Management of an Academic HPC & Research Computing Facility: The ULHPC Experience 2.0

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https://hpc.uni.lu

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High Performance Computing & Big Data Services

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Summary

1. **Overview of the Managed Facility**
   - Network Organisation
   - Tiered Shared Storage infrastructure
   - Computing Performance Evaluation and Acceptance Tests
2. **User Software Environment**
3. **User Job Management and the Slurm infrastructure**
4. **Conclusion and Perspectives**

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Network Organisation
Tiered Shared Storage infrastructure
Computing Performance Evaluation and Acceptance Tests

2 User Software Environment

3 User Job Management and the Slurm infrastructure

4 Conclusion and Perspectives

University of Luxembourg

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UNIVERSITÉ DU LUXEMBOURG

- **Created in 2003**, moved to Belval (South of the country) in 2015
- Among the top 250 universities in the Times Higher Education (THE) Rankings 2021
  - ↪ N°1 worldwide in the THE "international outlook" Rankings
  - ↪ N°20 worldwide in the THE Young University Rankings 2021.
    - ✓ N°4 (out of 64) in the THE Millennials Rankings 2021.

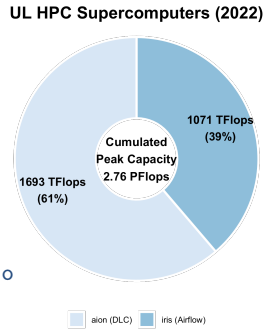
Uni.lu HPC (UL HPC) Facility

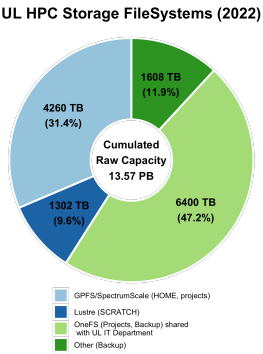
- **Managed and operated since 2007** (Dr. S. Varrette & Co.)
  ↪ 2nd Largest HPC facility in Luxembourg after EuroHPC MeluXina

`hpc.uni.lu`

Technical Docs:
`hpc-docs.uni.lu`

ULHPC Tutorials:
`ulhpc-tutorials.rtfd.io`





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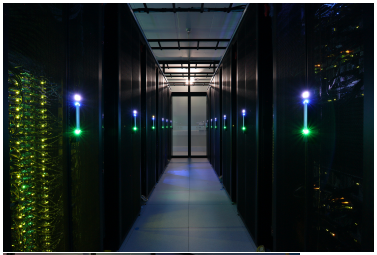
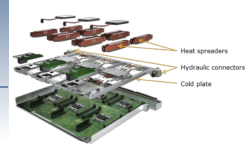
UL HPC Supercomputers: iris cluster



hpc-docs.uni.lu/systems/iris/

- **Dell/Intel** supercomputer *Air-flow cooling*
  - ↪ 196 compute nodes, **5824 cores**, 52.2 TB RAM
  - ↪ R_{peak}: **1,07 PetaFlop/s**
    - ✓ **regular** nodes (Dual CPU, 128 to 256 GB of RAM)
    - ✓ **GPU** nodes (Dual CPU, 4 NVidia accelerators, 768 GB RAM)
    - ✓ **Large-memory** nodes (Quad-CPU, 3072 GB RAM)
- Fast InfiniBand (IB) EDR network
  - ↪ **Fat-Tree** Topology blocking factor 1:1.5
- Stepwise deployment since 2017
  - ↪ two major upgrade phases (2018 and 2019)

UL HPC Supercomputers: aion cluster



`hpc-docs.uni.lu/systems/aion/`

- **Atos/AMD** supercomputer, DLC cooling
  - ↪ 4 BullSequana XH2000 adjacent racks
  - ↪ 318 **regular** nodes, **40704 cores**, 81.4 TB RAM
  - ↪ R_{peak}**: 1,693 PetaFLOP/s**
- Fast InfiniBand (IB) HDR network
  - ↪ **Fat-Tree** Topology blocking factor 1:2
- Acquisition by European Tender in 2020
  - ↪ **production release** in Oct 2021 (delayed by COVID)

