UL HPC School 2017 [bis]

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

Prof. Pascal Bouvry, Dr. Sebastien Varrette

and the UL HPC Team

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

Nov. 9th, 2017, MSA 3.070

University of Luxembourg (UL), Luxembourg

Welcome to the UL HPC School 2017

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

- **6th 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.)

Welcome to the UL HPC School 2017

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

- **6th 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.)

- **Next edition** planned for **June., 2018** in Belval
  - ↪ Full 2-days event, adressing advanced tutorials

Agenda Nov 9th, 2017

Time	Main Track (MSA 3.070)
9h00-10h00	**PS1a**: Getting Started on the UL HPC platform
10h00-10h30	**Coffee break**
10h30-11h45	**Keynote**: Overview and Challenges of the UL HPC Facility at the Belval and EuroHPC Horizon
11h45-12h30	**PS1b**: Getting Started on the UL HPC platform - continued
12h30-13h30	**LUNCH**
13h30-15h30	**PS2**: HPC workflow with sequential jobs (test cases on GROMACS, Java and Python)
15h30-16h00	**Coffee break**
16h00-17h00	**PS3**: UL HPC Monitoring in practice: why, what, how, where to look
17h00-18h00	**PS4**: HPC workflow with Parallel/Distributed MPI jobs

Time	Advanced Parallel Track (MSA 3.100)
13h30-14h30	**PS5**: Advanced Scheduling (Slurm, OAR)
14h30-15h30	**PS6**: Debugging, profiling and performance analysis
15h30-16h00	**Coffee break**
16h00-17h00	**PS7**: [Advanced] Prototyping with Python
17h00-18h00	**PS8**: MATLAB (interactive, passive and sequential jobs)

PS = *Practical Session using your laptop*

Summary

Summary

Summary

Prerequisites

- **HPC**: **H**igh **P**erformance **C**omputing

Main HPC Performance Metrics

- Computing Capacity/speed: often measured in **flops** (or **flop/s**)
  - ↪ **Fl**oating **p**oint **o**perations per **s**econds (often in DP)
  - ↪ **GFlops** $= 10^9$ Flops **TFlops** $= 10^{12}$ Flops **PFlops** $= 10^{15}$ Flops
- Storage Capacity: measured in multiples of **bytes** = 8 **bits**
  - ↪ **GB** $= 10^9$ bytes **TB** $= 10^{12}$ bytes **PB** $= 10^{15}$ bytes
  - ↪ **GiB** $= 1024^3$ bytes **TiB** $= 1024^4$ bytes **PiB** $= 1024^5$ bytes
- Transfer rate on a medium measured in **Mb/s** or **MB/s**
- Other metrics: Sequential vs Random **R/W speed**, **IOPS** ...

Why High Performance Computing ?

The country that out-computes will be the one that out-competes — *Council on Competitiveness*

- **Accelerates** research by accelerating **computation**

$\simeq$ 64 **G**Flops	206.772 **T**Flops
(Dual-core i5 2GHz)	(602 computing nodes,8452 cores)

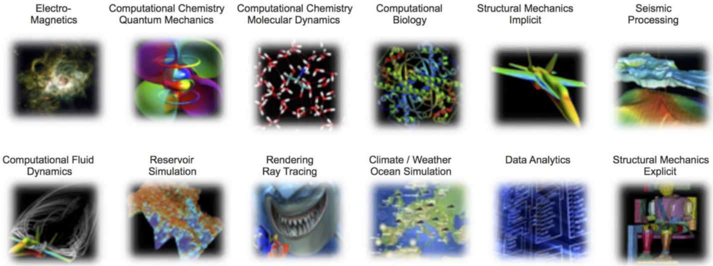
- Increases **storage** capacity and velocity for Big Data processing

4 TB	7952.4TB
(1 disk, 250 MB/s)	(2015 disks, 10 GB/s)

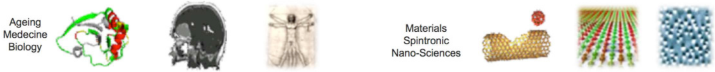
- **Communicates faster** — 1 GbE (1 Gb/s) vs Infiniband EDR (100 Gb/s)

HPC at the Heart of our Daily Life

- **Today**: Research, Industry, Local Collectivities

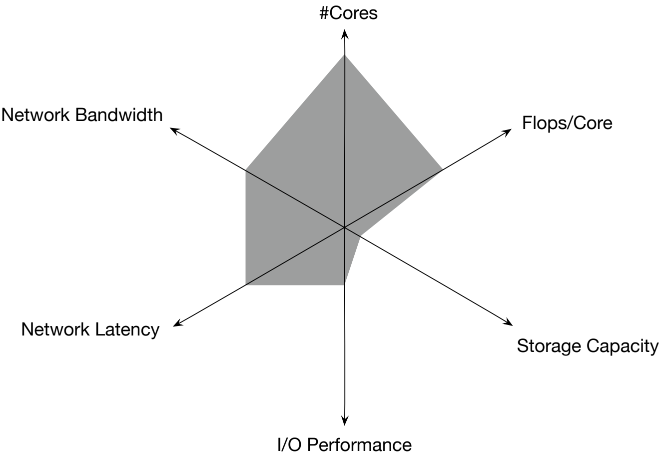


- ... **Tomorrow**: applied research, digital health, nano/bio tech.



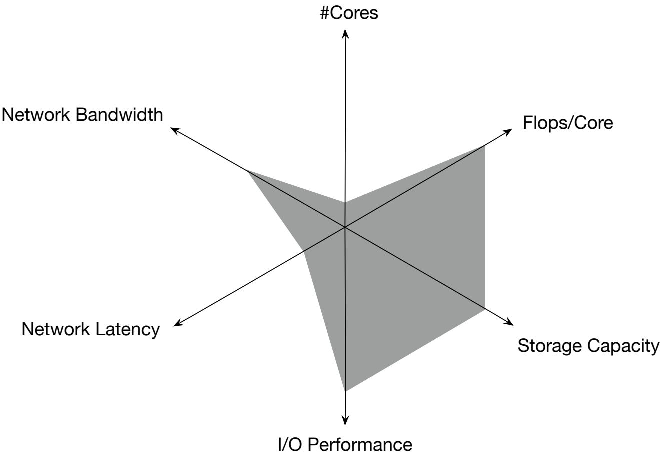
Different HPC Needs per Domains

Material Science & Engineering



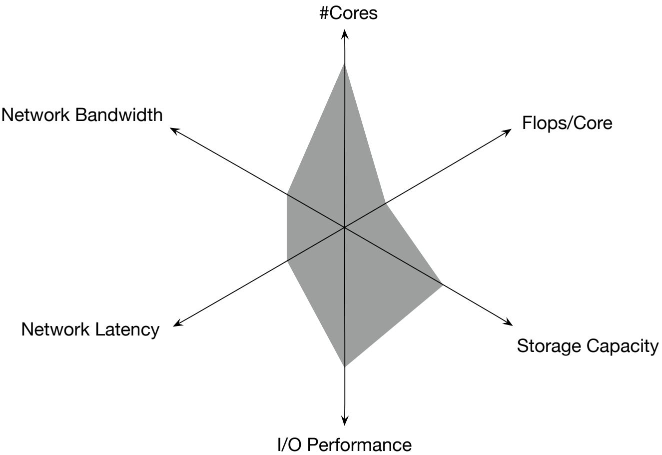
Different HPC Needs per Domains

Biomedical Industry / Life Sciences



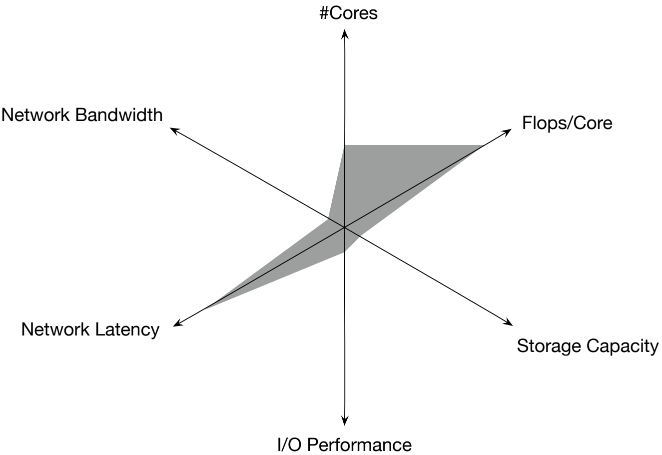
Different HPC Needs per Domains

Deep Learning / Cognitive Computing



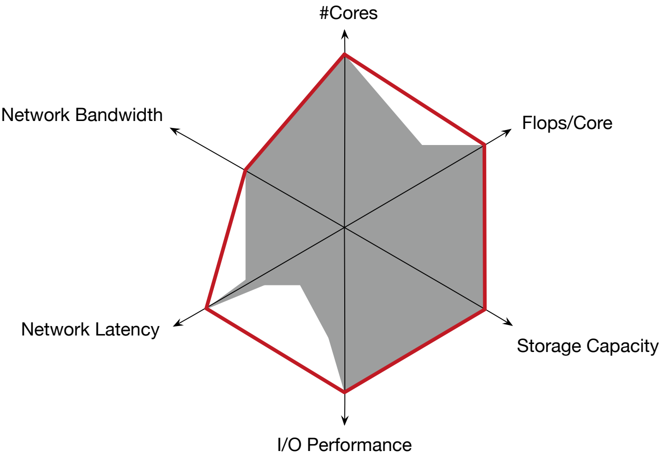
Different HPC Needs per Domains

IoT, FinTech



Different HPC Needs per Domains

ALL Research Computing Domains



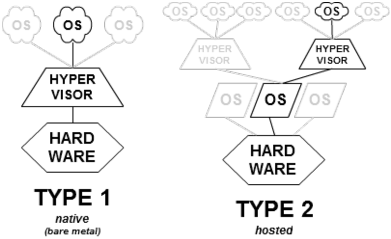
Summary

Computing for Researchers: Laptop

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

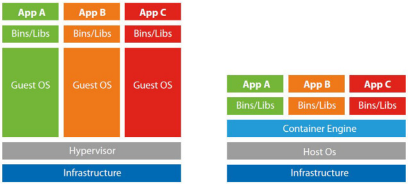
Computing for Researchers: Laptop

- **Regular PC / Local Laptop / Workstation**
  - ↪ **Native OS** (Windows, Linux, Mac etc.)
- Virtualized OS (**VM**) through an **hypervisor**
  - ↪ *Hypervisor*: core virtualization engine / environment
    - ✓ Ex: Xen, VMWare ESXi, KVM, VirtualBox
    - ✓ Non-negligible Performance loss: $\geq$ 20%



