

High Performance Computing & Big Data Services

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ULHPC Annual Report 2020

University of Luxembourg
High Performance Computing



University of Luxembourg High Performance Computing (ULHPC) Annual Report 2020

Dr. S. Varrette

2020 was a challenging year for everyone that will stay in our memory. The pandemic disrupted our economies, societies, and all our best laid-out plans. However, COVID-19 also taught us several lessons for the future, in particular the (real) necessity to adapt, to be nimble and to expect the unexpected while supporting cutting-edge excellence in science with the best performing and most flexible tools to unleash research potential.

One thing is certain - the strategic developments for accelerated digitalisation and the role that HPC will play to ensure a smarter and more connected University will be in focus in 2021 and the years to come. 2020 was thus a very fruitful and productive year for the ULHPC team which has seen unprecedented changes and challenges.

The following pages provide a recap of the 2020 highlights for the University's HPC facility.

HPC: A Key Strategic Asset

HPC is crucial in academic environments to achieve high-quality results in all application areas. All world-class universities require this type of facility to accelerate their research and ensure cutting-edge results in time to face the global competition.

Since 2007, the University of Luxembourg (UL) has invested tens of millions of euros into its own HPC facilities to respond to the growing needs for increased computing and storage. ULHPC (sometimes referred to as Uni.lu HPC) is the entity providing High Performance Computing and Big Data Storage services and support for UL researchers and external partners.

Led by Dr. Varrette, the HPC facility is a strategic asset of the university and an important factor for the scientific and economic competitiveness of the Grand Duchy of Luxembourg. It is one element of the extensive digital research infrastructure and expertise developed by the University over the last years.



High Performance
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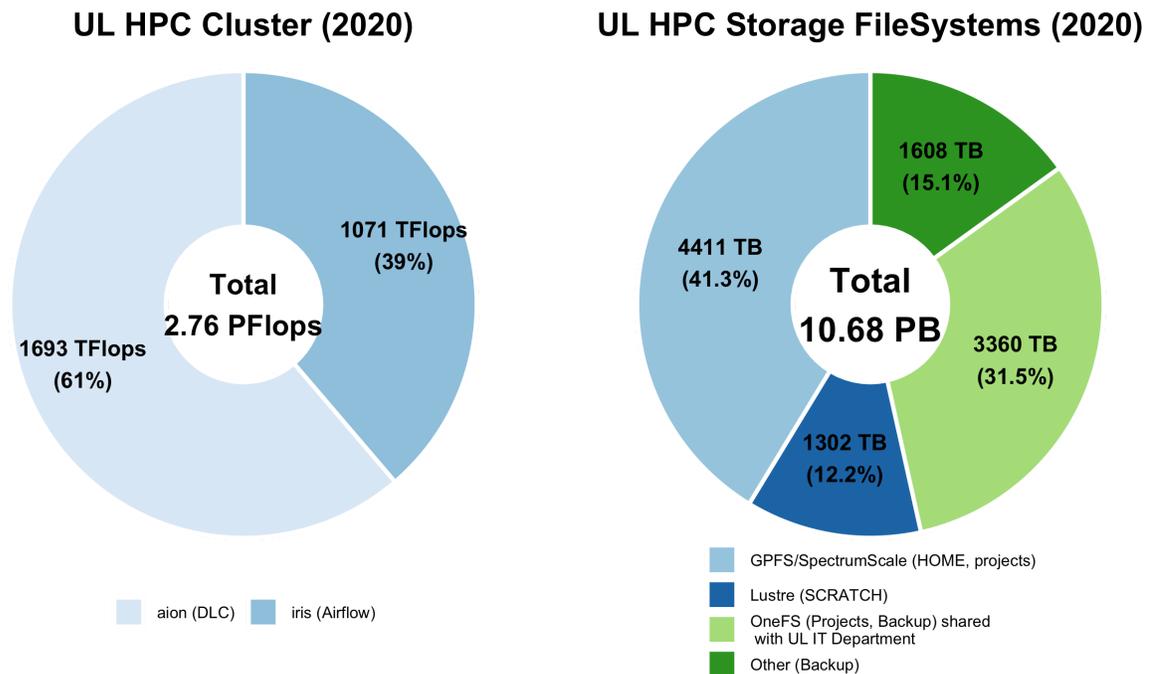


Figure 1: Overview of UL HPC computing and storage capacities.

