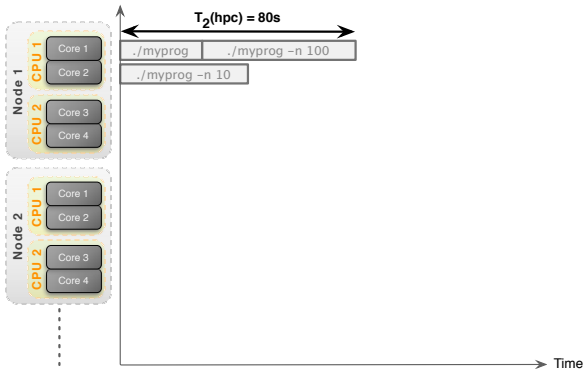
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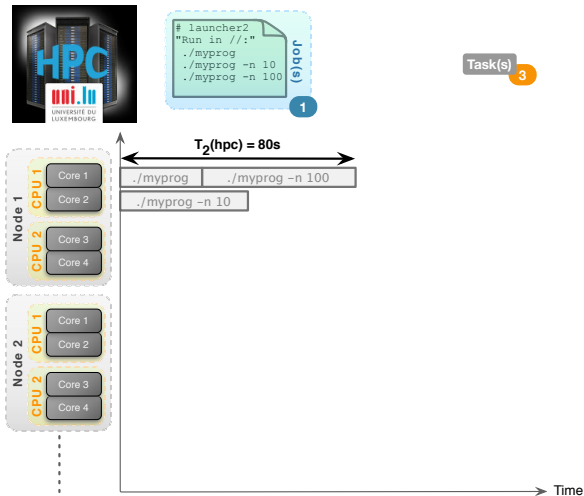
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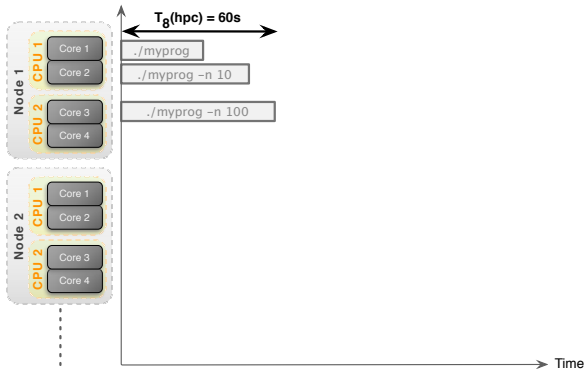
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Job(s) 1

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## Local vs. HPC Executions

Context	Local PC	HPC
Sequential	$T_1(\text{local}) = 100$	$T_1(\text{hpc}) = 120\text{s}$
Parallel/Distributed	$T_2(\text{local}) = 70\text{s}$	$T_2(\text{hpc}) = 80\text{s}$ $T_8(\text{hpc}) = 60\text{s}$

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- Sequential runs **WON'T BE FASTER** on HPC  
 ↪ Reason: Processor Frequency (typically  $\geq 3\text{GHz}$  vs  $\geq 2\text{GHz}$ )

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- Sequential runs **WON'T BE FASTER** on HPC  
 ↪ Reason: Processor Frequency (typically  $\geq 3\text{GHz}$  vs  $\geq 2\text{GHz}$ )
- Parallel/Distributed runs **DO NOT COME FOR FREE**  
 ↪ runs **will be sequential** even if you reserve  $\geq 2$  cores/nodes  
 ↪ you have to **explicitly** adapt your jobs to benefit from the multi-cores/nodes



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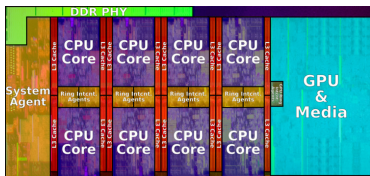
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# HPC Computing Hardware

Base

- CPU** (Central Processing Unit) *Highest software flexibility*
  - ↪ High performance across all computational domains
  - ↪ Ex: Intel Core i9-9900K (Q4'18)  $R_{peak} \simeq 922$  GFlops (DP)
    - ✓ 8 cores @3.6GHz (14nm, 95W,  $\simeq$  3.5 billion transistors) + integ. graphics



Intel Coffee Lake die

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Accelerators

- **GPU** (Graphics Processing Unit):

*Ideal for ML/DL workloads*

↳ Ex: Nvidia **Tesla V100 SXM2** (Q2'17)  $R_{peak} \simeq 7.8$  TFlops (DP)

✓ 5120 cores @ 1.3GHz (12nm, 250W, 21 billion transistors)



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  - ↳ High performance across all computational domains
  - ↳ Ex: Intel **Core i9-9900K** (Q4'18)  $R_{peak} \simeq 922$  GFlops (DP)
    - ✓ 8 cores @3.6GHz (14nm, 95W,  $\simeq 3.5$  billion transistors) + integ. graphics

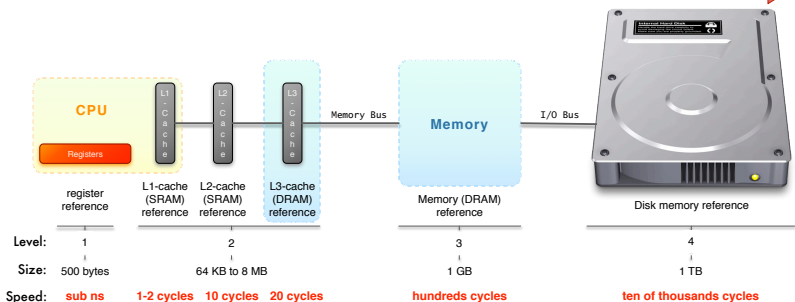
Accelerators

- **GPU** (Graphics Processing Unit): *Ideal for ML/DL workloads*
  - ↳ Ex: Nvidia **Tesla V100 SXM2** (Q2'17)  $R_{peak} \simeq 7.8$  TFlops (DP)
    - ✓ 5120 cores @ 1.3GHz (12nm, 250W, 21 billion transistors)
- Intel MIC (Many Integrated Core) Accelerator
- **ASIC** (Application-Specific Integrated Circuits), **FPGA** (Field Programmable Gate Array)
  - ↳ least software flexibility
  - ↳ highest performance for specialized problems
    - ✓ Ex: AI, Mining, Sequencing. . .

⇒ toward hybrid platforms w. DL enabled accelerators

# HPC Components: Local Memory

**Larger, slower and cheaper**

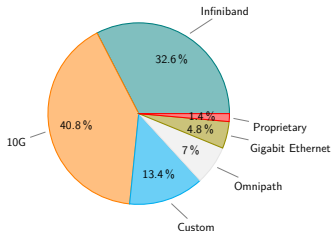


- SSD (SATA3) R/W: 550 MB/s; 100000 IOPS **450 €/TB**
- HDD (SATA3 @ 7,2 krpm) R/W: 227 MB/s; 85 IOPS **54 €/TB**

# HPC Components: Interconnect

- **latency**: time to send a minimal (0 byte) message from A to B
- **bandwidth**: max amount of data communicated per unit of time

Technology	Effective Bandwidth		Latency
Gigabit Ethernet	1 Gb/s	125 MB/s	40 $\mu$ s to 300 $\mu$ s
10 Gigabit Ethernet	10 Gb/s	1.25 GB/s	4 $\mu$ s to 5 $\mu$ s
Infiniband QDR	40 Gb/s	5 GB/s	1.29 $\mu$ s to 2.6 $\mu$ s
Infiniband EDR	100 Gb/s	12.5 GB/s	0.61 $\mu$ s to 1.3 $\mu$ s
Infiniband HDR	200 Gb/s	25 GB/s	0.5 $\mu$ s to 1.1 $\mu$ s
100 Gigabit Ethernet	100 Gb/s	1.25 GB/s	30 $\mu$ s
Intel Omnipath	100 Gb/s	12.5 GB/s	0.9 $\mu$ s

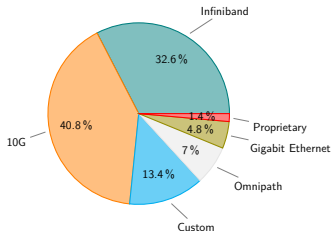


[Source : [www.top500.org](http://www.top500.org), Nov. 2017]

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# Network Topologies

- **Direct** vs. **Indirect** interconnect

- ↪ *direct*: each network node attaches to at least one compute node
- ↪ *indirect*: compute nodes attached at the edge of the network only
  - ✓ many routers only connect to other routers.

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## Main HPC Topologies

- **CLOS Network / Fat-Trees** [Indirect]
  - ↪ can be fully non-blocking (1:1) or blocking (x:1)
  - ↪ typically enables **best performance**
    - ✓ Non blocking bandwidth, lowest network latency





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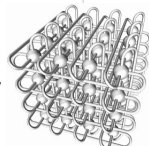
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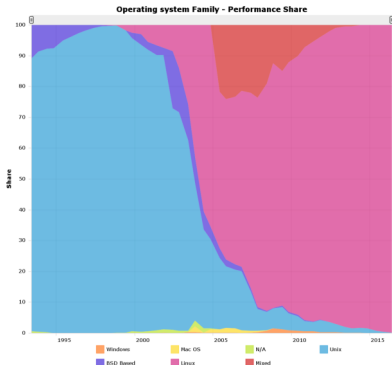


- **Mesh or 3D-torus** [Direct]

- ↳ Blocking network, cost-effective for systems at scale
- ↳ Great performance solutions for applications with locality
- ↳ Simple expansion for future growth

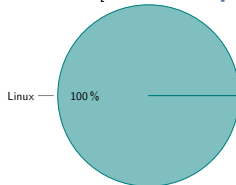


# HPC Components: Operating System



- Exclusively Linux-based (**really** 100%)
- Reasons:
  - ↳ stability
  - ↳ development flexibility

[Source : [www.top500.org](http://www.top500.org), Nov 2017]





# HPC Components: Software Stack

- **Remote connection to the platform** SSH
- **Identity Management / SSO:** LDAP, Kerberos, IPA...
- **Resource management:** job/batch scheduler
  - ↪ SLURM, OAR, PBS, MOAB/Torque...
- **(Automatic) Node Deployment:**
  - ↪ FAI, Kickstart, Puppet, Chef, Ansible, Kadeploy...
- **(Automatic) User Software Management:**
  - ↪ Easybuild, Environment Modules, LMod
- **Platform Monitoring:**
  - ↪ Nagios, Icinga, Ganglia, Foreman, Cacti, Alerta...