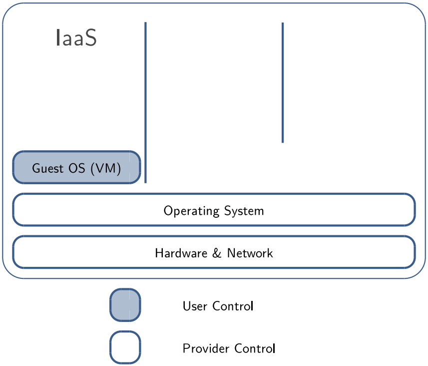
Computing for Researchers: Laptop

- **Regular PC / Local Laptop / Workstation**
  - ↪ **Native OS** (Windows, Linux, Mac etc.)
- Virtualized OS (**VM**) through an **hypervisor**
  - ↪ *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



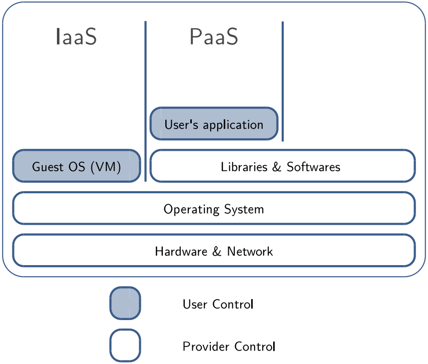
Computing for Researchers: Cloud

- **Cloud Computing**
  - ↪ access to shared *(generally virtualized)* resources
  - ↪ pay-per-use approach
  - ↪ **Infrastructure** as a Service (**I**aaS)



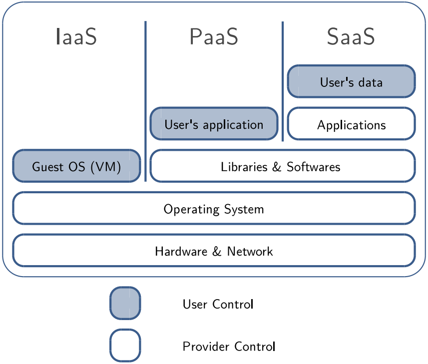
Computing for Researchers: Cloud

- **Cloud Computing**
  - ↪ access to shared *(generally virtualized)* resources
  - ↪ pay-per-use approach
  - ↪ **Platform** as a Service (**P**aaS)



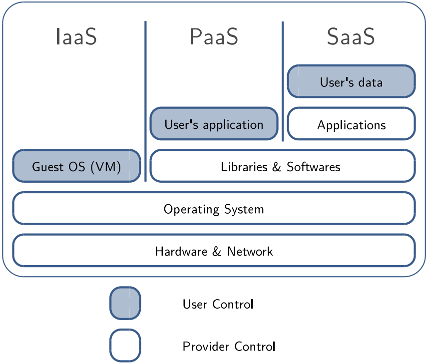
Computing for Researchers: Cloud

- **Cloud Computing**
  - ↪ access to shared *(generally virtualized)* resources
  - ↪ pay-per-use approach
  - ↪ **Software** as a Service (**S**aaS)



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**

Computing for Researchers: HPC

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

YET...

$$\textbf{PC} \neq \textbf{Cloud} \neq \textbf{HPC}$$

Computing for Researchers: HPC

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

YET...

PC ≠ Cloud ≠ HPC

- HPC ≃ 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
```

Jobs, Tasks & Local Execution

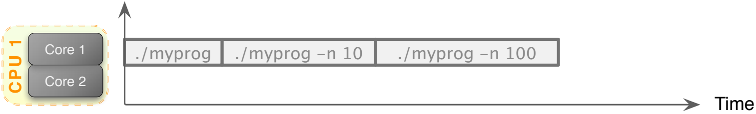
```
$> ./myprog
$> ./myprog -n 10
```

Jobs, Tasks & Local Execution

```
$> ./myprog
$> ./myprog -n 10
$> ./myprog -n 100
```

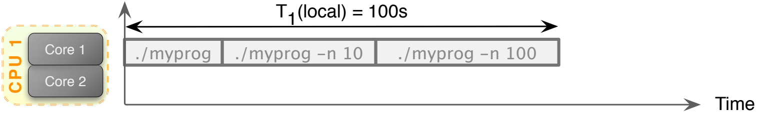
Jobs, Tasks & Local Execution

```
$> ./myprog
$> ./myprog -n 10
$> ./myprog -n 100
```

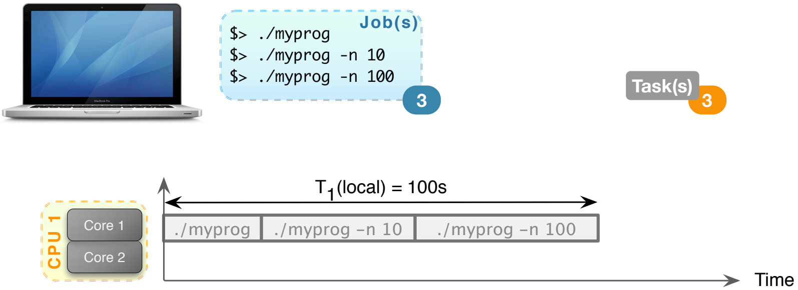


Jobs, Tasks & Local Execution

```
$> ./myprog
$> ./myprog -n 10
$> ./myprog -n 100
```



Jobs, Tasks & Local Execution



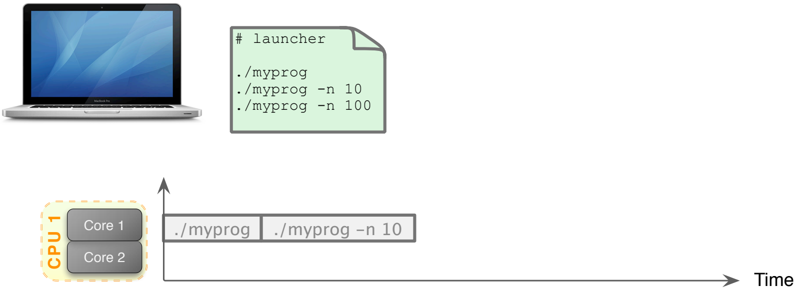
Jobs, Tasks & Local Execution

```
# launcher

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

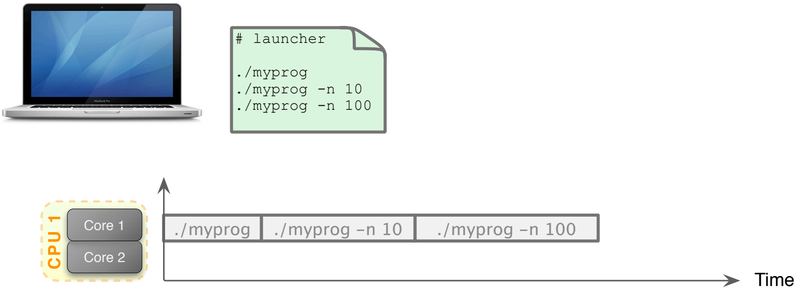
Jobs, Tasks & Local Execution

```
# launcher

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

Jobs, Tasks & Local Execution

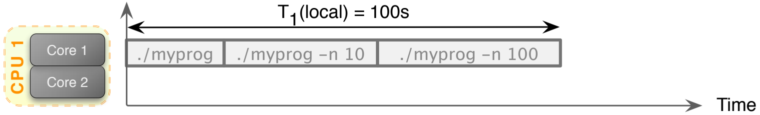


Jobs, Tasks & Local Execution

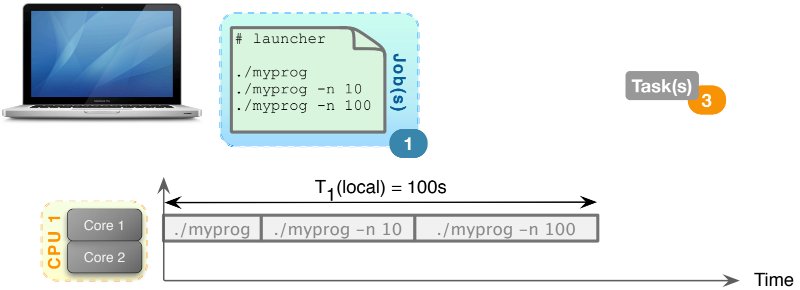


Jobs, Tasks & Local Execution