Production Machines

- [Iris](#): Dell/Intel supercomputer, 196 compute nodes, 5824 cores, 96 GPU accelerators, 1,07 PetaFLOP/s.
- [Aion](#)¹: Atos/AMD supercomputer, 318 compute nodes, 40704 cores, 1,693 PFlops

User Community

- 2020: 630 active users (1518 registered)
- 2019: 415 active users (1230 registered)

Granted resources

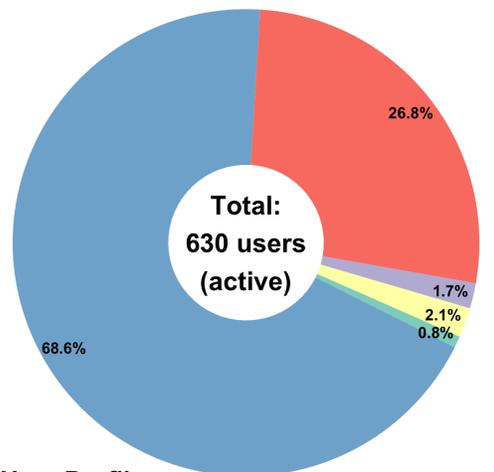
- 2020: 667 520 jobs scheduled, totalling **4319 CPU Years** (37 835 309 CPU hours)
- 2019: 1 031 739 jobs scheduled, totalling 3699 CPU Years (32 411 373 CPU hours)

User repartition and their corresponding usage of the ULHPC facility in 2020 are depicted in the below figures.

¹ Release for general availability initially planned for 2020, postponed to 2021 due to the pandemic.

By User Profile

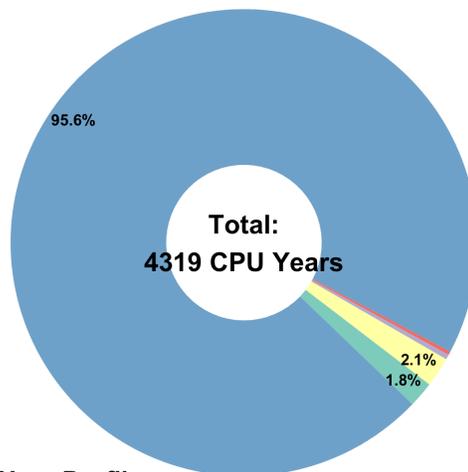
Repartition of Uni.lu HPC users (2020)



User Profile



Uni.lu HPC Facility Usage (2020)