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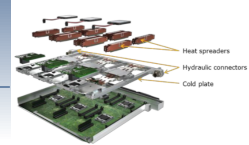

`hpc-docs.uni.lu/systems/aion/`

- **Atos/AMD** supercomputer, DLC cooling **(EOY update)**
  - ↪ 4 BullSequana XH2000 adjacent racks
  - ↪ 354 **regular** nodes, **45312 cores**, 90.6 TB RAM
  - ↪ R_{peak}: **1,885 PetaFLOP/s**
- Fast InfiniBand (IB) HDR network
  - ↪ **Fat-Tree** Topology — blocking factor 1:2
- Acquisition by European Tender in 2020
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  - ↪ **First upgrade EOY 2022** +36 **regular** nodes

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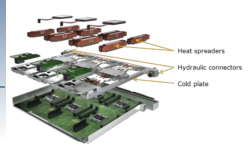

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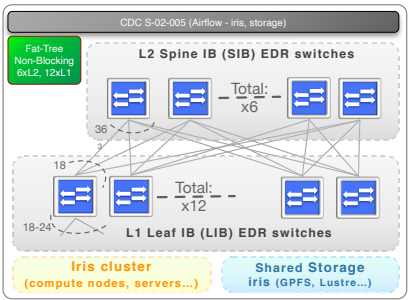
- **In this talk**:
  - ↪ design choices & config. changes when **integrating** aion, with performance evaluation

Fast Local Infiniband (IB) Interconnect Network

`hpc-docs.uni.lu/interconnect/ib/`

- **before** integration of `aion` (`iris` alone)

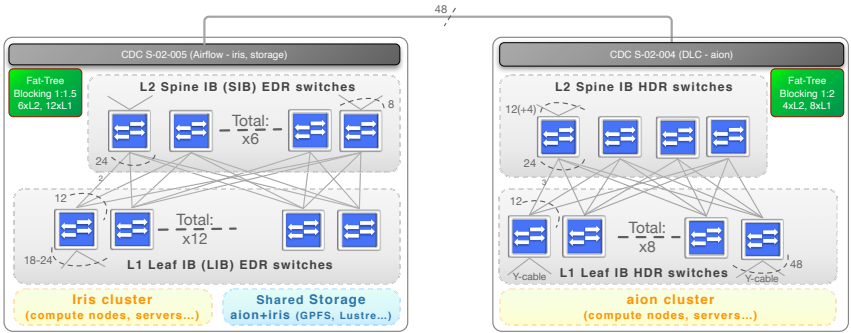


[PEARC22] S. Varrette, H. Cartiaux, T. Valette and A. Olloh, "*Aggregating and Consolidating two High Performant Network Topologies: The ULHPC Experience*" in ACM Practice and Experience in Advanced Research Computing (PEARC'22), Boston, USA, 2022.

Fast Local Infiniband (IB) Interconnect Network

- **after** merging `iris` and `aion` IB islands

`hpc-docs.uni.lu/interconnect/ib/`



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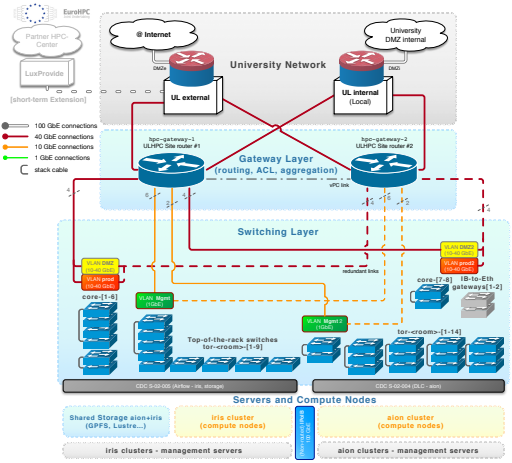
Complementary Ethernet Network

`hpc-docs.uni.lu/interconnect/ethernet/`



- Flexibility of Ethernet-based networks still required
- **2-layers** topology
  - ↪ *Upper* level: **Gateway Layer**
    - ✓ routing, switching features, network isolation and filtering (ACL) rules
    - ✓ meant to interconnect only switches.
    - ✓ allows to interface University network (LAN/WAN)
  - ↪ *bottom* level: **Switching Layer**
    - ✓ [stacked] core switches
    - ✓ TOR (Top-the-rack) switches
    - ✓ meant to interface HPC servers and compute nodes