```
# launcher

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



Jobs, Tasks & Local Execution



Jobs, Tasks & Local Execution

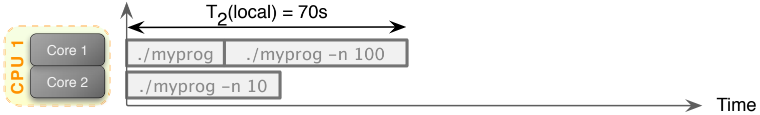
```
# launcher

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

Jobs, Tasks & Local Execution

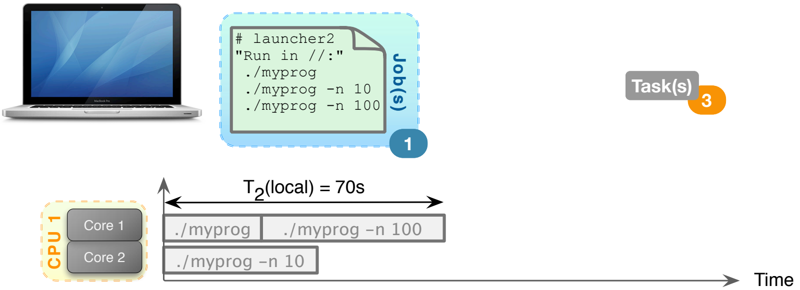
```
# launcher2
"Run in //:"
 ./myprog
 ./myprog -n 10
 ./myprog -n 100
```

Jobs, Tasks & Local Execution

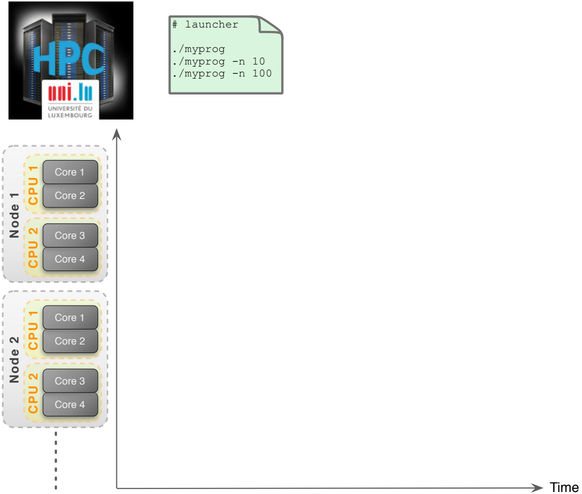
```
# launcher2
"Run in //:"
 ./myprog
 ./myprog -n 10
 ./myprog -n 100
```



Jobs, Tasks & Local Execution

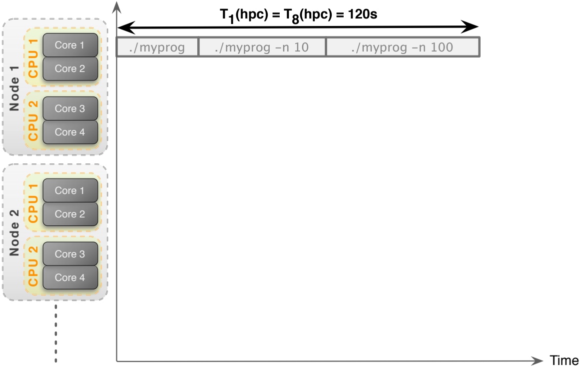


Jobs, Tasks & HPC Execution

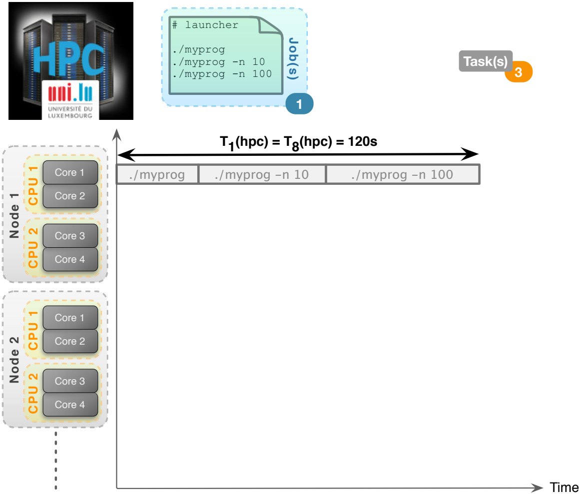


Jobs, Tasks & HPC Execution

```
# launcher

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

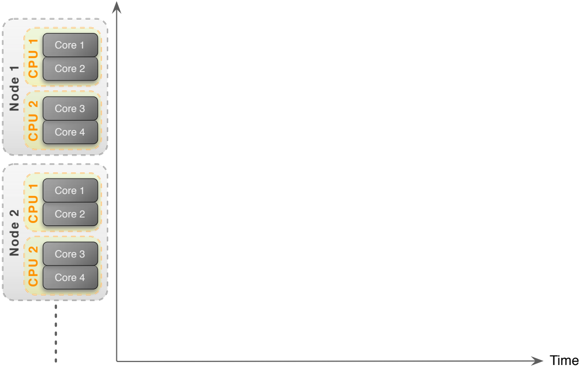


Jobs, Tasks & HPC Execution



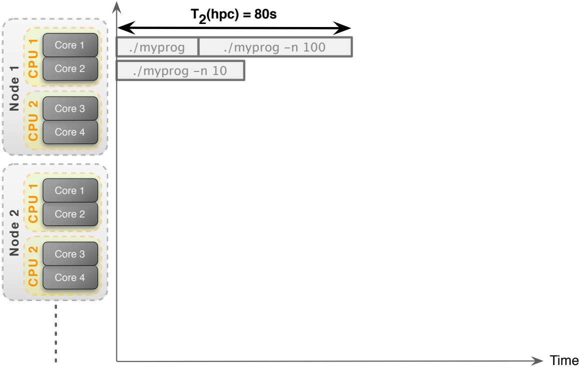
Jobs, Tasks & HPC Execution

```
# launcher2
"Run in //:"
 ./myprog
 ./myprog -n 10
 ./myprog -n 100
```

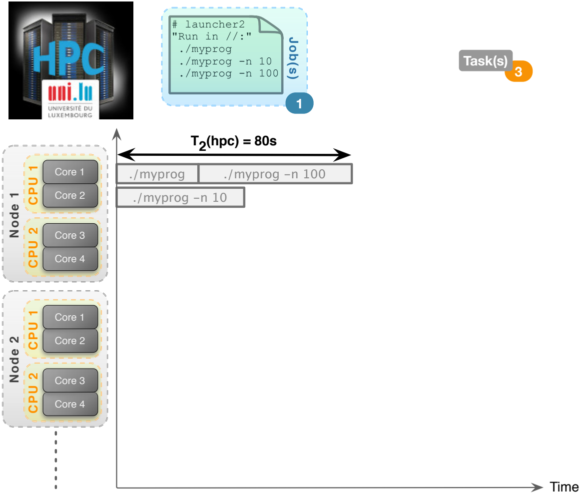


Jobs, Tasks & HPC Execution

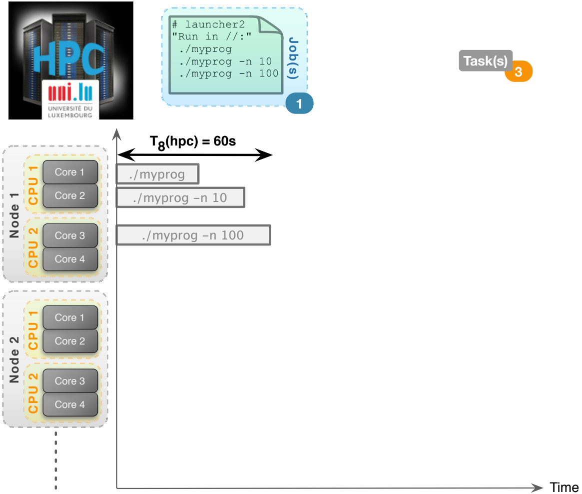
```
# launcher2
"Run in //:"
 ./myprog
 ./myprog -n 10
 ./myprog -n 100
```



Jobs, Tasks & HPC Execution



Jobs, Tasks & HPC Execution



Local vs. HPC Executions

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

Local vs. HPC Executions

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

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

Local vs. HPC Executions

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

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

- **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

Summary

HPC Components: [GP]CPU

CPU

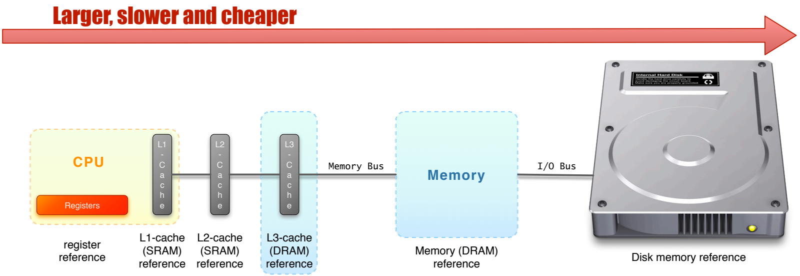
- Always multi-core
- Ex: Intel Core i7-7700K (Jan 2017) $R_{peak} \simeq$ 268.8 GFlops (DP)
  - ↪ 4 cores @ 4.2GHz (14nm, 91W, 1.75 billion transistors)
  - ↪ + integrated graphics (24 EUs) $R_{peak} \simeq$ +441.6 GFlops

GPU / GPGPU

- Always multi-core, optimized for vector processing
- Ex: Nvidia Tesla V100 (Jun 2017) $R_{peak} \simeq$ 7 TFlops (DP)
  - ↪ 5120 cores @ 1.3GHz (12nm, 250W, 21 billion transistors)
  - ↪ focus on Deep Learning workloads $R_{peak} \simeq$ 112 TFLOPS (HP)

$\simeq$ **100 Gflops** for 130$ (CPU), 214$? (GPU)

HPC Components: Local Memory



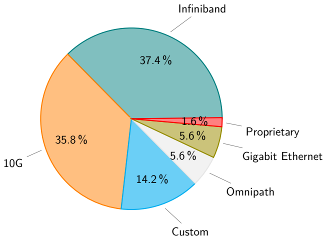
Level:	1	2			3	4
Size:	500 bytes	64 KB to 8 MB			1 GB	1 TB
Speed:	sub ns	1-2 cycles	10 cycles	20 cycles	hundreds cycles	ten of thousands cycles

- 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	40μs to 300μs
10 Gigabit Ethernet	10 Gb/s	1.25 GB/s	4μs to 5μs
Infiniband QDR	40 Gb/s	5 GB/s	1.29μs to 2.6μs
Infiniband EDR	100 Gb/s	12.5 GB/s	0.61μs to 1.3μs
100 Gigabit Ethernet	100 Gb/s	1.25 GB/s	30μs
Intel Omnipath	100 Gb/s	12.5 GB/s	0.9μs

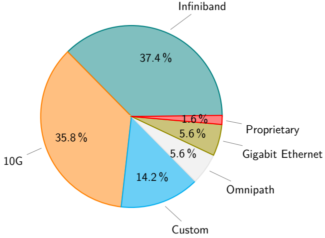


[Source : www.top500.org, Nov. 2016]

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	40μs to 300μs
10 Gigabit Ethernet	10 Gb/s	1.25 GB/s	4μs to 5μs
Infiniband QDR	40 Gb/s	5 GB/s	1.29μs to 2.6μs
Infiniband EDR	100 Gb/s	12.5 GB/s	0.61μs to 1.3μs
100 Gigabit Ethernet	100 Gb/s	1.25 GB/s	30μs
Intel Omnipath	100 Gb/s	12.5 GB/s	0.9μs



[Source : www.top500.org, Nov. 2016]

Network Topologies

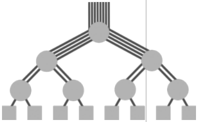
- **Direct** vs. **Indirect** interconnect
  - ↪ *direct*: each network node attaches to at least one compute node
  - ↪ *indirect*: compute nodes attached at the edge of the network only
    - ✓ many routers only connect to other routers.