# [Big]Data Management: Disk Encl.



- $\simeq$  120 K€ - enclosure - 48-60 disks (4U)  
↳ incl. redundant (i.e. 2) RAID controllers (master/slave)



# [Big]Data Management: FS Summary

- **File System (FS):** Logical manner to *store, organize & access* data
  - ↪ (local) **Disk FS** : FAT32, NTFS, HFS+, ext4, {x,z,btr}fs...
  - ↪ **Networked FS:** NFS, CIFS/SMB, AFP
  - ↪ **Parallel/Distributed FS:** SpectrumScale/GPFS, Lustre
    - ✓ typical FS for HPC / HTC (High Throughput Computing)



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## Main Characteristic of Parallel/Distributed File Systems

Capacity and Performance increase with #servers

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## Main Characteristic of Parallel/Distributed File Systems

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Name	Type	Read* [GB/s]	Write* [GB/s]
ext4	Disk FS	0.426	0.212
nfs	Networked FS	0.381	0.090
gpfs (iris)	Parallel/Distributed FS	<b>11.25</b>	<b>9.46</b>
lustre (iris)	Parallel/Distributed FS	<b>12.88</b>	<b>10.07</b>
gpfs (gaia)	Parallel/Distributed FS	7.74	6.524
lustre (gaia)	Parallel/Distributed FS	4.5	2.956

\* maximum **random** read/write, per IOZone or IOR measures, using concurrent nodes for networked FS.



# HPC Components: Data Center

## Definition (Data Center)

- Facility to house computer systems and associated components
  - ↳ Basic storage component: **rack** (height: 42 RU)



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## Definition (Data Center)

- Facility to house computer systems and associated components
  - ↳ Basic storage component: **rack** (height: 42 RU)

## Challenges: Power (UPS, battery), Cooling, Fire protection, Security

- Power/Heat dissipation per rack:
  - ↳ HPC **computing** racks: **30-120 kW**
  - ↳ **Storage** racks: **15 kW**
  - ↳ **Interconnect** racks: **5 kW**
- Various **Cooling** Technology
  - ↳ Airflow
  - ↳ Direct-Liquid Cooling, Immersion...

## Power Usage Effectiveness

$$PUE = \frac{\text{Total facility power}}{\text{IT equipment power}}$$



## Summary

- 1 Introduction**
  - Preliminaries
  - [Parallel] Computing for Enhanced Research
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# Univ. of Luxembourg & HPC

- *With regards to HPC, Univ. of Luxembourg offers:*

↪ **People**

- ✓ Domain experts
- ✓ Computational and data scientists
- ✓ Specialists in parallel algorithmics

↪ **Services**

- ✓ HPC clusters and management team
- ✓ IT team (SIU)
- ✓ Infrastructure team in collab. w. Fonds Belval

↪ **Infrastructure**

- ✓ Data center and a set of high-end clusters

↪ **Education & Training**



High Performance  
Computing &  
Big Data Services

 [hpc.uni.lu](http://hpc.uni.lu)

 [hpc@uni.lu](mailto:hpc@uni.lu)

 @ULHPC

 **UNIVERSITE DU LUXEMBOURG**  
LET'S MAKE IT HAPPEN



# High Performance Computing @ UL



## • Started in 2007

- ↳ under resp. of Prof P. Bouvry & Dr. S. Varrette
- ↳ expert Uni.lu HPC team
  - ✓ *S. Varrette, V. Plugaru, S. Peter, H. Cartiaux, C. Parisot...* and multiple domain experts per RU
- ↳ Largest HPC facility in Luxembourg w. GoodYear



<https://hpc.uni.lu>

High Performance Computing & Big Data Services

- [hpc.uni.lu](https://hpc.uni.lu)
- [hpc@uni.lu](mailto:hpc@uni.lu)
- @ULHPC

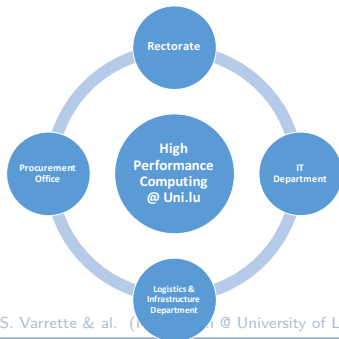




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High Performance  
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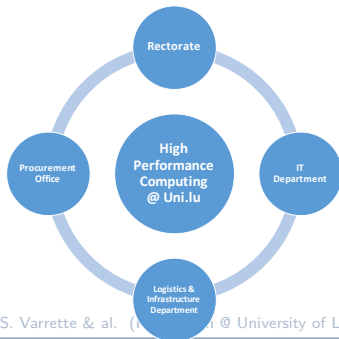




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HPC/Computing Capacity

1062.142 TFlops  
(incl. 637.82 GPU TFlops)

HTC/Storage Capacity

9852.4 TB storage

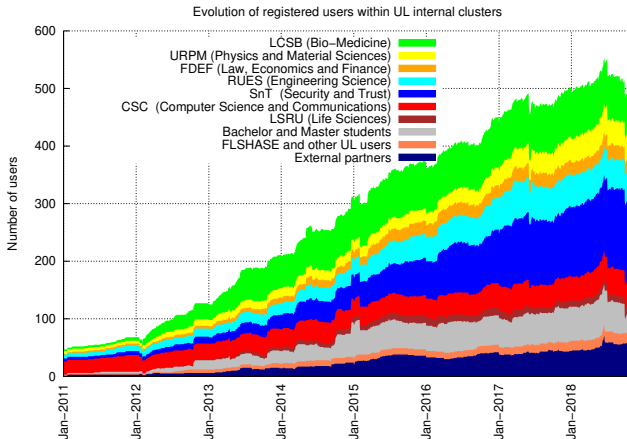
High Performance Computing & Big Data Services

- [hpc.uni.lu](http://hpc.uni.lu)
- [hpc@uni.lu](mailto:hpc@uni.lu)
- @ULHPC



# UL HPC User Base

● **496 Active HPC Users**





## UL HPC Beneficiaries

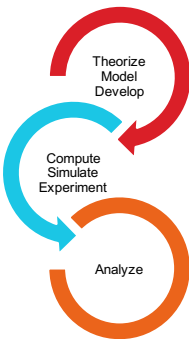
### 23 computational domains accelerated on UL HPC

- for the UL Faculties, Research Units and Interdisciplinary Centres
  - ↳ incl. LCSB, SnT... and now C2DH thematics
  - ↳ UL **strategic research priorities**
    - ✓ computational sciences, finance (fintech)
    - ✓ systems biomedicine, security, reliability and trust
- UL HPC features special systems targeting specific workloads:
  - ↳ **Machine Learning & AI**: GPU accelerators
    - ✓ 10 Tesla K40 + 16 Tesla K80 + 24 Tesla M20\*: **76 GPU Tflops**
    - ✓ **Q4 2018**: 18\*4 V100 (part of RFP 180027): **561 GPU Tflops**
  - ↳ **BigData analytics & data driven science**: large memory systems
    - ✓ Large SMP systems with 1, 2, 3 & 4 TB RAM
  - ↳ **Scale-out workloads**: 90 HP Moonshot servers + 96 viridis ARM-based systems

# Accelerating UL Research



- **over 200 software packages** available for researchers  
 ↪ via **Environment modules/LMod** from **Easybuild**



Domain	Software
Compiler Toolchains	(2018a) FOSS, Intel, PGI
MPI suites	OpenMPI, Intel MPI, MVAPICH2
<b>Machine Learning</b>	PyTorch, TensorFlow, Keras, Apache Spark...
<b>Math &amp; Optimization</b>	Matlab, Mathematica, R, CPLEX, Gurobi...
<b>Physics &amp; Chemistry</b>	GROMACS, QuantumESPRESSO, ABINIT, NAMD, VASP...
<b>Bioinformatics</b>	SAMtools, BLAST+, ABySS, mpiBLAST, TopHat, Bowtie2...
<b>Computer aided engineering</b>	ANSYS, ABAQUS, OpenFOAM...
<b>General purpose</b>	Allinea/ARM Forge & Perf Reports, Python, Go, Rust...
<b>Container systems</b>	Singularity
<b>Visualisation</b>	ParaView, OpenCV, XCS portal
...	