[PEARC22] S. Varrette, H. Cartiaux, T. Valette and A. Olloh, "*Aggregating and Consolidating two High Performant Network Topologies: The ULHPC Experience*" in ACM Practice and Experience in Advanced Research Computing (PEARC'22)

UL HPC Storage Systems

- Two types of **distributed & parallel FS**
  - ↪ **IBM Spectrum Scale** (formelly GPFS)
  - ↪ **Lustre** `$SCRATCH` storage
- Complementary storage infrastructure
  - ↪ **OneFS** (Dell/EMC Isilon)
    - ✓ project data, backup & archival

`hpc-docs.uni.lu/filesystems/`

File System	Vendor	#Disks	Raw/Effective capacity
GPFS (2017-)	DDN	710 HDDs + 38 SSDs	4260 / 3408 TB
Lustre (2018-)	DDN	Object Storage Targets: 167 HDDs Meta-Data Targets: 19 SSDs	1300 / 920 TB
OneFS (2014-)	Dell/EMC	n/a (NDA)	7100 / 6400 TB

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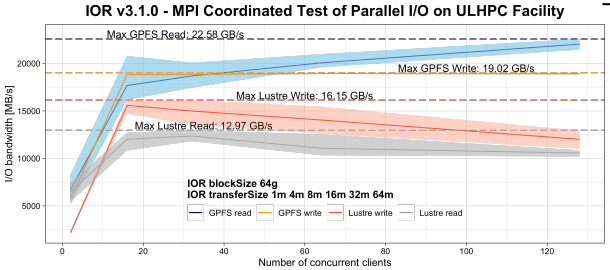

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- EU's **GDPR** *(General Data Protection Regulation)* and Open Science compliance [APF21]

[APF21] L. Paseri, S. Varrette, "*Protection of Personal Data in HPC Platform for Scientific Research Purposes*", in Proc. of the EU Annual Privacy Forum (APF) 2021, LNCS vol. 12703, pp. 123–142.

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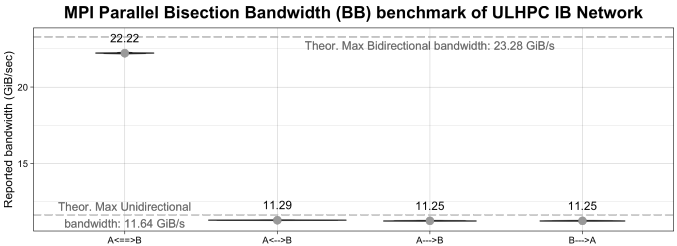
    - ✓ project data, backup & archival
- EU's **GDPR** *(General Data Protection Regulation)* and Open Science compliance [APF21]
- Specific **quota and purging policy** depending on usage pattern/sustaining FS

	Directory	File System	Backup	Default **Quota**	Default **Inode quota**	**Purging time**
`$HOME`	`/home/users/<login>`	GPFS/Spectrumscale	yes (daily)	500 GB	1 M	-
	`/work/projects/<name>`	GPFS/Spectrumscale	yes (daily)	n/a	0	-
`$SCRATCH`	`/scratch/users/<login>`	Lustre	no	10 TB	1 M	60 days
	`/mnt/isilon/projects/<name>`	OneFS	yes (snapshot, weekly)	1.14 PB globally	-	-

UL HPC Performance Evaluations *[selected benchs]*

- Bisection Bandwidth (**BB**) benchmarks: **96,99% efficiency**



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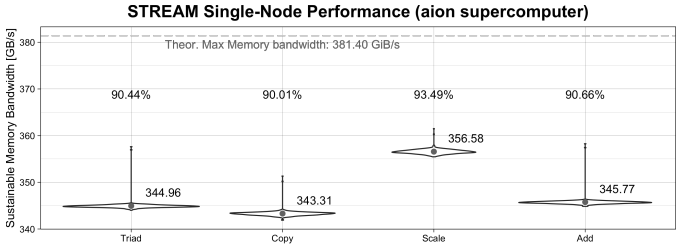
- **STREAM** sustainable **Memory Bandwidth** performance
  ↪ **above 90,01% efficiency** for 4 highly-intensive memory access pattern