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.

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

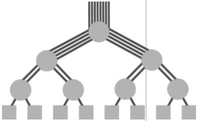


Network Topologies

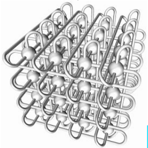
- **Direct** vs. **Indirect** interconnect
  - ↪ *direct*: each network node attaches to at least one compute node
  - ↪ *indirect*: compute nodes attached at the edge of the network only
    - ✓ many routers only connect to other routers.

Main HPC Topologies

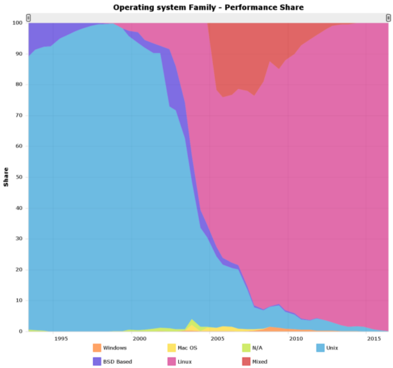
- **CLOS Network / Fat-Trees** [Indirect]
  - ↪ can be fully non-blocking (1:1) or blocking (x:1)
  - ↪ typically enables **best performance**
    - ✓ Non blocking bandwidth, lowest network latency



- **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

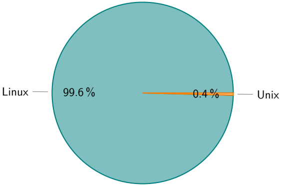


HPC Components: Operating System



- Exclusively Linux-based (99.6%)
  - ↪ . . . or Unix (0.4%)
- Reasons:
  - ↪ stability
  - ↪ prone to devels

[Source : www.top500.org, Nov 2016]



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)

[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)

Main Characteristic of Parallel/Distributed File Systems

Capacity and Performance increase with #servers

[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)

Main Characteristic of Parallel/Distributed File Systems

Capacity and Performance increase with #servers

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	**10.14**	**8,41**
`gpfs` (gaia)	Parallel/Distributed FS	7.74	6.524
`lustre`	Parallel/Distributed FS	4.5	2.956

* maximum **random** read/write, per IOZone or IOR measures, using 15 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)

HPC Components: Data Center

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

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

Summary

Summary

High Performance Computing @ UL

- **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)*
  - ↪ **8,173,747€** cumulative investment in hardware

Key numbers

- 416 users
- 602 computing nodes
  - ↪ 8452 cores, **206.772 TFlops**
  - ↪ 50 accelerators (+ **76.22 TFlops**)
- **7952.4 TB** storage
- 130 (+ 71) servers
- 5 sysadmins
- 2 sites: Kirchberg / Belval

http://hpc.uni.lu

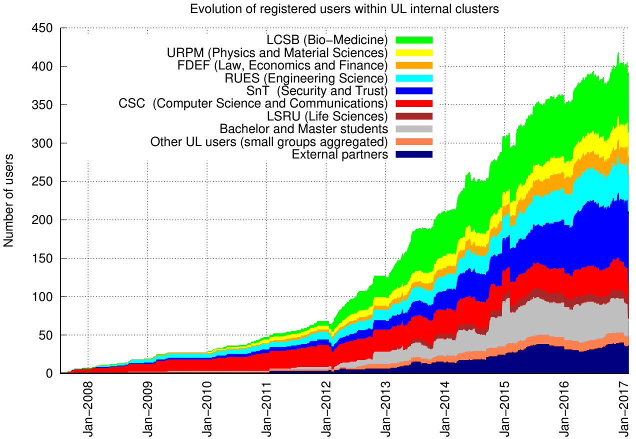
High Performance Computing @ UL

- **Enables & accelerates** scientific discovery and innovation
- **Largest facility** in Luxembourg (after GoodYear R&D Center)

Country	Institute	#Nodes	(CPU) #Cores	TFlops R_{peak}	TB (Shared) Storage
Luxembourg	**UL HPC** (Uni.lu)	**602**	**8452**	**206.772**	**7952.4**
	LIST	58	800	6.21	144
France	LORIA (G5K), Nancy	320	2520	26.98	82
	ROMEO, Reims	174	3136	49.26	245
Belgium	NIC4, University of Liège	128	2048	32.00	20
	Université Catholique de Louvain	112	1344	13.28	120
	UGent / VSC, Gent	440	8768	275.30	1122
Germany	bwGrid, Heidelberg	140	1120	12.38	32
	bwForCluster, Ulm	444	7104	266.40	400
	bwHPC MLS&WISO, Mannheim	604	9728	371.60	420

UL HPC User Base

- **416 Active** HPC Users



UL HPC Beneficiaries

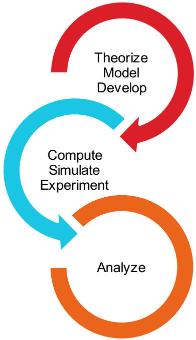
23 computational domains accelerated on UL HPC

- 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 feat. special systems targeting specific workloads:
  - ↪ **Machine Learning & AI**: GPU accelerators
    - ✓ 10 Tesla K40 + 16 Tesla K80 + 24 Tesla M20*: **76 GPU Tflops**
  - ↪ **BigData analytics & data driven science**: large memory systems
    - ✓ Large SMP systems with 1, 2, 3 & 4 TB RAM
  - ↪ **Scale-out workloads**: energy efficient systems
    - ✓ 90 HP Moonshot servers + 96 viridis ARM-based systems

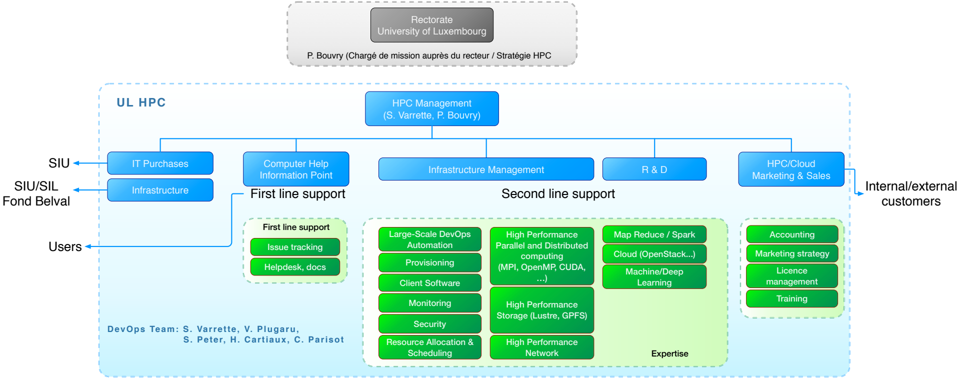
Accelerating UL Research

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



- >140 **software packages** available for researchers
  - ↪ **General purpose**, statistics, optimization:
    - ✓ Matlab, Mathematica, R, Stata, CPLEX, Gurobi Optimizer. . .
  - ↪ **Bioinformatics**
    - ✓ BioPython, STAR, TopHat, Bowtie, mpiHMMER. . .
  - ↪ **Computer aided engineering**:
    - ✓ ANSYS, ABAQUS, OpenFOAM. . .
  - ↪ **Molecular dynamics**:
    - ✓ NAMD, ABINIT, Q.ESPRESSO, GROMACS. . .
  - ↪ **Visualisation**: ParaView, VisIt, VMD, XCS portal
  - ↪ Compilers, libraries, performance modeling tools
  - ↪ [Parallel] debugging tools aiding development

ULHPC Governance



UL HPC Team

Prof. Pascal Bouvry
Director of DS-CSCE, Leader of PCO Group
Senior advisor for the president as regards the HPC strategy

Sébastien Varrette, PhD
CDI, Research Scientist (CSC, FSTC)

Valentin Plugaru, MSc.
CDI, Research Associate (CSC, FSTC)

Sarah Peter, MSc.
CDD, Research Associate (LCSB)

Hyacinthe Cartiaux
CDI, Support (SIU)

Clément Parisot
CDI, Support (CSC, FSTC)

Sites / Data centers

Kirchberg	Belval
CS.43, AS. 28	Biotech I, CDC/MSA

2 sites, $\geq$ 4 server rooms

Sites / Data centers

Kirchberg

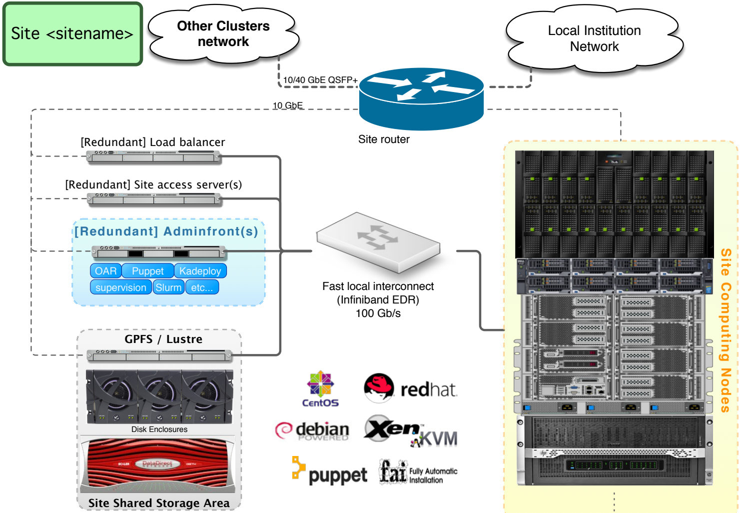
CS.43, AS. 28

Belval

Biotech I, CDC/MSA

2 sites, $\geq$ 4 server rooms

UL HPC: General cluster organization



UL HPC Computing capacity

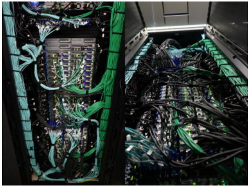
5 clusters

206.772 TFlops

602 nodes

8452 cores

34512GPU cores



INFINIBAND TRADE ASSOCIATION intel

UL HPC Computing Clusters

Cluster	Location	**#N**	**#C**	**Rpeak**	GPU Rpeak
iris	CDC S-01	108	3024	116.12	0
gaia	BT1	273	3440	69.296	76
chaos	Kirchberg	81	1120	14.495	0
g5k	Kirchberg	38	368	4.48	0
nyx (experimental)	BT1	102	500	2.381	0
	TOTAL:	**602**	**8452**	**206.772**	**+ 76 TFlops**