<https://hpc.uni.lu/users/software/>

## UL HPC Team



**Prof. Pascal Bouvry**  
Senior advisor for the president as regards the HPC strategy  
Leader of PCO Group, Head Uni.lu HPC



**Dr. Sébastien Varrette**  
Research Scientist, Deputy head Uni.lu HPC



**Valentin Plugaru, MSc.**  
R&D Specialist, Senior HPC Architect

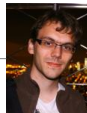


**Sarah Peter, MSc.**  
R&D Specialist, HPC/LCSB Support Liaison



**Hyacinthe Cartiaux**  
HPC System administrator

**Clément Parisot**  
HPC System administrator



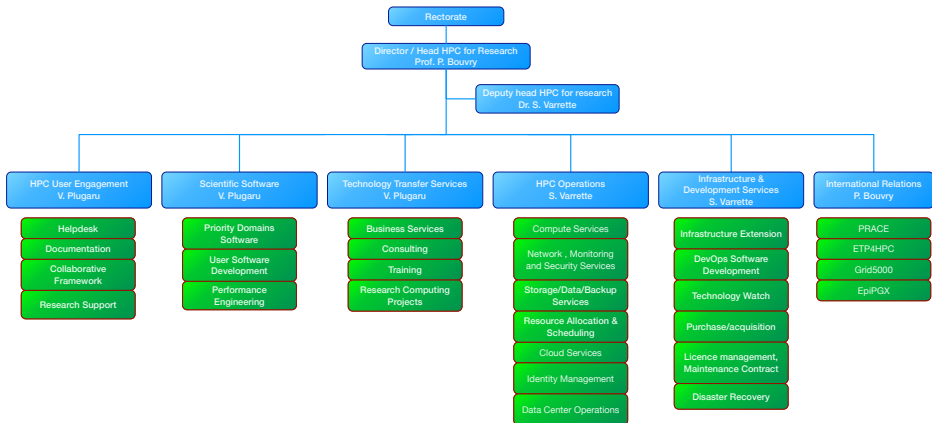
... and computational scientists / domain experts from  
across **ALL** the University



# UL HPC Functional Governance

## Functional Organization Chart - Uni.lu HPC department

rc5 Draft version



## Sites / Data centers



Kirchberg

CS.43, AS. 28

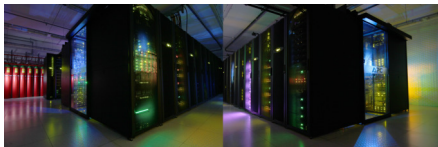


Belval

Biotech I, CDC/MSA

2 sites,  $\geq$  4 server rooms

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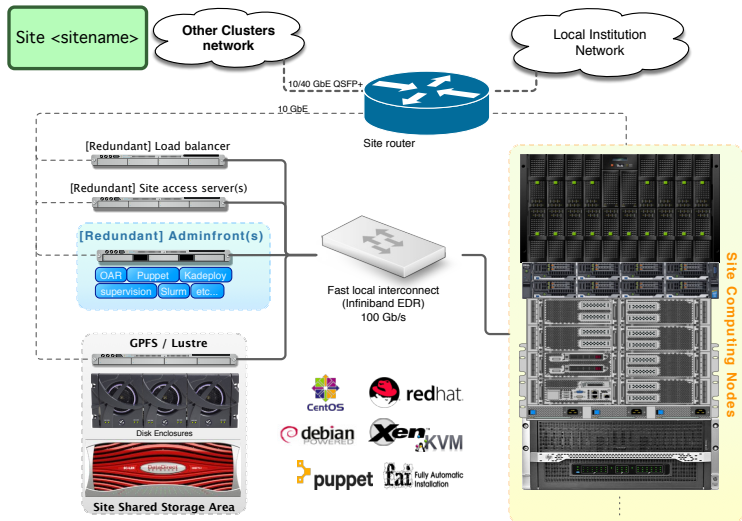
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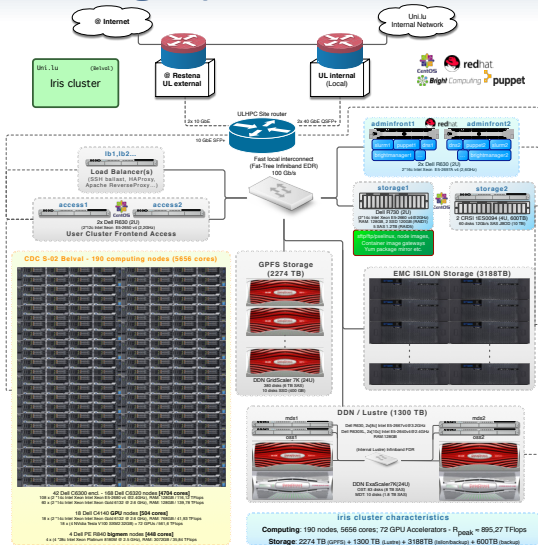
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# UL HPC: General cluster organization



## The flagship iris cluster





# UL HPC Computing capacity



5 clusters / 2 sites



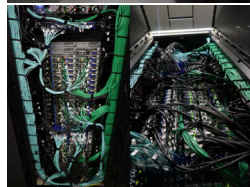
**1062.142 TFlops**

(incl. 637.82 GPU TFlops)

684 nodes

**11084 CPU cores**

(+ 489344 GPU cores)



- IB interconnect
- Fat tree topo. in general





## UL HPC Computing Clusters

Cluster	Location	#N	#C	$R_{\text{peak}}$ [TFlops]	GPU $R_{\text{peak}}$ [TFlops]
iris	CDC S-01	190	5656	333.67	561.6
gaia*	BT1	273	3440	69.296	76.22
chaos*	Kirchberg	81	1120	14.495	0
g5k	Kirchberg	38	368	4.48	0
nyx* (experimental)	BT1	102	500	2.381	0
<b>TOTAL:</b>		<b>684</b>	<b>11084</b>	<b>424.322</b>	<b>+ 637.82 TFlops</b>

\*: *Deprecated mid-2019!!*

**Uni.lu HPC Total Computing Capacity:**  
**1062.142 TFlops**

# UL HPC - Detailed Computing Nodes

	#N	#C	R <sub>peak</sub>
<b>Uni.lu HPC TOTAL:</b>	<b>684</b>	<b>11084</b>	<b>1062.142 TFlops</b>
			(incl. 637.82 GPU TFlops)

Cluster	Date	Vendor	Proc. Description	#N	#C	R <sub>peak</sub>
iris	2017	Dell	Intel Xeon E5-2680 v4@2.4GHz 2 × 14C,128GB	108	3024	116,12 TFlops
	2018	Dell	Intel Xeon Gold 6132 @ 2.6 GHz 2 × 14C,128GB	60	1680	139,78 TFlops
	2018	Dell	Intel Xeon Gold 6132 @ 2.6 GHz 2 × 14C,768GB Per node: 4x NVIDIA Tesla V100 SXM2 32GB	18 72 GPUs	504 368640	41,93 TFlops 561,6 GPU TFlops
	2018	Dell	Intel Xeon Platinum 8180M @ 2.5 GHz 4 × 28C,3072GB	4	448	35,84 TFlops
<b>iris TOTAL:</b>				<b>190</b>	<b>5656</b>	<b>333.67 TFlops</b>
				<b>72 GPUs</b>	<b>368640</b>	<b>+561.6 GPU TFlops</b>

g5k	2008	Dell	Intel Xeon L5335@2GHz 2 × 4C,16GB	22	176	1.408 TFlops
	2012	Dell	Intel Xeon E5-2630L@2GHz 2 × 6C,24GB	16	192	3.072 TFlops
<b>granduc/petitprince TOTAL:</b>				<b>38</b>	<b>368</b>	<b>4.48 TFlops</b>

### Testing cluster:

nyx, viridis, pyro...	2012	Dell	Intel Xeon E5-2420@1.9GHz 1 × 6C,32GB	2	12	0.091 TFlops
	2013	Viridis	ARM A9 Cortex@1.1GHz 1 × 4C,4GB	96	384	0.422 TFlops
	2015	Dell	Intel Xeon E5-2630Lv2@2.4GHz 2 × 6C,32GB	2	24	0.460 TFlops
	2015	Dell	Intel Xeon E5-2660v2@2.2GHz 2 × 10C,32GB	4	80	1.408 TFlops
<b>nyx/viridis TOTAL:</b>				<b>102</b>	<b>500</b>	<b>2.381 TFlops</b>

### Decommissioned clusters (Planned MID-2019)

Cluster	Start	End	Vendors	#N	#C	R <sub>peak</sub>
gaia	[2011-2016]	2019	Bull/Dell/HPE/SGI/Delta	273	3440	69.296 TFlops
			Intel architecture (Gulftown, Sandy/Ivy Bridge, Haswell) incl. 21 GPU nodes (2 to 4 NVidia Tesla per node)	50 GPUs	120704	+76.22 GPU TFlops
chaos	[2010-2012]	2019	Dell/HPE	81	1120	14.495 TFlops

## UL HPC Storage capacity



**9852.4 TB** (incl. 1020TB for Backup)  
2425 disks

- 4 distributed/parallel FS
  - ↪ GPFS : 3244 TB
  - ↪ Lustre: 1940 TB
  - ↪ OneFS: 3188 TB...

# UL HPC Shared Storage Capacities

Cluster	GPFS	Lustre	Other	Backup
<b>iris</b>	2284	1280	6/3188 <sup>2</sup>	600
gaia <sup>1</sup>	960	660	0/3188 <sup>2</sup>	240
chaos <sup>1</sup>	0	0	180	180
g5k	0	0	32.4	0
nyx <sup>1</sup> (experimental)	0	0	242	0
<b>TOTAL:</b>	<b>3244 TB</b>	<b>1940 TB</b>	<b>3648.4 TB</b>	<b>1020 TB</b>

<sup>1</sup>: *Deprecated mid-2019!!*

<sup>2</sup>: *Common Isilon/OneFS shared storage mounted on gaia and iris*

**Uni.lu HPC Total Storage Capacity:**  
**9852.4 TB**



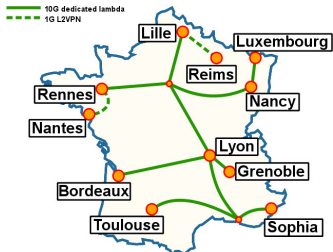
## UL HPC Software Stack

- **Operating System:** **Linux** CentOS 7 (*iris*), Debian 8 (others)
- **Remote connection to the platform:** SSH
- **User SSO:** IPA, OpenLDAP
- **Resource management:** job/batch scheduler: **Slurm**(*iris*), **OAR**
- **(Automatic) Computing Node Deployment:**
  - ↪ FAI (Fully Automatic Installation)(*gaia*, *chaos clusters*)
  - ↪ Bright Cluster Manager (*iris*)
  - ↪ Puppet
  - ↪ Kadeploy
- **Platform Monitoring:**
  - ↪ OAR Monika/Drawgantt, Ganglia, Allinea Perf Report, SLURM
  - ↪ Icinga, NetXMS, PuppetBoard etc.
- **Commercial Softwares:**
  - ↪ ANSYS, ABAQUS, MATLAB, Intel Cluster Studio XE, Allinea DDT, Stata etc.