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- **Single-node HPL** performance

Processor/GPU Model	#Cores	Freq.	R_{peak}	Avg. R_{max}
AMD ROME 7H12 *(epyc)*	64	2.6 GHz	2.66 TFlops	2.09 TFlops
Intel Xeon E5-2680v4 *(broadwell)*	14	2.4 GHz	0.54 TFlops	0.46 TFlops
Intel Xeon Gold 6132 *(skylake)*	14	2.3 GHz*	1.03 TFlops	0.94 TFlops
Intel Xeon Platinum 8180M *(skylake)*	28	2.3 GHz*	2.06 TFlops	1.76 TFlops
NVidia Tesla V100-SXM2	5120*+640*	1.3 GHz	7.80 TFlops	5.59 TFlops

*: AVX-512 Turbo Frequency

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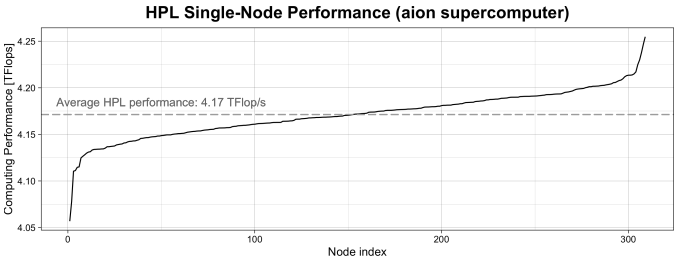
- Bisection Bandwidth (**BB**) benchmarks: **96,99% efficiency**
- **STREAM** sustainable **Memory Bandwidth** performance
  ↪ **above 90,01% efficiency** for 4 highly-intensive memory access pattern
- **Single-node HPL** performance (sorted distribution within `aion` nodes)



UL HPC Performance Evaluations *[selected benchs]*

	Benchmark	#N	*(Main parameters)*	Best Performance	Efficiency	Improvement*	Equivalent Worldwide Rank
	HPL (Top500)	**318**	*(NB=192,P×Q=48×53)*	$R_{\max}$ = **1255.36 TFlops**	**74.10%**	+1.9%	>500 (Nov 2021) **#490** (Jun 2020)
Aion	Green500	318		5.19 GFlops/W		+12.83%	**#71** (Jun 2022) **#56** (Jun 2021)
Aion	**HPCG**	318		16.842 TFlops		+15.35%	**#144** (Nov 2021) **#135** (Jun 2021)
Aion	**Graph500** BFS	2^8=256	*(Scale: 36,Edge:16)*	975 GTEPS		+64%	**#31** (Jun 2022) **#23** (Jun 2021)
Aion	GreenGraph500	2^8=256		6.14 MTEPS/W		+180%	**#43** (Jun 2022) **#36** (Jun 2021)
				: performance improvement with the minimal acceptance threshold set in the Aion *tender document*			
	IO500 (`isc21` release)	128		**11.345219**			**#42** (Nov 2020 - latest release)
Iris	HPL *(CPU/broadwell)*	108		84.75 TFlops	72.98%		
Iris	HPL *(GPU/V100 16G)*	72	*(NB=320,P×Q=12×6)*	283.6 TFlops	52.87%		
Iris	HPCG *(GPU/V100 16G)*	72		8.74 TFlops			
Iris	HPL *(GPU/V100 32G)*	24	*(NB=288,P×Q=6×4)*	135.2 TFlops	75.61%		
Iris	HPCG *(GPU/V100 32G)*	24		2.90 TFlops			

- Reference benchmarks: HPL, HPCG, Graph500, Green500, GreenGraph500
  - ↪ I/O specific: IO500, IOR
- *(not presented)* Unified European Application Benchmark Suite (UEABS)

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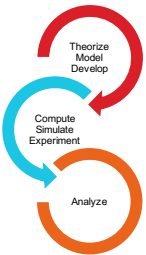
Accelerating Research - User Software Sets