UL HPC - Detailed Computing Nodes

	Date	Vendor	Proc. Description		#N	#C	R_{peak}
iris	2017	Dell	Intel Xeon E5-2680 v4@2.4GHz	2 × 14C,128GB	108	3024	116,12 TFlops
				iris **TOTAL:**	**108**	**3024**	**116.12 TFlops**
gaia	2011	Bull	Intel Xeon L5640@2.26GHz	2 × 6C,48GB	72	864	7.811 TFlops
	2012	Dell	Intel Xeon E5-4640@2.4GHz	4 × 8C, 1TB	1	32	0.614 TFlops
	2012	Bull	Intel Xeon E7-4850@2GHz	16 × 10C,1TB	1	160	1.280 TFLops
	2013	Dell	Intel Xeon E5-2660@2.2GHz	2 × 8C,64GB	5	80	1.408 TFlops
	2013	Bull	Intel Xeon X5670@2.93GHz	2 × 6C,48GB	40	480	5.626 TFlops
	2013	Bull	Intel Xeon X5675@3.07GHz	2 × 6C,48GB	32	384	4.746 TFlops
	2014	Delta	Intel Xeon E7-8880@2.5 GHz	8 × 15C,1TB	1	120	2.4 TFlops
	2014	SGi	Intel Xeon E5-4650@2.4 GHz	16 × 10C,4TB	1	160	3.072 TFlops
	2015	Dell	Intel Xeon E5-2680@2.5 GHz	2 × 12C,128GB	28	672	26.88 TFlops
	2015	HP	Intel E3-1284Lv3, 1.8GHz	1 × 4C,32GB	90	360	10.368 TFlops
	2016	Dell	Intel Xeon E7-8867@2.5 GHz	4 × 16C,2TB	2	128	5.12 TFlops
				gaia **TOTAL:**	**273**	**3440**	**69.296 TFlops**
chaos	2010	HP	Intel Xeon L5640@2.26GHz	2 × 6C,24GB	32	384	3.472 TFlops
	2011	Dell	Intel Xeon L5640@2.26GHz	2 × 6C,24GB	16	192	1.736 TFlops
	2012	Dell	Intel Xeon X7560@2,26GHz	4 × 6C, 1TB	1	32	0.289 TFlops
	2012	Dell	Intel Xeon E5-2660@2.2GHz	2 × 8C,32GB	16	256	4.506 TFlops
	2012	HP	Intel Xeon E5-2660@2.2GHz	2 × 8C,32GB	16	256	4.506 TFlops
				chaos **TOTAL:**	**81**	**1120**	**14.495 TFlops**
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
				granduc/petitprince **TOTAL:**	**38**	**368**	**4.48 TFlops**

Testing cluster:

	Date	Vendor	Proc. Description		#N	#C	R_{peak}
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
				nyx/viridis **TOTAL:**	**102**	**500**	**2.381 TFlops**

UL HPC Storage capacity

4 distributed/parallel FS
2015 disks
7952.4 TB
(incl. 2116TB for Backup)

UL HPC Shared Storage Capacities

Cluster	GPFS	Lustre	Other (NFS...)	Backup	TOTAL
iris	1440	0	6	600	**2046** TB
gaia	960	480	0	1336	**2776** TB
chaos	0	0	180	180	**360** TB
g5k	0	0	32.4	0	**32.4** TB
nyx (experimental)	0	0	242	0	**242** TB
TOTAL:	**2400**	**480**	**2956.4**	**2116**	**7952.4 TB**

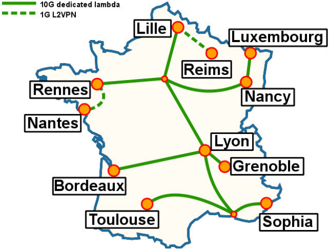
UL HPC Software Stack

- **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.

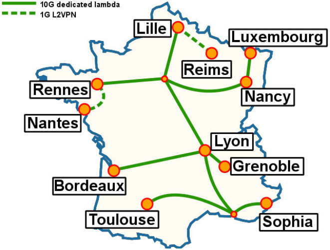


- 10 sites in France
  - ↪ **Abroad**: Luxembourg, Porto Allegre
  - ↪ Total: **7782** cores over **26** clusters
- 1-10GbE / Myrinet / Infiniband
  - ↪ **10Gb/s dedicated** between all sites
- Unique software stack
  - ↪ **kadeploy, kavlan, storage5k**

The case of Grid'5000

http://www.grid5000.fr

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

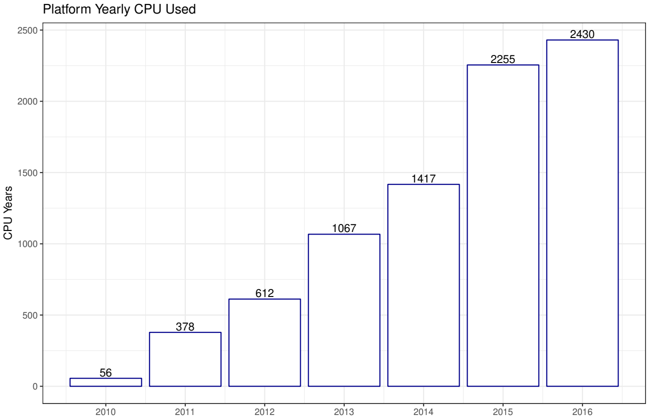


- 10 sites in France
  - ↪ **Abroad**: Luxembourg, Porto Allegre
  - ↪ Total: **7782** cores over **26** clusters
- 1-10GbE / Myrinet / Infiniband
  - ↪ **10Gb/s dedicated** between all sites
- Unique software stack
  - ↪ **kadeploy, kavlan, storage5k**

- **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

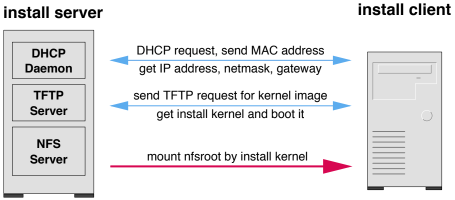
Computing nodes Management

Node deployment by FAI/Bright Manager

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

Fully Automatic Installation

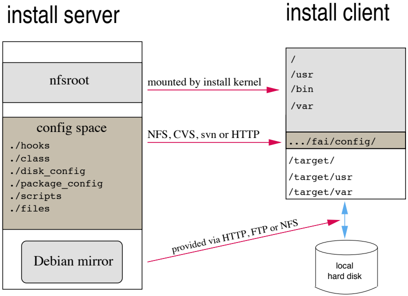
Bright Computing



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

Fully Automatic Installation
Bright Computing

- 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 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 command
  - ↪ configure OS and additional software
  - ↪ save log files to install server, then reboot new system

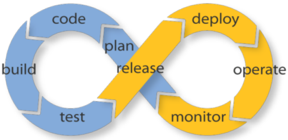
Average reinstallation time: $\simeq$ 500s

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 architecture
  - ↪ cross-platform through Puppet Resource Abstraction Layer (RAL)
  - ↪ Git-based workflow
  - ↪ PKI-based security (X.509)
- DevOps tool of choice for configuration management
  - ↪ Declarative Domain Specific Language (DSL)



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

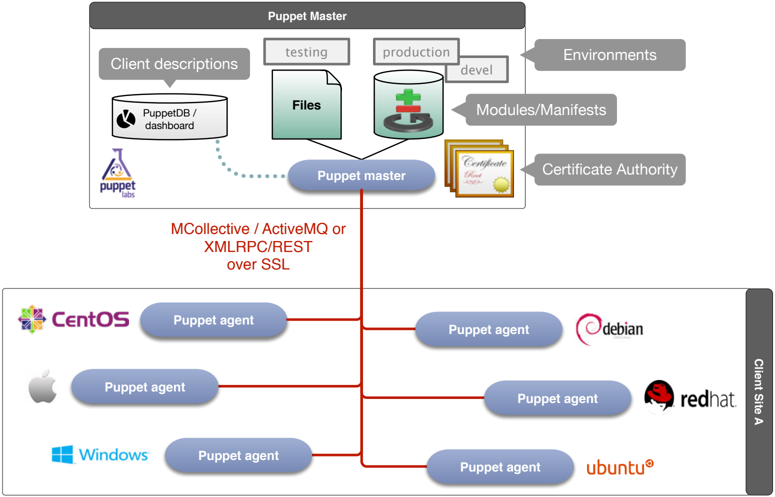
Server/Service configuration by Puppet

http://puppetlabs.com

- **IT Automation** for configuration management
  - ↪ idempotent
  - ↪ agent/master OR stand-alone architecture
  - ↪ cross-platform through Puppet Resource Abstraction Layer (RAL)
  - ↪ Git-based workflow
  - ↪ PKI-based security (X.509)
- DevOps tool of choice for configuration management
  - ↪ Declarative Domain Specific Language (DSL)

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:
  - ↪ $>$ **140 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

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

- Easybuild: open-source framework to (automatically) build scientific software
- **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

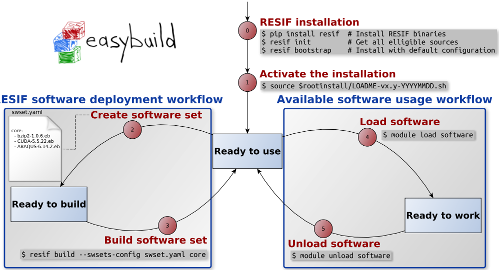
```
$> module use /path/to/easybuild
$> module load tools/EasyBuild
$> eb -S HPL    # Search for recipes for HPL software
$> eb HPL-2.2-intel-2017a.eb # Install HPL 2.2 w. Intel toolchain
```