# The case of Grid'5000

<http://www.grid5000.fr>

- Large scale nation wide infrastructure
  - ↳ for large scale parallel and distributed computing research.

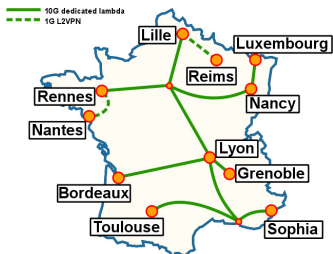


- 10 sites in France
  - ↳ **Abroad:** Luxembourg, Porto Allegre
  - ↳ Total: **7782** cores over **26** clusters
- 1-10GbE / Myrinet / Infiniband
  - ↳ **10Gb/s dedicated** between all sites
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  - ↳ **kadeploy, kavlan, storage5k**

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- Unique software stack
  - ↳ **kadeploy, kavlan, storage5k**

## • Out of scope for this talk

↳ General information:

<https://hpc.uni.lu/g5k>

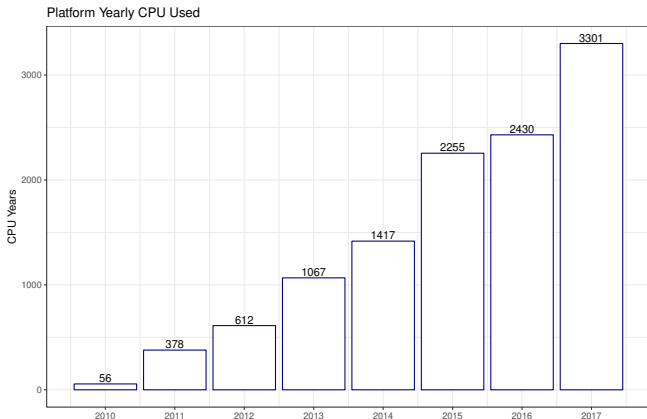
↳ Grid'5000 website and documentation:

<https://www.grid5000.fr>



## CPU-year usage since 2010

- **CPU-hour**: *work* done by a CPU in **one hour** of wall clock time





## Summary

- 1 Introduction**
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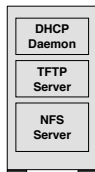
# Computing nodes Management

## Node deployment by FAI/Bright Manager

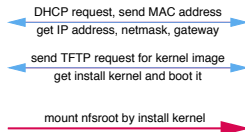
- Boot via network card (PXE)
  - ↔ ensure a running diskless Linux OS



install server



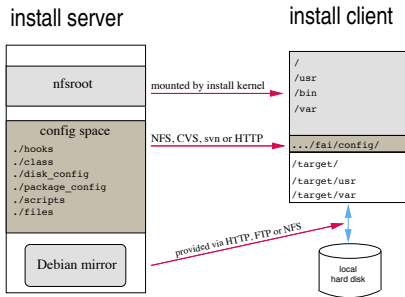
install client



# Computing nodes Management

## Node deployment by FAI/Bright Manager

- Boot via network card (PXE)
  - ↳ ensure a running diskless Linux OS
- Get configuration data (NFS/other)



# Computing nodes Management

## Node deployment by FAI/Bright Manager

- Boot via network card (PXE)
  - ↪ ensure a running diskless Linux OS
- Get configuration data (NFS/other)
- Run the installation
  - ↪ partition local hard disks and create filesystems
  - ↪ install software using apt-get/yum command
  - ↪ configure OS and additional software
  - ↪ save log files to install server, then reboot new system



# Computing nodes Management

## Node deployment by FAI/Bright Manager



- Boot via network card (PXE)
  - ↪ ensure a running diskless Linux OS
- Get configuration data (NFS/other)
- Run the installation
  - ↪ partition local hard disks and create filesystems
  - ↪ install software using apt-get/yum command
  - ↪ configure OS and additional software
  - ↪ save log files to install server, then reboot new system

**Average (full) reinstallation time:  $\simeq$  600s**

# IT Serv[er|ice] Management: Puppet

## Server/Service configuration by Puppet



<http://puppetlabs.com>

- **IT Automation** for configuration management

- ↳ idempotent, agent/master OR stand-alone
- ↳ cross-platform through Puppet Resource Abstraction Layer (RAL)
- ↳ git-based workflow with *r10k* (*role & profiles* workflow)
- ↳ PKI-based security (X.509)

- **DevOps** tool of choice for configuration management

- ↳ Reusable modules
- ↳ per-environment hierarchy lookup with *hier*a

<https://forge.puppet.com/>



Endless Possibilities: DevOps can create an infinite loop of release and feedback for all your code and deployment targets.

# IT Serv[er|ice] Management: Puppet

## Server/Service configuration by Puppet



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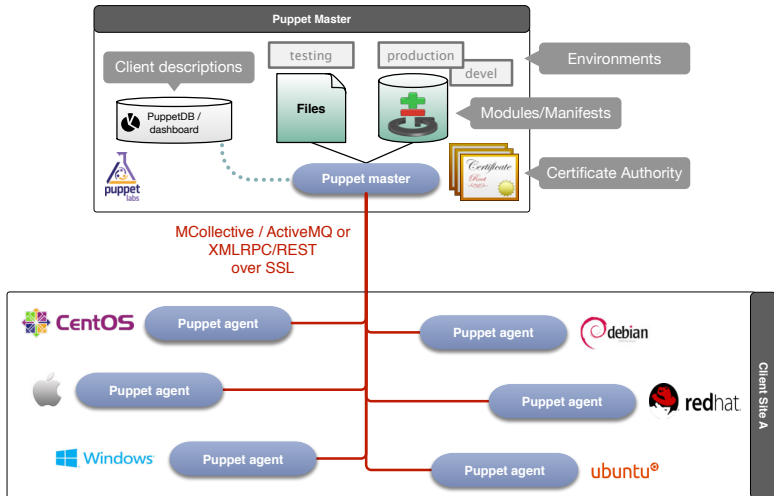
- **DevOps** tool of choice for configuration management

- ↪ Reusable modules <https://forge.puppet.com/>
- ↪ per-environment hierarchy lookup with `hier`

**Average server installation/configuration time:  $\simeq$  3-6 min**



# General Puppet Infrastructure





# Software/Modules Management

<https://hpc.uni.lu/users/software/>

- Based on **Environment Modules / LMod**
  - ↪ convenient way to dynamically change the users environment \$PATH
  - ↪ permits to easily load software through `module` command
- Currently on **UL HPC**:
  - ↪ > **200 software packages**, in *multiple* versions, within **18 categ.**
  - ↪ reworked software set for `iris` cluster and now deployed everywhere
    - ✓ RESIF v2.0, allowing [real] semantic versioning of released builds
  - ↪ hierarchical organization **Ex:** `toolchain/{foss,intel}`

```
$> module avail # List available modules
```

```
$> module load <category>/<software>[/<version>]
```



## Software/Modules Management

- Key module variable: `$MODULEPATH` / where to look for modules  
↳ altered with `module use <path>`. **Ex:**

```
export EASYBUILD_PREFIX=$HOME/.local/easybuild
export LOCAL_MODULES=$EASYBUILD_PREFIX/modules/all
module use $LOCAL_MODULES
```

## Software/Modules Management

- Key module variable: `$MODULEPATH` / where to look for modules  
↳ altered with module use `<path>`. **Ex:**

```
export EASYBUILD_PREFIX=$HOME/.local/easybuild
export LOCAL_MODULES=$EASYBUILD_PREFIX/modules/all
module use $LOCAL_MODULES
```

### Main modules commands:

Command	Description
<code>module avail</code>	Lists all the modules which are available to be loaded
<code>module spider &lt;pattern&gt;</code>	Search for among available modules ( <b>Lmod only</b> )
<code>module load &lt;mod1&gt; [mod2...]</code>	Load a module
<code>module unload &lt;module&gt;</code>	Unload a module
<code>module list</code>	List loaded modules
<code>module purge</code>	Unload all modules (purge)
<code>module display &lt;module&gt;</code>	Display what a module does
<code>module use &lt;path&gt;</code>	Prepend the directory to the <code>MODULEPATH</code> environment variable
<code>module unuse &lt;path&gt;</code>	Remove the directory from the <code>MODULEPATH</code> environment variable

# Software/Modules Management

<http://hpcugent.github.io/easybuild/>

- Easybuild: open-source framework to (automatically) build scientific SW
- **Why?:** *"Could you please install this software on the cluster?"*
  - ↪ Scientific software is often **difficult** to build
    - ✓ non-standard build tools / incomplete build procedures
    - ✓ hardcoded parameters and/or poor/outdated documentation
  - ↪ EasyBuild helps to facilitate this task
    - ✓ **consistent** software **build and installation** framework
    - ✓ includes testing step that helps validate builds
    - ✓ **automatically generates LMod modulefiles**

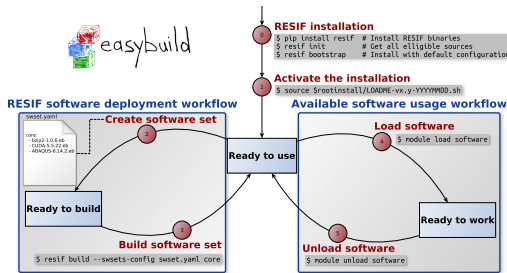
```
$> module use $LOCAL_MODULES
$> module load tools/EasyBuild
# Search for recipes for HPL software
$> eb -S HPL
$> eb HPL-2.2-intel-2018a.eb -Dr # Dry-run install HPL 2.2
$> eb HPL-2.2-intel-2018a.eb -r
```