- **Over 280 software packages** available for researchers
  - ↪ software environment generated using **RESIF 3.0 framework** [PEARC21] over Easybuild
    - ✓ **optimized builds** organized by architecture, exposed through Environment Modules/Lmod
    - ✓ Categorized Naming Scheme <category>/<name>/<version>-<toolchain><versionsuffix>



	Software set release <version>		
Component	**2019b** legacy	**2020b** prod	**2021b** devel
binutils	2.32	2.35	2.37
GCCCore	8.3.0	10.2.0	11.2.0
foss	2019b	2020b	2021b
- OpenMPI	3.1.4	4.0.5	4.1.2
intel	2019b	2020b	2021a
- Compilers/MKL	2019.5.281	2020.1.217	2021.4.0
- Intel MPI	2018.5.288	2019.7.217	2021.4.0
Python	3.7.4	3.8.6	3.9.6
RESIF version	3.0	3.0	3.1
#Software Modules	<arch>: 269 gpu: 135	<arch>: 274 gpu: 151	<arch>: 282 gpu: 157

[PEARC21] S. Varrette, E. Kieffer, F. Pinel, E. Krishnasamy, S. Peter, H. Cartiaux, and X. Besseron. "*RESIF 3.0: Toward a Flexible & Automated Management of User Software Environment on HPC facility*". In ACM Practice & Experience in Advanced Research Computing (PEARC'21) pdf – code

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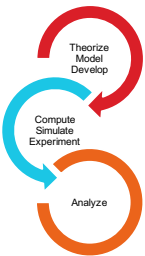

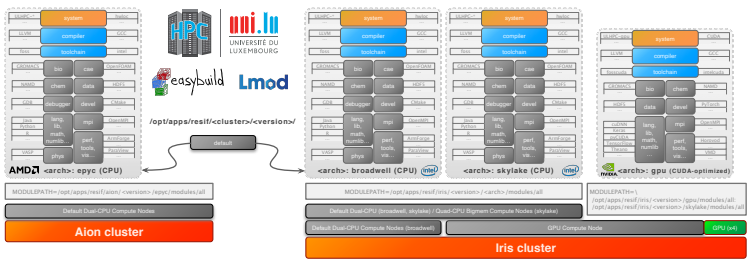

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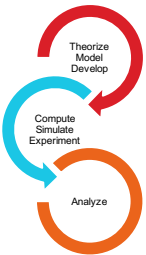

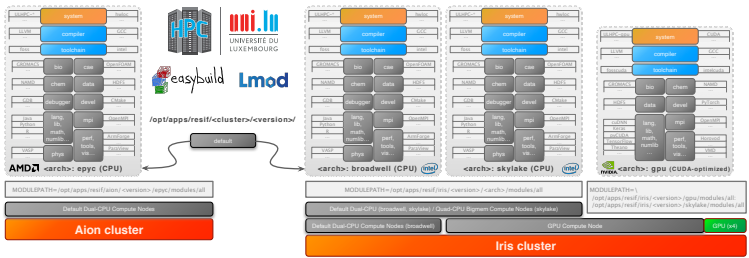

  - ↪ containerized applications delivered with Singularity system
  - ↪ user web/application portal (ouside regular SSH access): Open OnDemand

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ULHPC Slurm Partitions and QOS 2.0

AION Partition	**Type**	**#Node**	**PriorityTier**	**DefaultTime**	**MaxTime**	**MaxNodes**
interactive	floating	318	100	30min	2h	2
batch		318	1	2h	48h	64
IRIS Partition	**Type**	**#Node**	**PriorityTier**	**DefaultTime**	**MaxTime**	**MaxNodes**
interactive	floating	196	100	30min	2h	2
batch		168	1	2h	48h	64
gpu		24	1	2h	48h	4
bigmem		4	1	2h	48h	1

[ISPDC22] S. Varrette, E. Kieffer and F. Pinel, "*Optimizing the Resource and Job Management System of an Academic HPC and Research Computing Facility*" in 21st IEEE Intl. Symp. on Parallel and Distributed Computing (ISPDC'22)