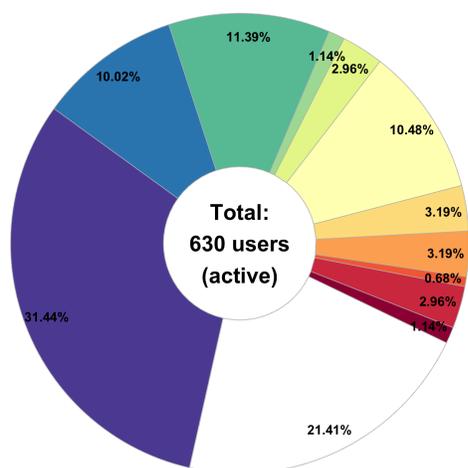


User Profile

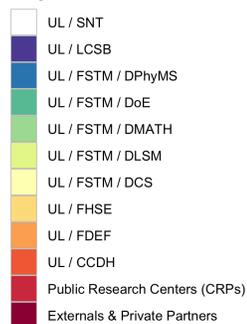


By Faculty, ICs and Departements of FSTM²

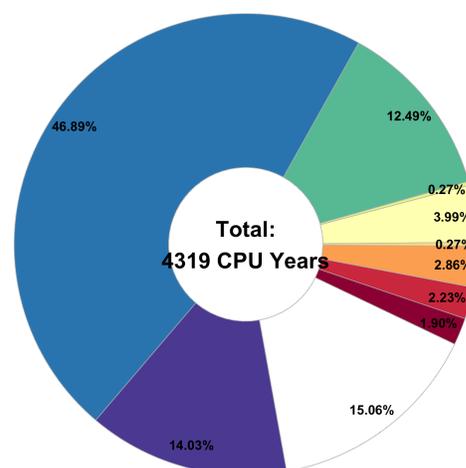
Repartition of Uni.lu HPC users (2020)



Departement / Center



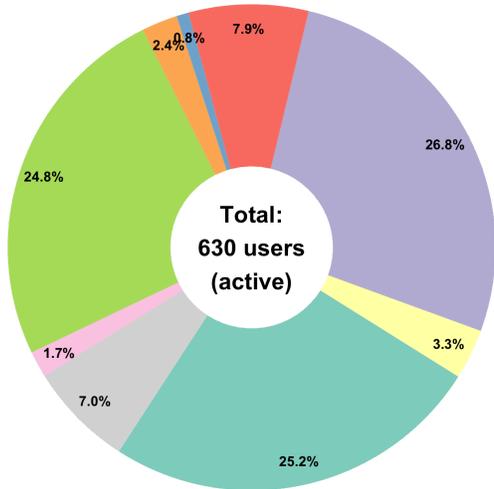
Uni.lu HPC Facility Usage (2020)



² FSTM: Faculty of Science, Technology and Medicine

By Research Domains

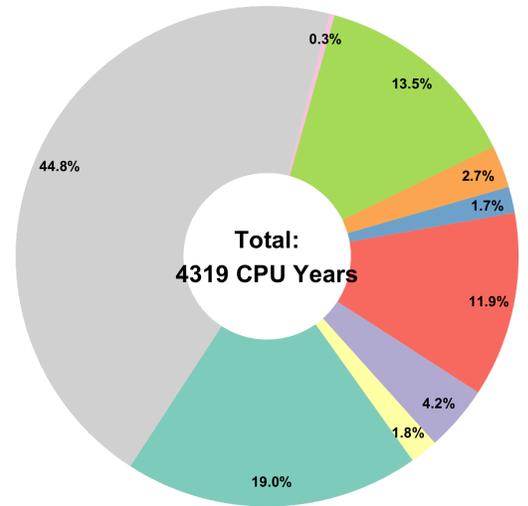
Repartition of Uni.lu HPC users (2020)