# Software/Modules Management

- **RESIF**: Revolutionary EasyBuild-based Software Installation Framework
  - ↳ Automatic Management of **software sets**
  - ↳ Fully automates software builds and supports all available toolchains
  - ↳ Clean (hierarchical) modules layout to facilitate its usage
  - ↳ (`_incoming_`) per-release module, per-ISA builds,

MODULEPATH=/opt/apps/resif/data/{devel,production,stable,testing}/default/modules/all/

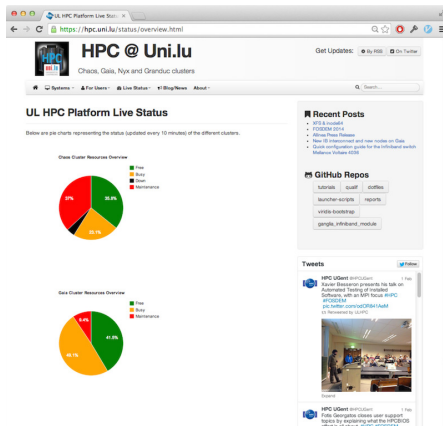
## RESIF: Revolutionary EasyBuild-based Software Installation Framework



## Platform Monitoring

### ● General Live Status

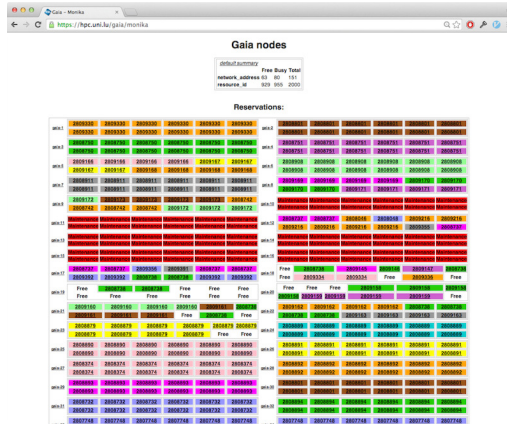
<http://hpc.uni.lu/status/overview.html/>



# Platform Monitoring

- **Monika (OAR)**

<http://hpc.uni.lu/{gaia,chaos,g5k}/monika>

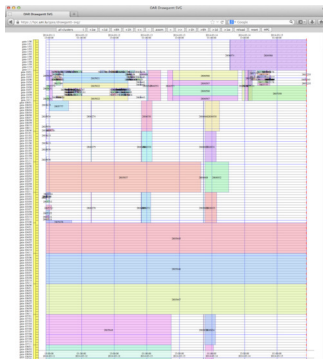




# Platform Monitoring

- Drawgantt (OAR)

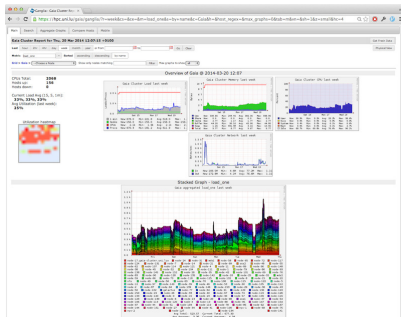
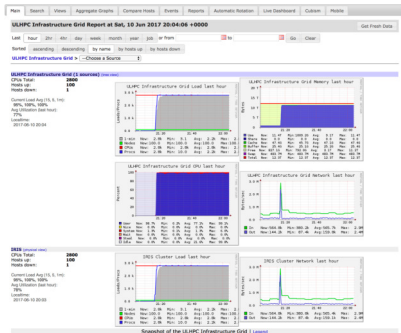
<http://hpc.uni.lu/{gaia,chaos,g5k}/drawgantt>



## Platform Monitoring

### ● Ganglia

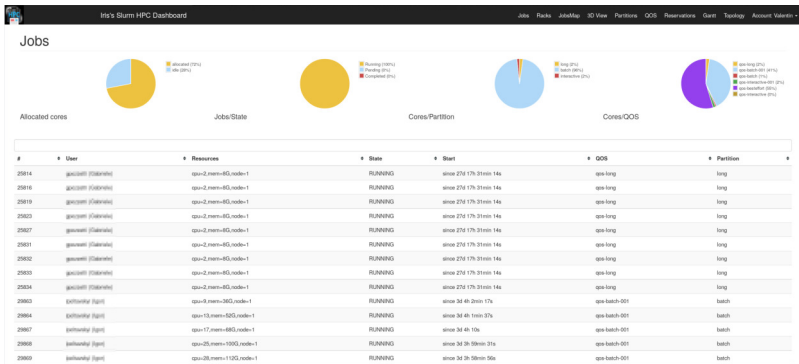
<http://hpc.uni.lu/{gaia,chaos,g5k,iris}/ganglia>



## Platform Monitoring

### SLURM-Web

<http://hpc.uni.lu/iris/slurm/>



## Platform Monitoring

- CDash

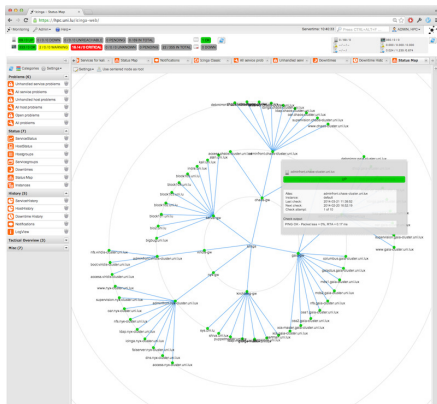
<http://cdash.uni.lu/>

The screenshot shows the CDash web interface for 'UL-HPC-Testing'. The page title is 'UL-HPC-Testing' and it shows the date 'Thursday, March 20 2014 11:55:01 CET'. The main content is a table titled 'Nightly' with columns for 'Site', 'Build Name', 'Update', 'Configure', 'Build', 'Test', and 'Build Time'. The 'Test' column is further divided into 'Files', 'Error', 'Warn', 'Not Pass', 'Fail', and 'Pass'. The table lists 20 build entries, each with a status indicator (green for success, red for failure, yellow for warning) and a '9 hours ago' timestamp.

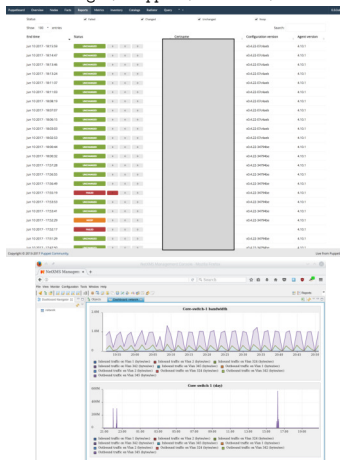
Site	Build Name	Update			Configure			Build			Test			Build Time
		Files	Error	Warn	Error	Warn	Not Pass	Fail	Pass	Files	Error	Warn		
Chaos cluster	MPI Module MPICH2_1.1-GCC-4.8.1	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Galix cluster	MPI Module MPICH2_1.1-GCC-4.8.1	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.8.3-iccfort-2011.13.387	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Galix cluster	MPI Module OpenMPI_1.8.3-iccfort-2011.13.387	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.8.4-GiangGCC-1.3.3	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Galix cluster	MPI Module OpenMPI_1.8.4-GiangGCC-1.3.3	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.8.4-GCC-4.8.4	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Galix cluster	MPI Module OpenMPI_1.8.4-GCC-4.8.4	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.8.4-GCC-4.7.2	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Galix cluster	MPI Module OpenMPI_1.8.4-GCC-4.7.2	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.8.5-GCC-4.7.2	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Galix cluster	MPI Module OpenMPI_1.8.5-GCC-4.7.2	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.7.3-gccouide-2.6.10	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Galix cluster	MPI Module OpenMPI_1.7.3-gccouide-2.6.10	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Chaos cluster	MPI Module imp_3.2.2.006	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Galix cluster	MPI Module imp_3.2.2.006	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Chaos cluster	MPI Module imp_4.0.0.028	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Galix cluster	MPI Module imp_4.0.0.028	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago
Chaos cluster	MPI Module imp_2.0.0.026.totw	0	0	0	0	0	0	0	0	0	0	0	0	9 hours ago

## Platform Monitoring

### Internal Monitoring

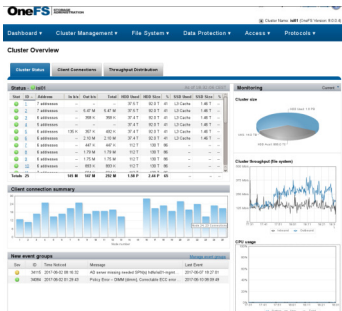


### Icinga / Puppet / NetXMS (networking)

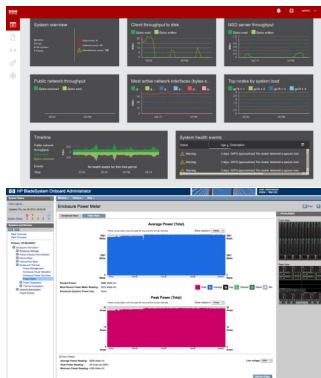


## Platform Monitoring

### Internal Monitoring



### [Disk] Enclosure status





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## Past Year Achievements / Technical

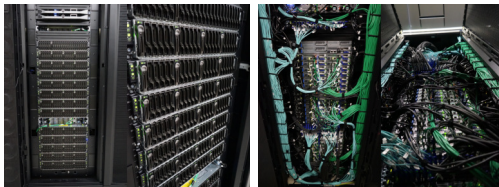
- **2017/2018: Installation of the new flagship iris cluster**

→ RFP 160020: **168 nodes**, 4707 cores **256 TFlops**

- ✓ Dell C6320, 128 GB RAM
- ✓ 108 × 2 Intel Xeon E5-2680v4@2.4 GHz [2x14c] (2017)
- ✓ 60 × 2 Intel Xeon Gold 6132@2.6 GHz [2x14c] (Q1 2018)