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QOS	**Partition**	**Allowed [L1] Account**	**Prio**	**GrpTRES**	**MaxTresPJ**	**MaxJobPU**	**Flags**
besteffort	*	**ALL**	1			100	NoReserve
low	*	**ALL** (default for CRP/externals)	10			2	DenyOnLimit
normal	*	**Default** (UL,Projects,...)	100			50	DenyOnLimit
long	*	UL,Projects,etc.	100	node=12	node=2	4	DenyOnLimit,PartitionTimeLimit
debug	interactive	**ALL**	150	node=8		2	DenyOnLimit
high	*	(**restricted**) UL,Projects,Industry	200			10	DenyOnLimit
urgent	*	(**restricted**) UL,Projects,Industry	1000			100	DenyOnLimit

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Fairsharing and Accounting 2.0

- **New configuration with Multifactor Priority Plugin and Fair tree algorithm**
  - ↪ migration from Depth-Oblivious Fair-share (*initial* setup)
  - ↪ new jobs are immediately assigned a priority fairshare levels

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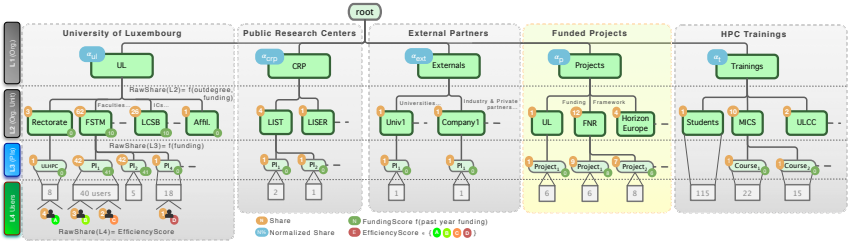
  - ↪ new jobs are immediately assigned a priority fairshare levels
- **Accounting records re-organized as a hierarchical tree** (3 layers $L_{1,2,3}$ + leafs)
  - ↪ raw share attribution based on **funding score** and **job efficiency**



[ISPDC22] S. Varrette, E. Kieffer and F. Pinel, "*Optimizing the Resource and Job Management System of an Academic HPC and Research Computing Facility*" in 21st IEEE Intl. Symp. on Parallel and Distributed Computing (ISPDC'22)

Fairsharing and Accounting 2.0

- **New configuration with Multifactor Priority Plugin and Fair tree algorithm**
  - ↪ migration from Depth-Oblivious Fair-share (*initial* setup)
  - ↪ new jobs are immediately assigned a priority fairshare levels
- **Accounting records re-organized as a hierarchical tree** (3 layers $L_{1,2,3}$ + leafs)
  - ↪ raw share attribution based on **funding score** and **job efficiency**

Impact of the new Slurm configuration

- **Daily utilization increased by 12.64%** to reach 81.56% of available resources
  - ↪ measures from workload traces over several months of **uninterrupted** HPC services
- **Wall-time Request Accuracy (WRA)** of processed jobs **increased by 110,81%**
  - ↪ evaluation covering 1 year period **before** and **after** configuration change
- UL HPC **budget incomes increased in 2021 by 10%**

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Summary

1 Overview of the Managed Facility
Network Organisation
Tiered Shared Storage infrastructure
Computing Performance Evaluation and Acceptance Tests

2 User Software Environment

3 User Job Management and the Slurm infrastructure

4 Conclusion and Perspectives

Conclusion

- **In this talk**:
  - ↪ **Design choices** when **acquiring** & **integrating** a new supercomputer `aion`
    - ✓ smooth integration within the existing HPC ecosystem
  - ↪ **Overview of the managed HPC facility**
    - ✓ supercomputer architectures, network organization, tiered shared storage infrastructure
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- **Perspectives and Future directions**
  - ↪ **smooth integration with Euro-HPC infrastructures**
    - ✓ *transparently* outsource Research Computing/data analytic workflows to Tier-0 systems
  - ↪ **automatically offload of less-demanding jobs** onto **virtual cloud resources**

Thank you for your attention...

Questions?

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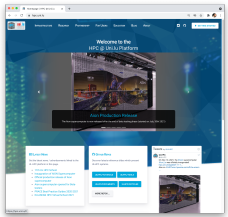

ULHPC Technical Docs

`hpc-docs.uni.lu`