Software/Modules Management

http://resif.readthedocs.io/en/latest/

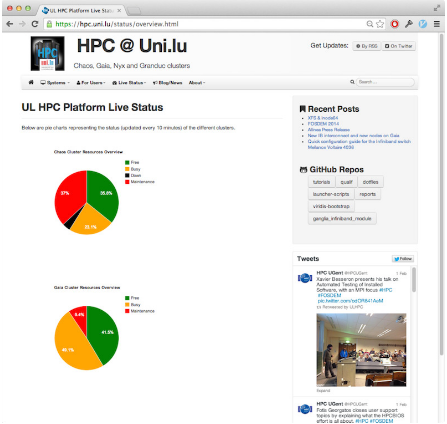
- **RESIF**: Revolutionary EasyBuild-based Software Installation Framework
  - ↪ Automatic Management of **software sets**
  - ↪ Fully automates software builds and supports all available toolchains
  - ↪ Clean (hierarchical) modules layout to facilitate its usage

RESIF: Revolutionary EasyBuild-based Software Installation Framework



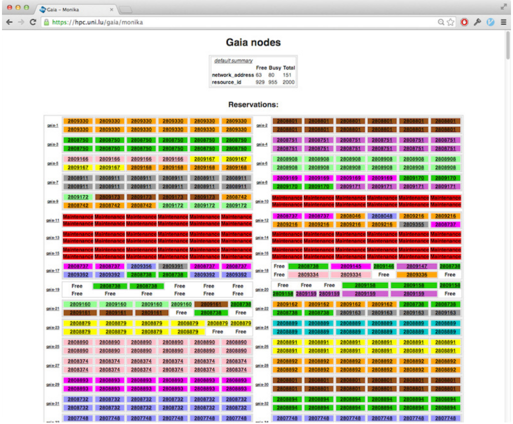
Platform Monitoring

- **General Live Status** http://hpc.uni.lu/status/overview.html/



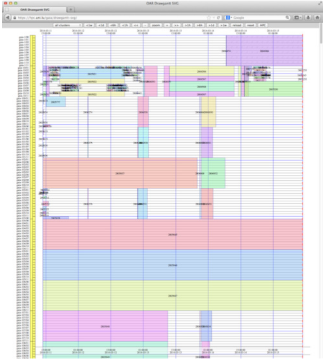
Platform Monitoring

- **Monika** http://hpc.uni.lu/{gaia,chaos,g5k}/monika



Platform Monitoring

- **Drawgantt** http://hpc.uni.lu/{gaia,chaos,g5k}/drawgantt



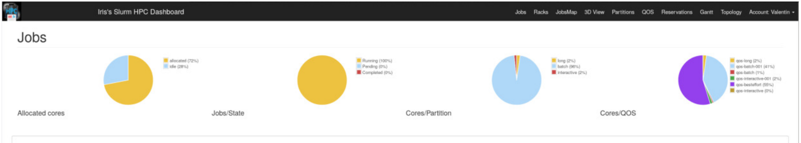
Platform Monitoring

- **Ganglia**

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

Platform Monitoring

- **SLURM-Web** http://hpc.uni.lu/iris/slurm/

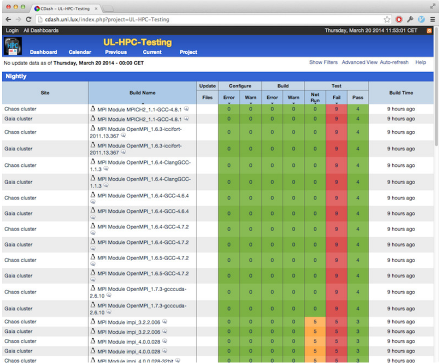


#	User	Resources	State	Start	QOS	Partition
25814	[illegible]	cpu=2,mem=8G,node=1	RUNNING	since 27d 17h 31min 14s	qos-long	long
25816	[illegible]	cpu=2,mem=8G,node=1	RUNNING	since 27d 17h 31min 14s	qos-long	long
25819	[illegible]	cpu=2,mem=8G,node=1	RUNNING	since 27d 17h 31min 14s	qos-long	long
25823	[illegible]	cpu=2,mem=8G,node=1	RUNNING	since 27d 17h 31min 14s	qos-long	long
25827	[illegible]	cpu=2,mem=8G,node=1	RUNNING	since 27d 17h 31min 14s	qos-long	long
25831	[illegible]	cpu=2,mem=8G,node=1	RUNNING	since 27d 17h 31min 14s	qos-long	long
25832	[illegible]	cpu=2,mem=8G,node=1	RUNNING	since 27d 17h 31min 14s	qos-long	long
25833	[illegible]	cpu=2,mem=8G,node=1	RUNNING	since 27d 17h 31min 14s	qos-long	long
25834	[illegible]	cpu=2,mem=8G,node=1	RUNNING	since 27d 17h 31min 14s	qos-long	long
29863	[illegible]	cpu=9,mem=36G,node=1	RUNNING	since 3d 4h 2min 17s	qos-batch-001	batch
29864	[illegible]	cpu=13,mem=52G,node=1	RUNNING	since 3d 4h 1min 37s	qos-batch-001	batch
29867	[illegible]	cpu=17,mem=68G,node=1	RUNNING	since 3d 4h 10s	qos-batch-001	batch
29868	[illegible]	cpu=25,mem=100G,node=1	RUNNING	since 3d 3h 59min 31s	qos-batch-001	batch
29869	[illegible]	cpu=28,mem=112G,node=1	RUNNING	since 3d 3h 58min 56s	qos-batch-001	batch

Platform Monitoring

- **CDash**

http://cdash.uni.lu/

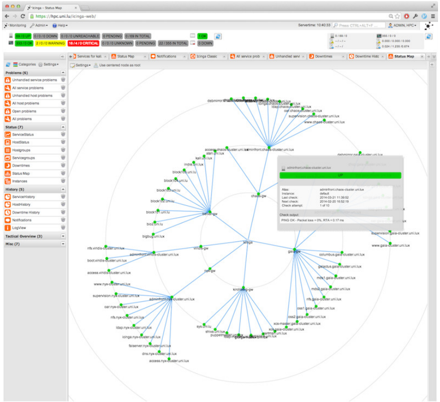


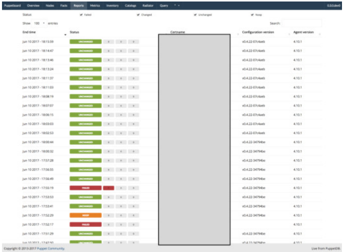
Site	Build Name	Update	Configure		Build		Test			Build Time
		Files	Error	Warn	Error	Warn	Not Run	Fail	Pass	
Chaos cluster	MPI Module MPICH2_1.1-GCC-4.8.1		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module MPICH2_1.1-GCC-4.8.1		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.3-iccifort-2011.13.367		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.3-iccifort-2011.13.367		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.4-ClangGCC-1.1.3		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.4-ClangGCC-1.1.3		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.4-GCC-4.6.4		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.4-GCC-4.6.4		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.4-GCC-4.7.2		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.4-GCC-4.7.2		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.6.5-GCC-4.7.2		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.6.5-GCC-4.7.2		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module OpenMPI_1.7.3-gcccuda-2.6.10		0	0	0	0	0	9	4	9 hours ago
Gaia cluster	MPI Module OpenMPI_1.7.3-gcccuda-2.6.10		0	0	0	0	0	9	4	9 hours ago
Chaos cluster	MPI Module impi_3.2.2.006		0	0	0	0	5	5	3	9 hours ago
Gaia cluster	MPI Module impi_3.2.2.006		0	0	0	0	5	5	3	9 hours ago
Chaos cluster	MPI Module impi_4.0.0.028		0	0	0	0	5	5	3	9 hours ago
Gaia cluster	MPI Module impi_4.0.0.028		0	0	0	0	5	5	3	9 hours ago
Chaos cluster	MPI Module impi_4.0.0.028-32bit		0	0	0	0	5	5	3	9 hours ago

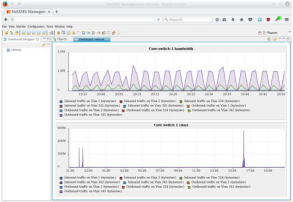
Platform Monitoring

- **Internal Monitoring**

Icinga / Puppet / NetXMS (networking)



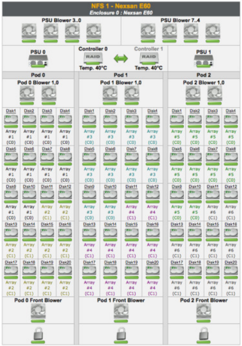


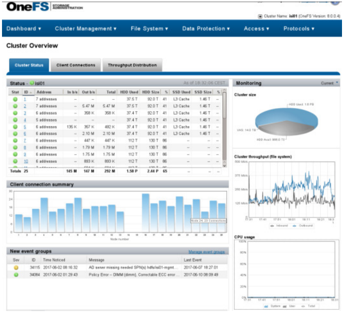


Platform Monitoring

- **Internal Monitoring**

[Disk] Enclosure status





Summary

Back to 2017 Achievements / Technical

- Installation of the new `iris` cluster
  - ↪ **108 nodes**, 3024 cores, **116.12 TFlops**
    - ✓ Dell C6320, Intel Xeon E5-2680v4@2.4 GHz [2x14c], 128 GB RAM
  - ↪ **SpectrumsScale GPFS**: **1440 TB raw**

Back to 2017 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)

Back to 2017 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)
- **Continuous OS / software modules Upgrade**
  - ↪ Migration to **Debian 8** on `gaia` and `chaos`
  - ↪ **RESIF v2**, updated software sets

Back to 2017 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)
- **Continuous OS / software modules Upgrade**
  - ↪ Migration to **Debian 8** on `gaia` and `chaos`
  - ↪ **RESIF v2**, updated software sets
- **Storage**:
  - ↪ **Spectrumscale/GPFS** Upgrades accross all clusters (to 4.2.2.X)
  - ↪ **Lustre (2.7.x)**: saturated ($>$ 95% storage capacity) thus unstable
    - ✓ update to new LTS version 2.10.X not possible without formatting

- **Drastic measures required for Lustre!!**
  - ↪ PENDING **formatting and new quota policy**

Back to 2017 Achievements

- **Feb. 2017 (HR)**: Clement Parisot joined the UL HPC Team
- **June. 2017**: UL HPC School