→ RFP 180027: **22 GPU/Bigmem nodes**, 952 cores **+77.77 TFlops**

- ✓ **18 GPU nodes** × 4 Nvidia V100 SXM2 32GB **+561.6 GPU TFlops**
- ✓ 4 × 4 Intel Xeon Platinum 8180M@2.5 GHz [4x28c, 3TB RAM]
- ✓ **Deployment planned Dec 2018**

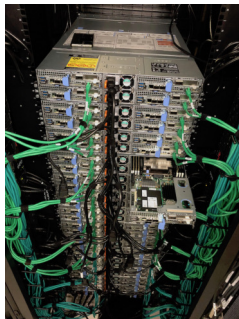




## Past Year Achievements / Technical

- Feb. 2018: Moving iris cluster

↔ CDC S-01 → S-02



## Past Year Achievements / Technical

- **April-Dec 2018: iris Storage (GPFS/Lustre)**

↪ RFP 160019: **SpectrumsScale GPFS** (DDN GridScaler) **2284 TB**

✓ Initial deployment June 2017

/mnt/irisgpfs

✓ Extension done in April 2018

↪ RFP 170035: **Lustre** (DDN Exascaler)

**1280 TB**

✓ Initial deployment April 2018

/mnt/lscratch

✓ Performance issue identified

✓ Lustre Exascaler 4.0 upgrade Oct 2018

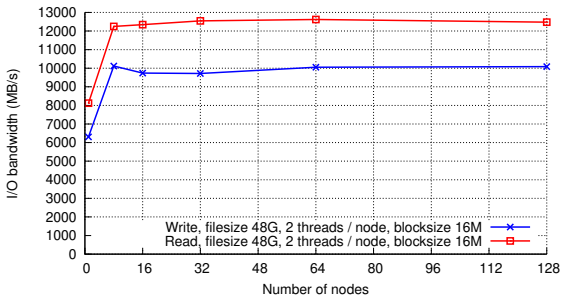
✓ Pending last HW upgrade/final validation (next week!)



# Past Year Achievements / Technical

- iris Storage Performances: Lustre

↳ Self Encrypting Disks (SED)-based storage





## Past Year Achievements / Technical

- **Aug 2018:** RESIF/2018 Software Set update
  - ↪ `toolchain/{foss,intel}/2018a`
  - ↪ **Machine Learning:**
    - ✓ PyTorch, TensorFlow, Keras, Apache Spark
  - ↪ **Math & Optimization:**
    - ✓ MATLAB, Mathematica, CPLEX
  - ↪ **Physics & Chemistry:**
    - ✓ GROMACS, ESPResSo, QuantumESPRESSO, Meep, ABINIT, NAMD, NWChem, VASP, CRYSTAL
  - ↪ **Bioinformatics:**
    - ✓ SAMtools, BEDTools, BWA, BioPerl, FastQC, PLINK, SNPTEST, FASTX-Toolkit, TopHat, Bowtie2, Trinity, BLAST+, ABySS, mpiBLAST, HTSlib
  - ↪ Computer Aided Design & Engineering, CFD: ANSYS, OpenFOAM
  - ↪ Container systems: Singularity
  - ↪ ...



## Past Year Achievements / Technical

- Beyond iris setup, we **introduced several new elements**
  - ↪ Migration to **SLURM**
  - ↪ Consolidation of the High Availability (HA) setup
  - ↪ **Improved system automation** (Puppet 4.x / hiera)



## Past Year Achievements / Technical

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  - ↪ **Improved system automation** (Puppet 4.x / hiera)
- **Continuous OS / software modules / security Upgrade**
  - ↪ Migration to **Debian 8** on gaia and chaos
  - ↪ **RESIF v2**, updated software sets (2018a toolchain & co.)
  - ↪ **Meltdown/Spectre** processor vulnerability **mitigation**

## Past Year Achievements / Technical

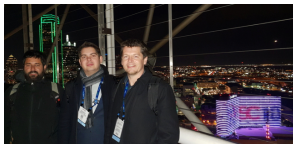
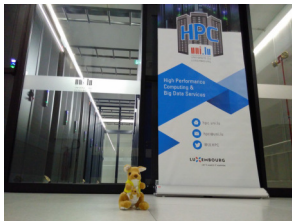
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  - ↪ **RESIF v2**, updated software sets (2018a toolchain & co.)
  - ↪ **Meltdown/Spectre** processor vulnerability **mitigation**
- **Storage:**
  - ↪ **Oct 2018:** EMC/Dell ISILON – ACL reconfiguration
  - ↪ **GPFS gaia: saturated and out of warranty**

- **chaos and gaia will be DECOMMISSIONED mid-2019**
  - ↪ migration guidelines to be released EOY
  - ↪ prepare the transition to iris!!!

## Past Year Events



- 7<sup>th</sup> Uni.lu HPC School Jun 2018
  - ↪ 2 days event (as today but with domain specialised parallel sessions)
- HPC conferences and exhibitions:
  - ↪ SC'18, Dallas, US Nov 2018
  - ↪ HPC User Forum, Stuttgart, DE Sep 2018
  - ↪ ISC'18, Frankfurt, DE Jun 2018







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  - ↪ SC'18, Dallas, US Nov 2018
  - ↪ HPC User Forum, Stuttgart, DE Sep 2018
  - ↪ ISC'18, Frankfurt, DE Jun 2018
- **Invited keynotes**
  - ↪ Data Science Meetup, *Financial Aspects of AI Innovation* Oct 2018
  - ↪ 10<sup>th</sup> anniversary *ISACA.lu* Luxembourg chapter Sep 2018
  - ↪ MVAICH MUG'18, Columbus, US Aug 2018
  - ↪ ISC Workshop HPC Collaboration Europe/Latin America Jun 2018
  - ↪ Data Conversation GDPR Avr 2018
  - ↪ cHiPSet Workshop Model/Simu. in the Data Deluge Era Mar 2018



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## General Guidelines



- The UL HPC is a **\*shared\*** resource
  - ↪ hundreds of users may be logged on at one time
  - ↪ hundreds of jobs may be running on all compute nodes,
- All users must practice **\*good citizenship\***
  - ↪ limit activities that may impact the system for other users.
  - ↪ **Do not abuse the shared filesystems**
    - ✓ Avoid too many simultaneous file transfers
    - ✓ regularly clean your directories from useless files
  - ↪ **Do not run programs on the login nodes**
  - ↪ Plan large scale experiments during night-time or week-ends
    - ✓ **no more than 120 cores** during working day and working hours

## General Guidelines



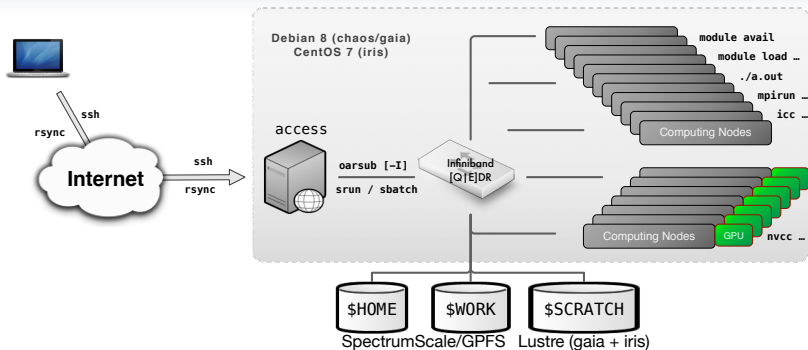
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  - ↪ Plan large scale experiments during night-time or week-ends
    - ✓ **no more than 120 cores** during working day and working hours
- For **ALL** publications having results produced using the UL HPC
  - ↪ Acknowledge / cite the UL HPC facility (using **official banner**)
  - ↪ Tag your publication upon registration on **ORBiLu**.



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# Compute Nodes Environment



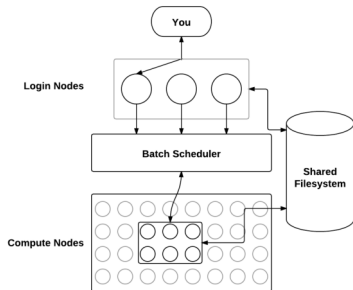
- OS: Debian 8 / CentOS 7
- **Storage usage:** `df-ulhpc`
- **Env. modules:** `modules`
  - ↳ **Not** available on frontends
  - ↳ **\*Only\*** on compute nodes

Directory	Max size	Max #files	Backup
\$HOME (chaos,gaia)	100 GB	1.000.000	YES
\$HOME (iris)	500 GB	1.000.000	YES
\$WORK (excl. iris)	3 TB		NO
\$SCRATCH	per request		NO

## Resource and Job Management Systems

- **Resource and Job Management System (RJMS)**

- ↳ *Glue* for a parallel computer to execute parallel jobs
- ↳ **Goal:** satisfy users demands for computation
  - ✓ assign resources to user jobs with an efficient manner





# Resource and Job Management Systems

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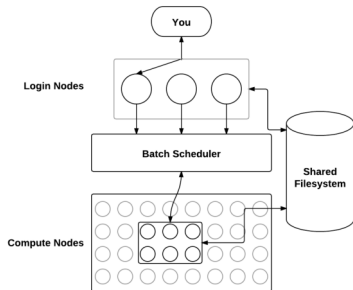
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- **HPC Resources:**

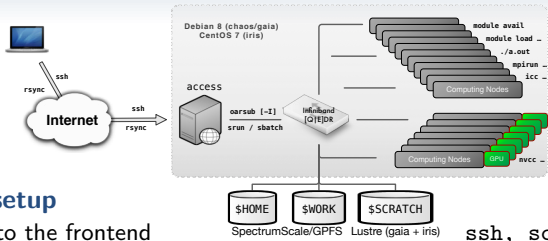
- ↪ Nodes (typically a unique IP address)
  - ✓ Sockets / Cores / Hyperthreads
  - ✓ Memory
  - ✓ Interconnect/switch resources
- ↪ Generic resources (e.g. GPUs)
- ↪ Licenses