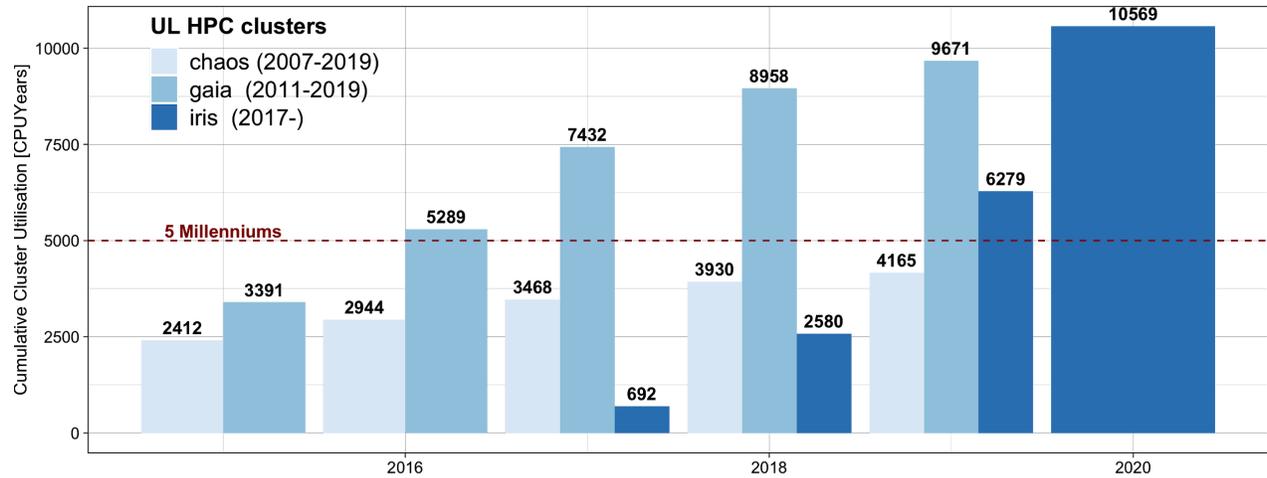
Research Domains

- Physics and Materials Science
- Misc. (projects)
- Life Sciences
- Law, Economics and Finance
- Industry and External Partners
- Engineering
- Education and Trainings
- Digital History, Social Sciences
- Computer Sciences

Uni.lu HPC Facility Usage (2020)



UL HPC Facility Usage (in CPU Years)



HPC Highlights in 2020

- **National HPC developments:** In order to boost Europe's supercomputing infrastructure, the European Commission has set up a call for hosting Peta-scale supercomputers in 2019. The Luxembourg proposal, **Meluxina**, elaborated by a consortium led by the Ministry of Economy and including LuxConnect, ULHPC, LIST, Jülich Supercomputing Centre (JSC) and Partec, was selected with 7 others (5 peta-scale, 2 pre-exascale).
Consisting of an 18 Petaflops supercomputer provided by Atos, Meluxina will be implemented by LuxProvide SA under the governance of the Ministry of Economy and the Ministry of State.
 - Meluxina will serve for 35% of its computing power for EuroHPC calls and for the 65 remaining percent for commercial access, with a specific focus on R&D projects in particular for SMEs and start-ups.
 - In addition to his professor duties at the university, Pascal Bouvry started acting as co-CEO of Luxprovide with Roger Lampach, while Valentin Plugaru took the CTO position.
 - Meluxina's launch is due for the Spring of 2021.
- In parallel, the University reinforces its internal HPC facility.
 - To replace the decommissioned systems Chaos and Gaia, the acquisition of a new supercomputer **Aion** was prepared during Summer 2019 with the [RFP 190027](#). With a target budget of 3,5M€, the tender (released in Sept 2019) was attributed to Atos in December 2019.
 - Initially planned April 2020, the **delivery and installation of the new Aion supercomputer was largely impacted by the COVID pandemic** and started only in Dec 2020, with a release for general availability expected for Q2 2021.
- 2020 has seen several updates in the UL HPC **access & usage policies**:
 - Updated [Acceptable Use Policy \(AUP\) 2.0](#)
 - New [HPC Cost Model](#) for FNR/H2020-funded projects & Externals partners, approved by rectorate in July 2020
 - Updated [model](#) for Fairshare, Account Hierarchy and Scheduler Limits
- **Newcomers and new strategic partnerships**
 - Following the departure of C. Parisot and V. Plugaru, the ULHPC team was reinforced with the arrival of T. Valette and A. Ollloh, who joined as Infrastructure & HPC Engineers.
 - Continued **strategic partnership**
 - [PRACE](#) - Partnership for Advanced Computing in Europe