Back to 2017 Achievements

- **Feb. 2017 (HR)**: Clement Parisot joined the UL HPC Team
- **June. 2017**: UL HPC School
- **Mar-Sep 2017**: **UL crisis**
  - ↪ . . . yet UL HPC Budget line maintained and part of 4Y plan
  - ↪ induced many delay in the delivery of CDC S-02
  - ↪ impact on UL credibility in general

Back to 2017 Achievements

- **Feb. 2017 (HR)**: Clement Parisot joined the UL HPC Team
- **June. 2017**: UL HPC School
- **Mar-Sep 2017**: **UL crisis**
  - ↪ . . . yet UL HPC Budget line maintained and part of 4Y plan
  - ↪ induced many delay in the delivery of CDC S-02
  - ↪ impact on UL credibility in general
- **Oct. 2017**: Luxembourg 25th country to join PRACE
  - ↪ Official representatives for Luxembourg from UL
    - ✓ Delegate: Prof. Pascal Bouvry
    - ✓ Advisor: Dr. Sebastien Varrette

Back to 2017 Achievements

- **Feb. 2017 (HR)**: Clement Parisot joined the UL HPC Team
- **June. 2017**: UL HPC School
- **Mar-Sep 2017**: **UL crisis**
  - ↪ . . . yet UL HPC Budget line maintained and part of 4Y plan
  - ↪ induced many delay in the delivery of CDC S-02
  - ↪ impact on UL credibility in general
- **Oct. 2017**: Luxembourg 25th country to join PRACE
  - ↪ Official representatives for Luxembourg from UL
    - ✓ Delegate: Prof. Pascal Bouvry
    - ✓ Advisor: Dr. Sebastien Varrette

- Still **pending**:
  - ↪ official structure enabling **Research computing @ UL & abroad**
  - ↪ National commitment for having next-gen HPC in CDC S-02

Summary

Summary

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

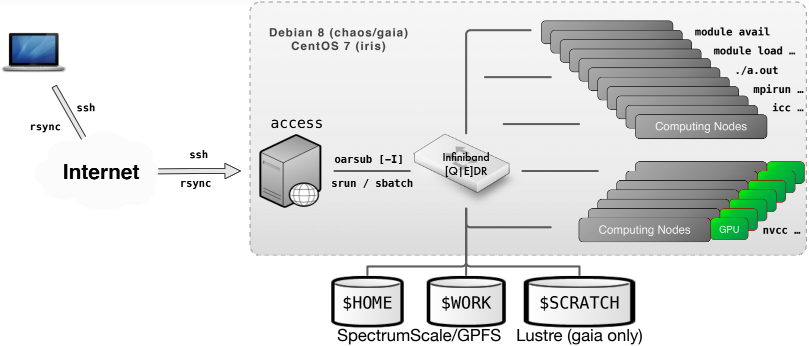
General Guidelines

- 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

- 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.

Summary

Compute Nodes Environment

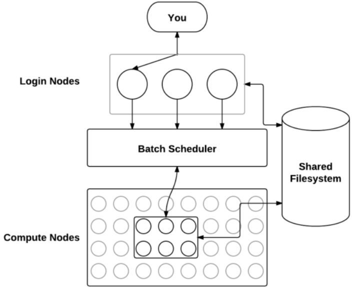


- *OS*: Debian 8 / CentOS 7
- **Storage usage**: `df-ulhpc`
- **Env. modules**: `modules`
  - ↪ **Not** available on frontends
  - ↪ ***Only*** on compute nodes

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

Resource and Job Management Systems

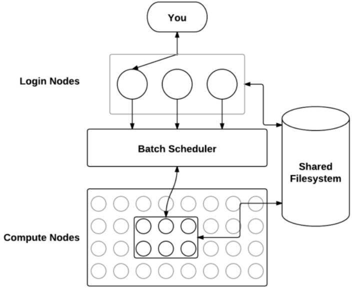
- **Resource and Job Management System (RJMS)**
  - ↪ *Glue* for a parallel computer to execute parallel jobs
  - ↪ **Goal**: satisfy users demands for computation
    - ✓ assign resources to user jobs with an efficient manner



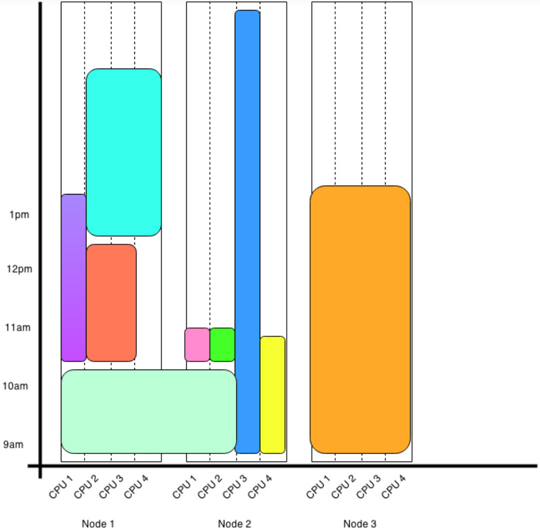
Resource and Job Management Systems

- **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

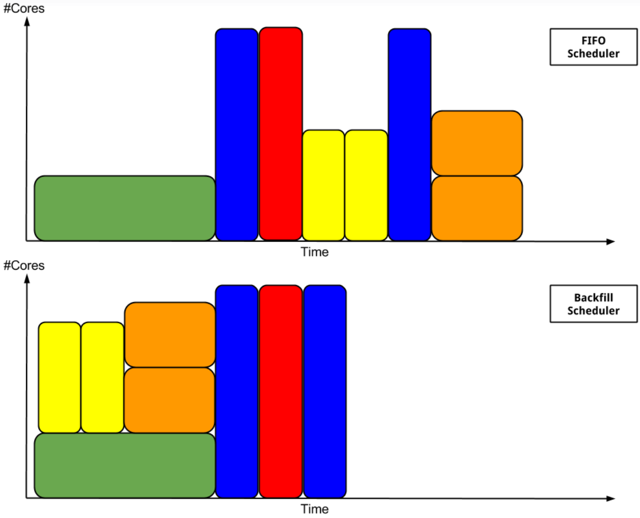
- **HPC Resources**:
  - ↪ Nodes (typically a unique IP address)
    - ✓ Sockets / Cores / Hyperthreads
    - ✓ Memory
    - ✓ Interconnect/switch resources
  - ↪ Generic resources (e.g. GPUs)
  - ↪ Licenses
- **Strategic Position**
  - ↪ Direct/constant knowledge of resources
  - ↪ Launch and otherwise manage jobs



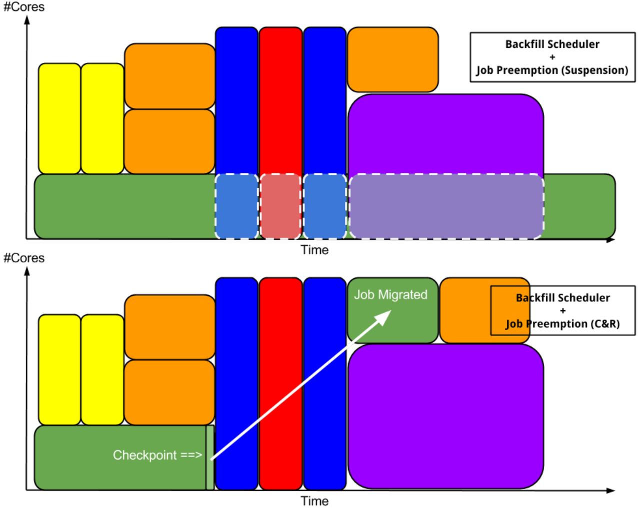
Job Scheduling



Job Scheduling (backfilling)



Job Scheduling (suspension & requeue)



List of the Main Job Schedulers

Name	Company	Version*
SLURM	SchedMD	17.02.9
LSF	IBM	10.1
OpenLava	LSF Fork	2.2
MOAB/Torque	Adaptative Computing	6.1
PBS	Altair	13.0
OAR (PBS Fork)	LIG	2.5.7
Oracle Grid Engine (formely SGE)	Oracle	

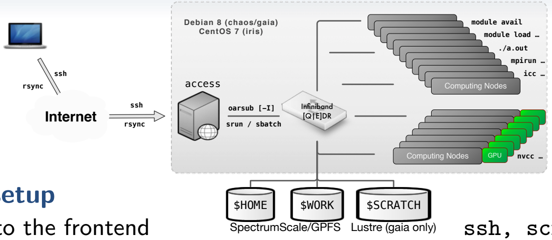
**: As of Nov. 2017*

List of the Main Job Schedulers

Name	Company	Version*
SLURM	SchedMD	17.02.9
LSF	IBM	10.1
OpenLava	LSF Fork	2.2
MOAB/Torque	Adaptative Computing	6.1
PBS	Altair	13.0
OAR (PBS Fork)	LIG	2.5.7
Oracle Grid Engine (formely SGE)	Oracle	

**: As of Nov. 2017*

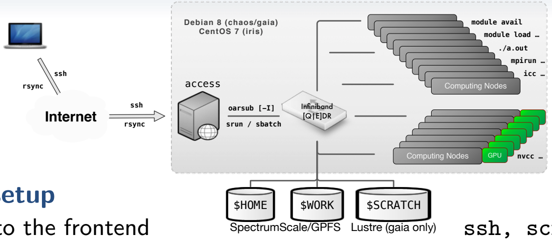
Typical Workflow on UL HPC resources



- **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



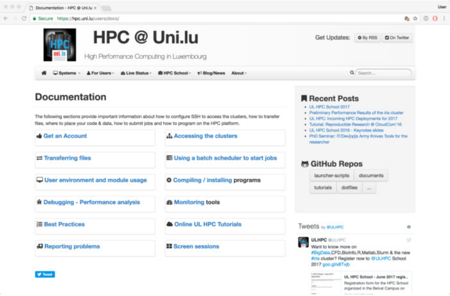
- **Preliminary setup**
  1. Connect to the frontend — `ssh, screen`
  2. Synchronize you code — `scp/rsync/svn/git`
  3. Reserve a few interactive resources — `oarsub -I [...]`
     or, on iris: `srun -p interactive [...]`
     - ✓ *(eventually)* build your program — `gcc/icc/mpicc/nvcc..`
     - ✓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