- **Strategic Position**

- ↪ Direct/constant knowledge of resources
- ↪ Launch and otherwise manage jobs



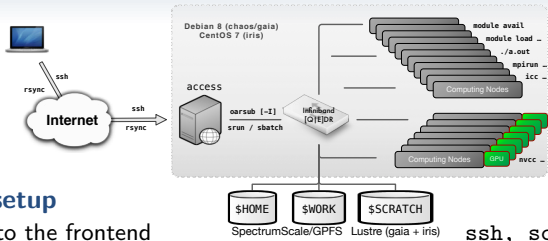
# Typical Workflow on UL HPC resources



## • Preliminary setup

- 1 Connect to the frontend ssh, screen
  - 2 Synchronize you code scp/rsync/svn/git
  - 3 Reserve a few interactive resources oarsub -I [...]
- or, on iris: srun -p interactive [...]
- ✓ (eventually) build your program gcc/icc/mpicc/nvcc..
  - ✓ Test on small size problem mpirun/srun/python/sh...
  - ✓ Prepare a launcher script <launcher>.{sh|py}

# Typical Workflow on UL HPC resources



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  - ✓ (eventually) build your program `gcc/icc/mpicc/nvcc..`
  - ✓ Test on small size problem `mpirun/srun/python/sh...`
  - ✓ Prepare a launcher script `<launcher>.{sh|py}`

## ● Real Experiment

- ① Reserve passive resources `oarsub [...]` `<launcher>`  
 or, on iris: `sbatch -p {batch|long} [...]` `<launcher>`
- ② Grab the results `scp/rsync/svn/git ..`



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## Documentation

[http://hpc.uni.lu/users/getting\\_started.html](http://hpc.uni.lu/users/getting_started.html)

... aka the **rtf<sub>ine</sub>m** paradigm

## Reference Documentation

<http://hpc.uni.lu/docs/>

## Online Tutorials

<http://ulhpc-tutorials.rtfid.io/>

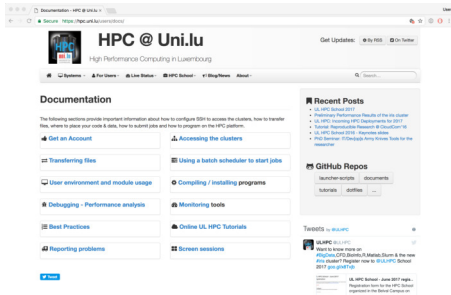
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### ● UL HPC Ticketing System

↔ <https://hpc-tracker.uni.lu/>

↔ [merge.service.uni.lu](https://merge.service.uni.lu/) ?

### ● Ask other users [hpc-users@uni.lu](mailto:hpc-users@uni.lu)

↔ ... OR US [hpc-sysadmins@uni.lu](mailto:hpc-sysadmins@uni.lu)



# Reporting Problems

[https://hpc.uni.lu/users/docs/report\\_pbs.html](https://hpc.uni.lu/users/docs/report_pbs.html)

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- 3 check the state of your nodes
  - ✓ `{ oarsub -C <jobid> | ssh <node>}; htop` *on active jobs*
  - ✓ `{ oarsub -f -j <jobid> }` *post-mortem*
  - ✓ **iris**: `scontrol show job <jobid> OR sacct --job <jobid> -l`
  - ✓ Ganglia on your node(s) <https://hpc.uni.lu/status/ganglia.html>



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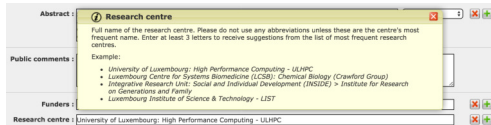
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- In all cases: **Carefully describe the problem and the context**

↪ Guidelines

## Reporting Obtained Results

- In your **scientific publications**: *as per Acceptable Use Policy (AUP)*
  - ↪ **acknowledge** your usage of the UL HPC platform
  - ↪ *(if possible)* **cite** the UL HPC paper `\cite{VBCG_HPCS14}`
- **More importantly**: add **ULHPC** Tag on your **ORBi<sup>lu</sup>** publication



```

@InProceedings{VBCG_HPCS14,
  author =      {S. Varrette and P. Bouvry and H. Cartiaux and F. Georgatos},
  title =      {Management of an Academic HPC Cluster: The UL Experience},
  booktitle =  {Proc. of the 2014 Intl. Conf. on High Performance Computing & Simulation (HPCS 2014)},
  year =      {2014},
  pages =     {959--967},
  month =     {July},
  address =   {Bologna, Italy},
  publisher =  {IEEE},
}
  
```



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# HPC International State of Affairs

## Global race toward Exascale Technology

### IDC-Projected Exascale Investment Levels (In Addition to System Purchases)

#### U.S.



- \$1 to \$2 billion a year in R&D (including NRE)
- Investments by both governments & vendors
- Plans are to purchase multiple exascale systems

#### EU



- About 5 billion euros in total
- Investments in multiple exascale and pre-exascale systems
- Investments mostly by country governments with a little from the EU

#### China



- Over \$1billion a year in R&D
- Investments by both governments & vendors
- Plans are to purchase multiple exascale systems each year
- Already investing in 3 pre-exascale systems by 2017/18

#### Japan



- Planned investment of just over \$1billion\* (over 5 years) for both the R&D and purchase of 1 exascale system
- To be followed by a number of smaller systems ~\$100M to \$150M each
- Creating a new processor and a new software environment

# HPC International State of Affairs

## Global race toward Exascale Technology

### IDC-Projected Exascale Dates and Suppliers

#### U.S.



- Sustained ES: 2023
- Peak ES: 2021
- Vendors: U.S.
- Processors: U.S.
- Initiatives: NSCI/ECP
- Cost: \$300-500M per system, plus heavy R&D investments

#### EU



- Sustained ES: 2023-24
- Peak ES: 2021
- Vendors: U.S., Europe
- Processors: U.S., ARM
- Initiatives: PRACE, ETP4HPC
- Cost: \$300-\$350 per system, plus heavy R&D investments

#### China



- Sustained ES: 2023
- Peak ES: ~~2020~~ 2019...
- Vendors: Chinese
- Processors: Chinese (plus U.S.?)
- 13<sup>th</sup> 5-Year Plan
- Cost: \$350-500M per system, plus heavy R&D

#### Japan



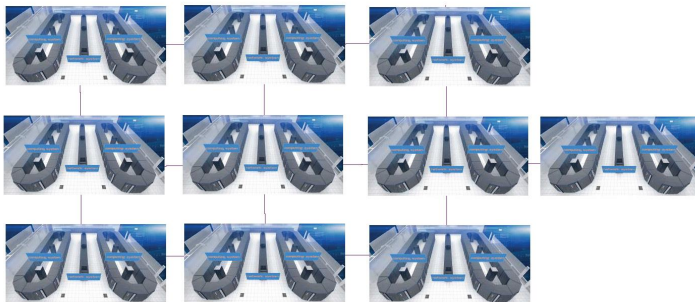
- Sustained ES: 2023-24
- Peak ES: Not planned
- Vendors: Japanese
- Processors: Japanese
- Cost: \$600-850M, this includes both 1 system and the R&D costs...will also do many smaller size systems

# Exascale Feasibility



## We Can Build an Exascale System Today?

Connect together 10 Sunway TaihuLight systems



Require **150 MW** of power, programming for **100 M threads**, and **\$2.7B** price tag

22



## European HPC strategy

- EU HPC strategy initiated in 2012
  - ↔ implementation within H2020 program

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- More recently:
  - ↔ IPCEI on HPC and Big Data (BD) Applications (Nov. 2015)
    - ✓ Luxembourg (leader), France, Italy & Spain
    - ✓ Testbed around Personalized Medicine, Smart Space, Industry 4.0, Smart Manufacturing, New Materials, FinTech, Smart City...

IMPORTANT PROJECT  
OF COMMON  
EUROPEAN INTEREST  
(IPCEI)

ON  
HIGH PERFORMANCE COMPUTING  
AND  
BIG DATA ENABLED APPLICATIONS  
(IPCEI-HPC-BDA)

European Strategic Positioning Paper

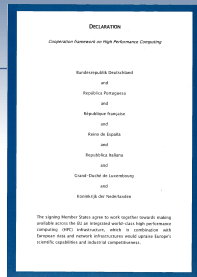
Luxembourg, France, Italy & Spain  
November 2015





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- Latest advances:
  - ↪ EU Member States sign EuroHPC (Mar. 2017)
    - ✓ common effort to create/grow European supercomputing ecosystem
    - ✓ Federation of national/regional HPC centers (see also PRACE2)
  - ↪ EU Objective with EuroHPC:
    - ✓ EuroHPC JU effectively operational starting **Jan 1st, 2019**
    - ✓ 2-3 **Pre-exascale** systems 2020, **2 exascale** systems by 2022





# EU HPC Strategy Implementation

- **European Technology Platform (ETP) for HPC**

- ↪ Industry-led forum feat. HPC stakeholders
- ↪ Providing EU framework to define HPC research priorities/actions
  - ✓ UL (P. Bouvry, S. Varrette, V.Plugaru) part of ETP4HPC (2016-)
  - ✓ See Strategic Research Agenda, 2017 European HPC Handbook...



EUROPEAN  
TECHNOLOGY  
PLATFORM  
FOR HIGH  
PERFORMANCE  
COMPUTING

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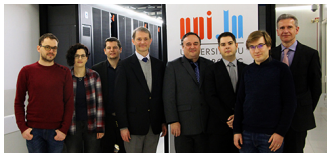
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  - ✓ See **Strategic Research Agenda, 2017 European HPC Handbook**...