- [ETP4HPC](#) - European Technology Platform (ETP) for HPC
 - **New strategic partnerships** were established within EU HPC projects:
 - NVidia AI Technology Center ([NVAITC](#)), coordinated by Dr. F. Pinel
 - H2020 [PRACE-6IP](#), where Dr. E. Krishnasamy joined as PostDoc
 - EuroHPC Competence Center [EuroCC and CASTIEL](#) projects, where A. Moinier-Vandeventer joined as Project Manager and Dr. L. Koutsantonis as postdoc
 - *Note:* As part of the **University Digital Strategy**, three newcomers will come and reinforce the HPC team in 2021 to provide support Levels 3 and 4:
 - Dr Marcu Ovidiu, Dr Joshgun Sirajzaden and Dr Tiago Carnerio will join as postdocs
- Continued **HPC Trainings and Education**
 - [ULHPC School](#), initiated and coordinated by Dr. S. Varrette
 - 9th ULHPC School 2019 (June 20-21, 2019) in Belval: 102 participants
 - 2 keynotes, 18 practical sessions, 10 lecturers
 - 10th ULHPC School 2020 (Dec 20-21, 2020), 153 online participants
 - 2 keynotes, 11 practical sessions, 11 lecturers
 - MICS Parallel & Grid Computing lecture (Dr. S. Varrette, Dr. F. Pinel)
 - PRACE Summer of HPC, coordinated by Dr. E. Krishnasamy
 - New NVIDIA Deep Learning Institute (DLI) Ambassador: Dr. F Pinel
 - Preparation of EuroHPC Master Program (Prof. P. Bouvry, Dr. F. Pinel, Dr. E. Kieffer)
- Communication and Technical Support:
 - Migration of the HPC HelpDesk support tracker to [Uni.lu Service NOW](#)
 - New UL HPC [Technical Documentation](#) online

Detailed Chronology 2020

January-February 2020

- To replace the [decommissioned](#) systems Chaos and Gaia, the acquisition of a **new supercomputer Aion** was prepared through the [RFP 190027](#). With a target budget of 3,5M€, the tender was attributed to Atos in December 2019.
- The Kickoff meeting with Atos team took place in January 2020
 - [Atos Press release](#): “Atos empowers researchers at the University of Luxembourg with its BullSequana XH2000 supercomputer”
 - Note: Initially planned for April 2020, the delivery and installation of the new Aion supercomputer was largely impacted by the COVID pandemic and started only in Dec 2020, with a release for general availability expected for Q2 2021.
- Updated [Acceptable Use Policy \(AUP\) 2.0](#)
- New [HPC Cost Model](#) for [FNR] Funded projects & External partners
 - Approved by Rectorate on July 7, 2020
 - For more details: see [ULHPC Usage Charging Policy](#)



March-June 2020

- Changes in ULHPC/PCOG Team
 - V. Plugaru left to join LuxProvide as CTO (Mar 2020)
 - Prof. P. Bouvry started a mandate as co-CEO of LuxProvide with Roger Lampach (June 2020). During this mandate:
 - Dr. S. Varrette leads the HPC and research computing operations team
 - Dr. F. Pinel co-leads the HPC Research and Training within the PCOG team



- **COVID-19 pandemic and global lockdown**
 - The ULHPC facility has significantly contributed to the fight against the COVID-19 pandemic since mid-March 2020 by offering dedicated access for seven projects within its computational resources.
 - [University's supercomputer supports fight against COVID-19](#)

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University's supercomputer supports fight against COVID-19

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Published on Friday, 26 June 2020

The University's High-Performance Computing (HPC) facility has significantly contributed to the fight against the COVID-19 pandemic since mid-March 2020.

The "supercomputer" and its team, led by Prof. Patrick Bouvry and Dr. Sébastien Varrette, has supported University researchers and external partners in more than seven projects with its computational resources.

HPC delivers high performance in order to solve large problems faster. Tasks which would typically require several weeks to be completed on a general desktop computer may only require a couple of hours, days or weeks over an HPC system. And for research conducted to fight the COVID-19 pandemic, accelerating time-to-solutions is a critical criterion to effectively fight the spread of the coronavirus on surfaces.

The University's supercomputer's and computing power and storage capacities were used for analyzing and simulating COVID-19 responses in the areas of infectious & bio-science, civil and natural sciences, engineering, mathematics, ecology, health, digital transformation, artificial intelligence, business ecosystem modeling and simulation techniques to inform economic policy-makers in Luxembourg and abroad, while allowing for computing future projections of the viability of the coronavirus on surfaces.