Summary

Documentation

http://hpc.uni.lu/users/getting_started.html

... aka the **rtf**$_{\textbf{ine}}$**m** paradigm



http://hpc.uni.lu

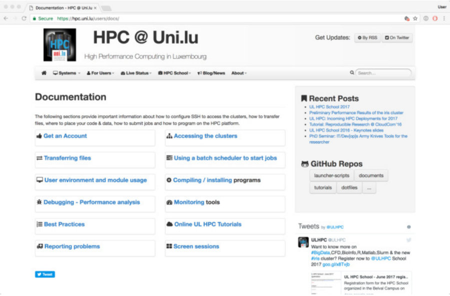
Reference Documentation

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

Documentation

http://hpc.uni.lu/users/getting_started.html

... aka the **rtf$_{\text{ine}}$m** paradigm



http://hpc.uni.lu

Reference Documentation

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

- Github Tutorials
  - ↪ http://ulhpc-tutorials.rtfd.io/
  - ↪ https://github.com/ULHPC/tutorials
- UL HPC Ticketing System
  - ↪ https://hpc-tracker.uni.lu/
- Ask other users hpc-users@uni.lu
  - ↪ ... or us hpc-sysadmins@uni.lu

Reporting Problems

https://hpc.uni.lu/users/docs/report_pbs.html

- **First checks**
  1. My issue is probably documented — see User Doc
  2. An event is on-going — cf mail from hpc-platform@uni.lu
  3. check the state of your nodes
     - ✓ `{ oarsub -C <jobid> | ssh <node>}; htop` — *on active jobs*
     - ✓ `{ oarsub -f -j <jobid> }` *post-mortem (check the events field)*
       iris: `scontrol show job <jobid>` OR `sacct --job <jobid> -l`
     - ✓ Ganglia on your node(s) — https://hpc.uni.lu/status/ganglia.html

Reporting Problems

https://hpc.uni.lu/users/docs/report_pbs.html

- **First checks**
  1. My issue is probably documented — see User Doc
  2. An event is on-going — cf mail from `hpc-platform@uni.lu`
  3. check the state of your nodes
     - ✓ `{ oarsub -C <jobid> | ssh <node>}; htop` — *on active jobs*
     - ✓ `{ oarsub -f -j <jobid> }` *post-mortem (check the events field)*
       iris: `scontrol show job <jobid>` OR `sacct --job <jobid> -l`
     - ✓ Ganglia on your node(s) — https://hpc.uni.lu/status/ganglia.html

- **ONLY NOW**, consider the following depending on the severity:
  - ↪ Open an new issue on http://hpc-tracker.uni.lu (**preferred**)
  - ↪ Mail (only now) us — `hpc-sysadmins@uni.lu`
  - ↪ **Ask the help of other users** — `hpc-users@uni.lu`

Reporting Problems

https://hpc.uni.lu/users/docs/report_pbs.html

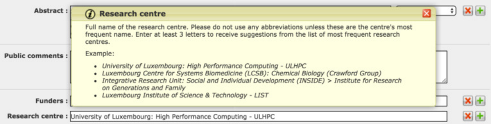
- **First checks**
  1. My issue is probably documented — see User Doc
  2. An event is on-going — cf mail from `hpc-platform@uni.lu`
  3. check the state of your nodes
     - ✓ `{ oarsub -C <jobid> | ssh <node>}; htop` — *on active jobs*
     - ✓ `{ oarsub -f -j <jobid> }` *post-mortem (check the events field)*
       iris: `scontrol show job <jobid>` OR `sacct --job <jobid> -l`
     - ✓ Ganglia on your node(s) — https://hpc.uni.lu/status/ganglia.html

- **ONLY NOW**, consider the following depending on the severity:
  - ↪ Open an new issue on `http://hpc-tracker.uni.lu` (**preferred**)
  - ↪ Mail (only now) us — `hpc-sysadmins@uni.lu`
  - ↪ **Ask the help of other users** — `hpc-users@uni.lu`

- 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^{lu} 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},
 }
```

Summary

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 purchases 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

** Note that this includes both the system and R&D*

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

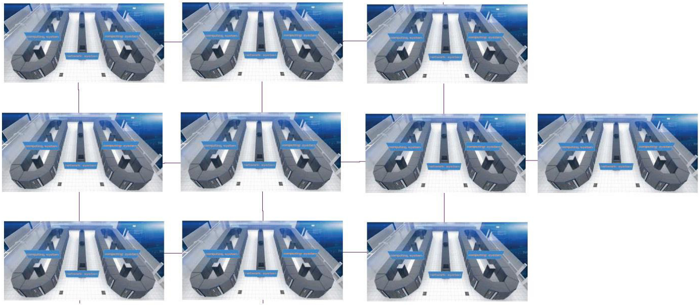
China
- Sustained ES: 2023
- Peak ES: ~~2020~~ 2019…
- Vendors: Chinese
- Processors: Chinese (plus ~~U.S.~~?)
- 13th 5-Year Plan
- Cost: $350-500M per system, plus heavy R&D

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

European HPC strategy


IMPORTANT PROJECT OF COMMON EUROPEAN INTEREST (IPCEI)

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

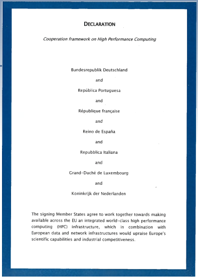
European Strategic Positioning Paper

Luxembourg, France, Italy (& Spain)
November 2015

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

- 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...

European HPC strategy


DECLARATION

Cooperation framework on High Performance Computing

Bundesrepublik Deutschland

and

República Portuguesa

and

République française

and

Reino de España

and

Repubblica Italiana

and

Grand-Duché de Luxembourg

and

Koninkrijk der Nederlanden

The signing Member States agree to work together towards making available across the EU an integrated world-class high performance computing (HPC) infrastructure, which in combination with European data and network infrastructures would upraise Europe's scientific capabilities and industrial competitiveness.

- EU HPC strategy initiated in 2012
  - ↪ implementation within H2020 program
- More recently:
  - ↪ IPCEI on HPC and Big Data (BD) Applications
    - ✓ Luxembourg (leader), France, Italy & Spain
    - ✓ Testbed around Personalized Medicine, Smart Space, Industry 4.0, Smart Manufacturing, New Materials, FinTech, Smart City. . .
- **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:
    - ✓ 2-3 **Pre-exascale** systems by 2019, **2 exascale** systems by 2021

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...

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...
- EU **COST Actions**
  - ↪ Ex: NESUS: Network for Sustainable Ultrascale Computing

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. . .
- EU **COST Actions**
  - ↪ Ex: NESUS: Network for Sustainable Ultrascale Computing
- **PRACE** - Partnership for Advanced Computing in Europe
  - ↪ Non-profit association, 25 member countries
  - ↪ Providing access to **Five EU Tier-0** compute & data resources

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...
- EU **COST Actions**
  - ↪ Ex: NESUS: Network for Sustainable Ultrascale Computing
- **PRACE** - Partnership for Advanced Computing in Europe
  - ↪ Non-profit association, 25 member countries
  - ↪ Providing access to **Five EU Tier-0** compute & data resources

- Luxembourg officially entered PRACE on **Oct. 17th, 2017**
  - ↪ Official Delegate/Advisor (P. Bouvry/S. Varrette) from UL

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

[Source : EuroLab-4-HPC]

This study was carried out for RIKEN by

IDC Analyze the Future

Special Study

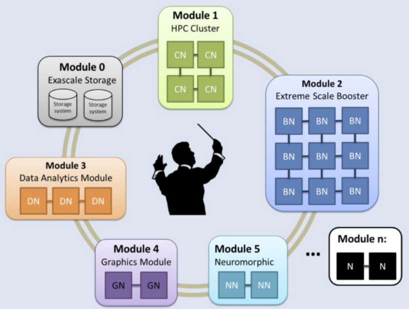
Analysis of the Characteristics and Development Trends of the Next-Generation of Supercomputers in Foreign Countries

Earl C. Joseph, Ph.D. Robert Sorensen
Steve Conway Kevin Monroe

[Source : IDC RIKEN report, 2016]

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; Data Analytics and AI



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

Summary

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)*
  - ↪ UL HPC (as of 2017): **206.772 TFlops, 7952.4TB (shared)**
  - ↪ consolidate and extend Europe efforts on HPC/Big Data

Conclusion

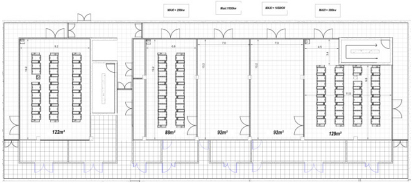
- **Luxembourg government priority on HPC**
  - ↪ sustained by University of Luxembourg HPC developments
    - ✓ started in 2007, under resp. of Prof P. Bouvry & Dr. S. Varrette
    - ✓ expert UL HPC team *(S. Varrette, V. Plugaru, S. Peter, H. Cartiaux, C. Parisot)*
  - ↪ UL HPC (as of 2017): **206.772 TFlops, 7952.4TB (shared)**
  - ↪ consolidate and extend Europe efforts on HPC/Big Data

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

Incoming Milestones

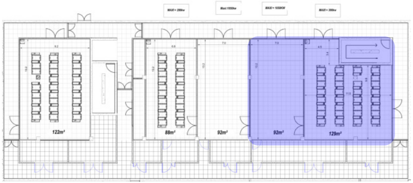
- MSA **CDC S-02** as the **new UL HPC Data Center (DC)**



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

Incoming Milestones

- MSA **CDC S-02** as the **new UL HPC Data Center (DC)**



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

- **Short term actions**
  - ↪ Official **Research computing @ UL & abroad** structure
  - ↪ `iris` cluster moving to CDC S-02-005
    - ✓ pending RFP 170035 (Lustre) + 60 nodes extension
  - ↪ **Luxembourg HPC-BD Competence Center** (exp. July 2018)
    - ✓ National commitment for having next-gen HPC in CDC S-02
  - ↪ Entering **PRACE2**

Questions?

http://hpc.uni.lu

Prof. Pascal Bouvry
Dr. Sebastien Varrette & The UL HPC Team
(V. Plugaru, S. Peter, H. Cartiaux & C. Parisot)
University of Luxembourg, Belval Campus:
Maison du Nombre, 4th floor
2, avenue de l'Université
L-4365 Esch-sur-Alzette
mail: hpc@uni.lu