- **PRACE** - Partnership for Advanced Computing in Europe

- ↪ Non-profit association, 25 member countries, now entering PRACE2
- ↪ Providing access to **Five EU Tier-0** compute & data resources
- ↪ (Oct. 2017) **Luxembourg 25th country to join PRACE**
  - ✓ Official Delegate/Advisor (P. Bouvry/S. Varrette) from UL



# EU HPC Strategy Implementation

## • European High-Performance Computing Joint Undertaking

↪ EuroHPC JU effectively operational starting **Jan 1st, 2019**

- ✓ administrative management from Luxembourg

↪ Public and private members

- ✓ EC, 25 MS, representatives from supercomputing/BD stakeholders
- ✓ Governing Board (public members)
- ✓ Industrial & Scientific Advisory Board (private members)

↪ EU Objective with EuroHPC:

- ✓ 2 **Pre-exascale** systems (2021), 2-3 **exascale** systems (2023)
- ✓ Pending decision on hosting countries



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**EuroHPC Budget:  $2 \times 486$  M€**

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- **European Processor Initiative (EPI)**

- ↳ Initial plan vs current plan. . .

- ↳ **120 M€** via Framework Partnership Agreement (FPA)



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## New Trends in HPC

- **Continued scaling** of scientific, industrial & financial applications
  - ↪ ... well beyond Exascale
- New trends changing the landscape for HPC
  - ↪ Emergence of **Big Data analytics**
  - ↪ Emergence of (*Hyperscale*) **Cloud Computing**
  - ↪ **Data intensive Internet of Things (IoT)** applications
  - ↪ **Deep learning & cognitive computing** paradigms

This study was carried out for RIKEN by



### Special Study

Analysis of the Characteristics and Development Trends of the Next-Generation of Supercomputers in Foreign Countries

Earl C. Joseph, Ph.D.  
Steve Conway

Robert Sorensen  
Kevin Monroe

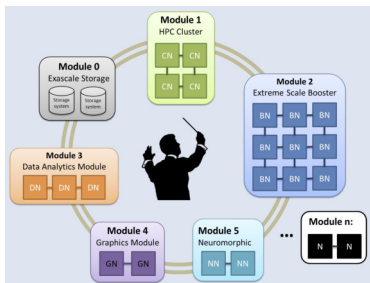
[Source : IDC RIKEN report, 2016]



[Source : EuroLab-4-HPC]

# Toward Modular Computing

- Aiming at **scalable, flexible HPC infrastructures**
  - ↪ *Primary processing on CPUs and accelerators*
    - ✓ **HPC & Extreme Scale Booster** modules
  - ↪ *Specialized modules for:*
    - ✓ **HTC & I/O intensive** workloads;
    - ✓ **[Big] Data Analytics & AI**



[Source : "Towards Modular Supercomputing: The DEEP and DEEP-ER projects", 2016]



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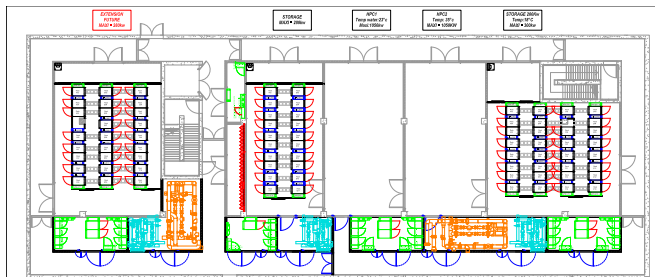
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# Uni.lu CDC (Centre de Calcul)

- **Toward Energy-Efficient HPC enabling DLC**

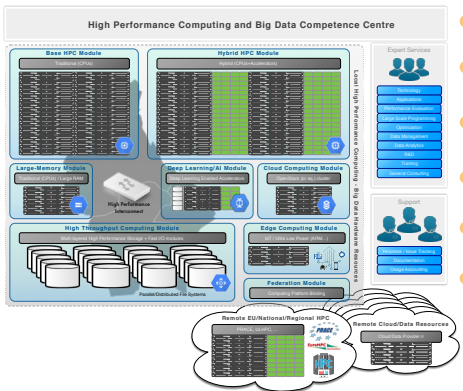
↪ 2x500 m<sup>2</sup> deployed since 2015, one floor for HPC developments

Location	Cooling	Usage	Max Capacity [kW]
CDC S-02-001	Airflow	<i>Future extension</i>	280 kW (120 m <sup>2</sup> )
CDC S-02-002	Airflow	Storage / Traditional HPC /Cloud/FPGA	280 kW (88 m <sup>2</sup> )
CDC S-02-003	<b>DLC</b>	<b>High Density/Energy efficient HPC</b>	<b>1050 kW (90 m<sup>2</sup>)</b>
CDC S-02-004	<b>DLC</b>	<b>High Density/Energy efficient HPC</b>	<b>1050 kW (92 m<sup>2</sup>)</b>
CDC S-02-005	Airflow	Storage / Traditional HPC (iris cluster)	300 kW (128 m <sup>2</sup> )



# National HPC-BD Competence Center

- Built by ministerial, academic, industrial stakeholders
- ↳ Inspired by national research computing centers



- Comprehensive centre:
  - ↳ HPC
  - ↳ data infrastructure
  - ↳ Techn. Expertise
  - ↳ Domain knowledge
- *More than just computing services*
- **Inspiration:**
  - ↳ **EU:** JSC, TGCC...
  - ↳ **US:** OSC, SDSC, TACC, LLNL...
  - ↳ **Singapore:** A\*STAR



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## Conclusion

- **Luxembourg government priority on HPC**

- ↪ sustained by University of Luxembourg HPC developments
  - ✓ started in 2007, under resp. of Prof P. Bouvry & Dr. S. Varrette
  - ✓ expert UL HPC team (*S. Varrette, V. Plugaru, S. Peter, H. Cartiaux, C. Parisot*)
  - ✓ computational scientists / domain experts across ALL the UL
- ↪ Uni.lu HPC (as of 2018): **1062.142 TFlops, 9852.4TB (shared)**

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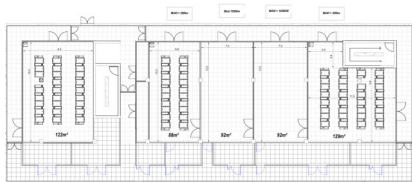
### Several On-going Strategic HPC efforts in Europe...

- ... in which **UL (HPC)** is involved ...

- ↪ ETP4HPC, EU COST Action NESUS etc.
- ↪ PRACE - Official representative for Luxembourg from UL
  - ✓ Delegate: Prof. Pascal Bouvry
  - ✓ Advisor: Dr. Sebastien Varrette
- ↪ EuroHPC / IPCEI on HPC and Big Data (BD) Applications
- ↪ **National HPC-BD Competence Center**

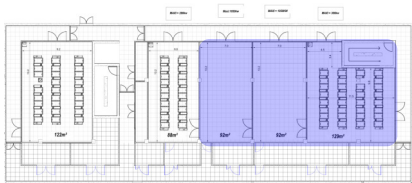


## Incoming Milestones in MSA CDC-02



- $\approx$  **1050kW** per **HPC** room
  - ↪ Direct Liquid Cooling (DLC)
- $\approx$  **300kW** per **storage** room
  - ↪ rooms 1, 2 & 5
  - ↪ Air-flow storage / HPC

## Incoming Milestones in MSA CDC-02

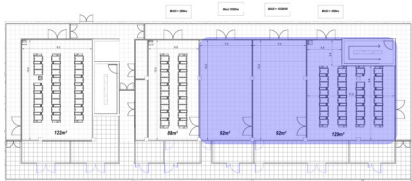


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- **Short term actions (by mid 2019)**

- ↪ Official **Research computing @ UL & abroad** structure

## Incoming Milestones in MSA CDC-02

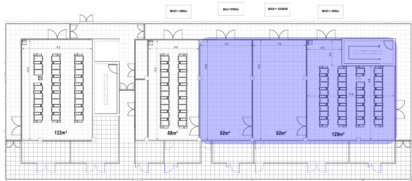


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  - ↪ rooms 1, 2 & 5
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### ● Short term actions (by mid 2019)

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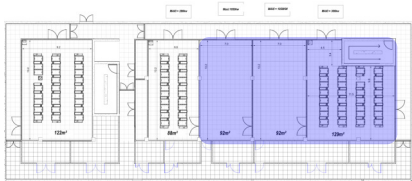


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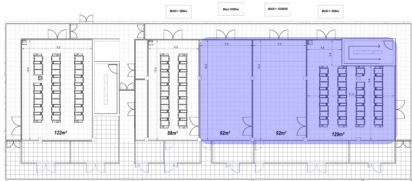


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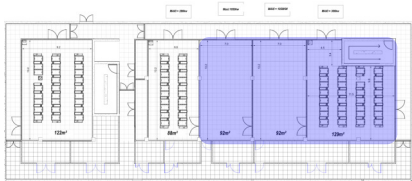


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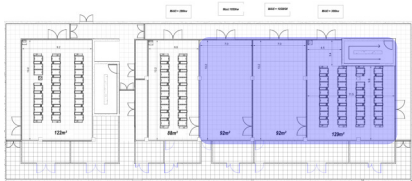


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- ↪ **UL HPC Service Contracts**





Thank you for your attention...

## Questions?

<http://hpc.uni.lu>

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- 1 Introduction**  
Preliminaries  
[Parallel] Computing for Enhanced Research  
Overview of the Main HPC Components
- 2 High Performance Computing (HPC) @ UL**  
Overview  
Platform Management  
Back to last achievements & incoming developments

- 3 UL HPC in Practice: Toward an [Efficient] Win-Win Usage**  
General Considerations  
Environment & Typical Workflow Overview  
Documentation & Reporting (problems or results)
- 4 HPC Strategy in Europe & Abroad**
- 5 Current and Future Developments in Luxembourg**  
Trends in HPC  
Incoming Milestones in Luxembourg
- 6 Conclusion & Perspectives**