The University's HPC services support four University-led projects funded by the FNR COVID-19 fund. These include: Call on projects from the Research Luxembourg COVID-19 fund. Four use case collaboration between the University Luxembourg Centre for Systems Biomedicine, TU

The HPC facility is one element of the extensive digital research infrastructure and expertise developed by the University over the last years. It also supports the University's wireless digital strategy and in particular the creation of a faculty for Data and HPC Sciences. This faculty aims to provide world-class research digital infrastructure and services by leveraging the combination of collaborative research models (Public-Research and Learning), the Centre of Computational and Data Science, including High-Performance Computing, Data Analytics, Big Data Applications, Artificial Intelligence and Machine Learning.

More than 1000 jobs were scheduled on the dedicated reservations set by the HPC team from the longer job running for 28 days. An overview of the associated load usage in the most critical period of the pandemic is depicted in Figure 8. The University's HPC resources allowed to provide resources and guidance to current and future COVID-19 research projects.

Resources utilization for the COVID-19 reservation

Figure 8: Overview of the computational resources used by the COVID-19 projects from middle of March to end of April.

The high utilization rate of the resources during the critical period shows the strong involvement and collaboration of all University partners to fight the pandemic. Below is a list of the most COVID-19 related projects which relied on the University's HPC computing resources.

Combined in Silico Molecular Docking And in Vitro Experimental Assessment Of Drug Receptor-Modulators For COVID-19 Treatment

- Support for Uni.lu LCSB research in the COVID-19 Lung CT Lesion Segmentation Challenge (ranked 5th)

Congratulations

MICCAI COVID-19 Lung CT Lesion Segmentation Challenge

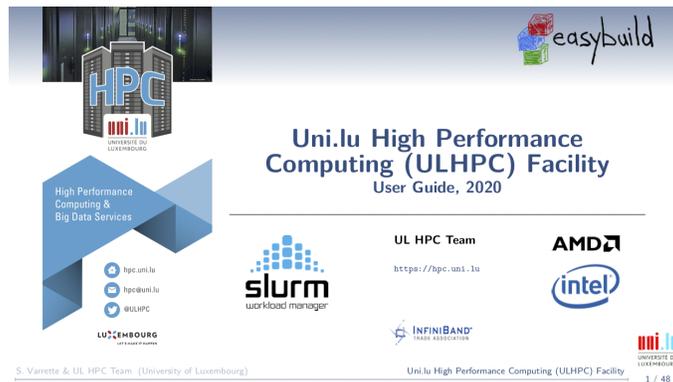


Out of over 1000 teams from all over the world, a team of LCSB researchers (Jan SÖLTER, Daniele PROVERBIO, Mehri BANIASADI, Matias Nicolas BOSSA, Beatriz GARCÍA SANTA CRUZ, Andreas HUSCH) [won the 5th place in the challenge](#). *Congratulations!*

- Reworked model for HPC User Software management
 - New model more robust, architecture optimised, and allows for 91% reduction of custom configurations in place

June-September 2020

- Reworked configuration for the Slurm Job Scheduler
 - Global accounting and billing implementing the new HPC Cost Model and allowing for the new cluster integration
 - Updated model for Fairshare, Account Hierarchy and Limits for Iris/Aion for an improved efficiency
 - Updated [ULHPC User guide](#) summarizing these changes

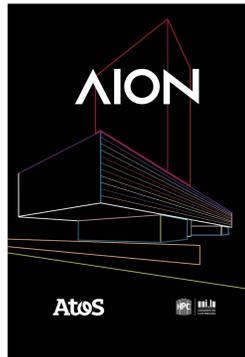


- HPC Helpdesk support tracker [migrated to Uni.lu Service NOW](#)

