



HPC & Big Data Analytics in Luxembourg

Application to Efficient Parallel Coupling of CFD-DEM simulations

High Performance
Computing &
Big Data Services



Dr. X. Besson and Dr. S. Varrette

University of Luxembourg (UL), Luxembourg

6th Annual MVAICH User Group (MUG) Meeting

Aug. 8th, 2018, Columbus, Ohio, US



MVAICH





Summary

- 1 Introduction**
 - Preamble Game
 - Research Excellence in Luxembourg
- 2 High Performance Computing (HPC) @ UL
- 3 Current and Future Developments
- 4 Example of Technical Scientific Achievement

Where is Wally?

Hint: in Luxembourg



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University of Luxembourg

<http://www.uni.lu>



An international university serving its country

- **Created in 2003**, moved to Belval (South of the country) in 2015
- **Ranked 12** among the **Young Universities**
 - ↪ cf. 2018 Times Higher Education (THE) Ranking
 - ↪ ranked 179 in the Worldwide University rankings





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High Performance Computing @ UL

• Started in 2007

- ↳ under resp. of Prof P. Bouvy & Dr. S. Varrette
- ↳ expert UL HPC team
 - ✓ S. Varrette, V. Plugaru, S. Peter, H. Cartiaux, C. Parisot... and multiple domain experts per RU
- ↳ **8,173,747€** cumulative HW investment , *excl. server rooms*
 - ✓ Largest HPC facility in Luxembourg w. GoodYear



<https://hpc.uni.lu>

High Performance Computing & Big Data Services



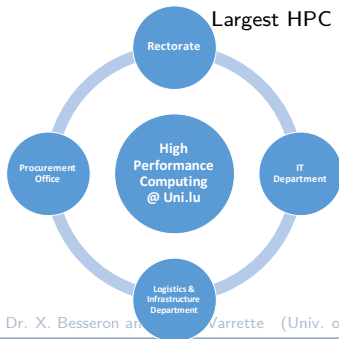


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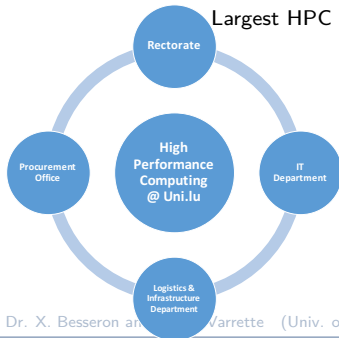


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HPC/Computing Capacity

422.872 TFlops
(incl. 76.22 GPU TFlops)

HTC/Storage Capacity

9852.4 TB storage



High Performance
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UL HPC Computing capacity



5 clusters / 2 sites



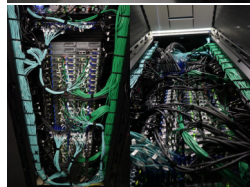
422.872 TFlops

(incl. 76.22 GPU TFlops)

662 nodes

10132 CPU cores

(+ 120704 GPU cores)



- IB interconnect
- Fat tree topo. in general

UL HPC Storage capacity



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

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

UL HPC Beneficiaries

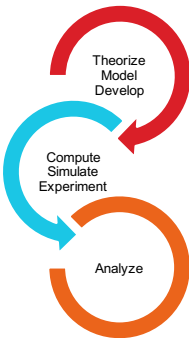
23 computational domains accelerated on UL HPC

- 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**
 - ✓ **Q4 2018**: 18*4 V100 (part of RFP 180027): **> 365 GPU Tflops**
 - ↪ **BigData analytics & data driven science**: large memory systems
 - ✓ Large SMP systems with 1, 2, 3 & 4 TB RAM
 - ↪ **Scale-out workloads**: 90 HP Moonshot servers + 96 viridis ARM-based systems

Accelerating UL Research



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



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

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



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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...



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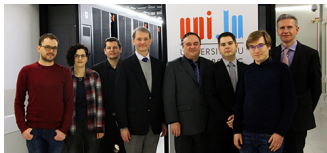
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- **PRACE** - Partnership for Advanced Computing in Europe

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



EU HPC Strategy Implementation

• European High-Performance Computing Joint Undertaking

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

- ✓ administrative management from Luxembourg

↪ Public and private members

- ✓ EC, 14 MS, representatives from supercomputing/BD stakeholders
- ✓ Governing Board (public members)
- ✓ Industrial & Scientific Advisory Board (private members)

↪ EU Objective with EuroHPC:

- ✓ 2-3 **Pre-exascale** systems (2020), **2 exascale** systems (2022)
- ✓ Pending decision on hosting countries



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EuroHPC Budget: 2×486 M€

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- **European Processor Initiative (EPI)**

- ↪ Initial plan vs current plan. . .

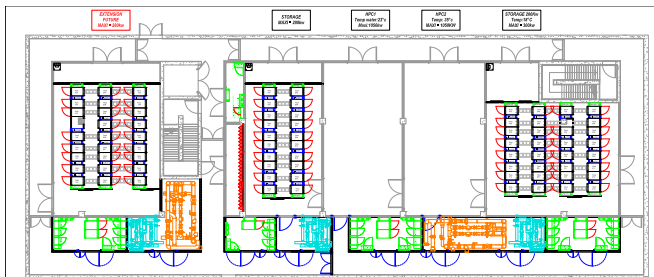
- ↪ **120 M€** via Framework Partnership Agreement (FPA)

Uni.lu CDC (Centre de Calcul)

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

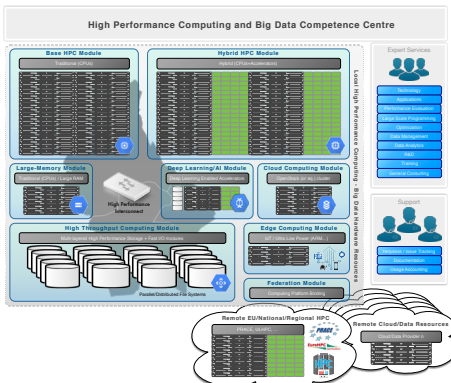
↪ 2x500 m² deployed since 2015, one floor for HPC developments

Location	Cooling	Usage	Max Capacity [kW]
CDC S-02-001	Airflow	<i>Future extension</i>	280 kW (120 m ²)
CDC S-02-002	Airflow	Storage / Traditional HPC /Cloud/FPGA	280 kW (88 m ²)
CDC S-02-003	DLC	High Density/Energy efficient HPC	1050 kW (90 m²)
CDC S-02-004	DLC	High Density/Energy efficient HPC	1050 kW (92 m²)
CDC S-02-005	Airflow	Storage / Traditional HPC (iris cluster)	300 kW (128 m ²)



National HPC-BD Competence Center

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



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

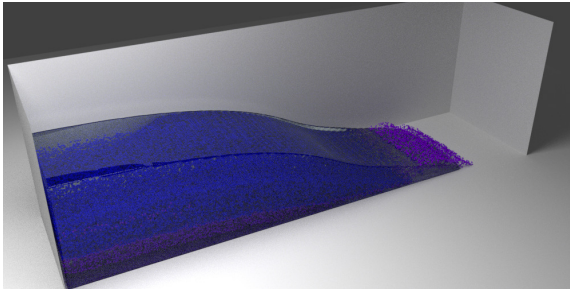


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Parallel Coupling CFD-DEM simulations

- Now time to dive into a more technical achievement
 - ↳ involving Uni.lu HPC platform
- Illustration of developments performed within LuxDEM team
 - ↳ **Efficient Parallel Coupling of CFD-DEM simulations**
 - ↳ Presented by **Dr. Xavier Besson**



Questions?

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Dr. Xavier Besson

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