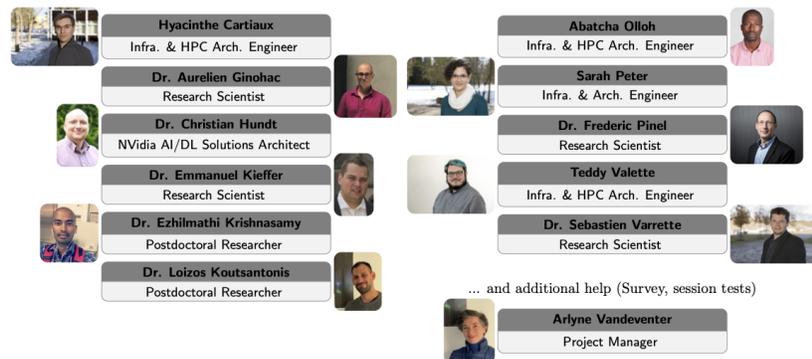
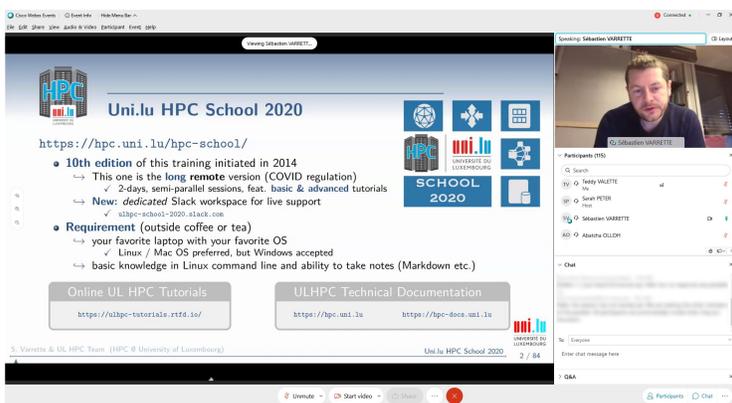
September-December 2020

- Changes in ULHPC/PCOG Team:
 - T. Valette and A. Olloh joined the HPC Team as Infrastructure & HPC Engineers (Sept 2020)
 - A. Moinier-Vandeventer (Project Manager), Dr. L. Koutsantonis (PostDoc) joined the PCOG team as part of the EuroCC project (Oct 2020)

- Main delivery of Aion equipment (Nov-Dec, 2020),
 - installation in progress in early 2021



- New version of the ULHPC reference websites
 - New UL HPC [Technical Documentation](#) online
- ULHPC School 2020 (Dec 20-21, 2020)
 - 10th edition, 2 keynotes, 11 practical sessions, 11 lecturers
 - 153 registered participants, fully online event



... and additional help (Survey, session tests)

Meet the ULHPC Team (2020)

		Prof. Stephane Pallage Rector		
Uni.lu HPC Team		Prof. Pascal Bouvry Head PCOG Research Group* <small>* half-time mandate: co-CEO LuxProvide</small>		
		Dr. Sebastien Varrette Research Scientist, Deputy Head, Uni.lu HPC		
Research Computing & HPC Operations <small>* Acting Head during mandate: Dr. S. Varrette</small>		HPC Research & Trainings <small>* Acting Deputy Head during mandate: Dr. F. Pinel</small>		Strategic Developments Partnership
Hyacinthe Cartiaux Infrastructure and HPC Architecture Engineer		Dr. Frederic Pinel Research Scientist, Coordinator NVidia Joint AI Lab		Administration & Information Arlyne Vandeventer Project Manager EuroHPC Comp. Center (EuroCC)
				
Abatcha Olloh Infrastructure and HPC Architecture Engineer		Dr. Emmanuel Kieffer Research Scientist		
				
Teddy Valette Infrastructure and HPC Architecture Engineer		Dr. Ezhilmathi Krishnasamy Postdoctoral Researcher, Coordinator H2020 PRACE-6IP		
				
Sarah Peter Infrastructure & Architecture Engineer LCSB BioCore sysadmins manager		Dr. Loizos Koutsantonis Postdoctoral Researcher, EuroCC		
		N/A Postdoctoral Researcher, EuroCC		



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