High Performance Computing & Big Data Services

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LUXEMBOURG
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HPC & BD Services @ Uni.lu

Building up High Performance Computing & Big Data Competence Center to support national priorities

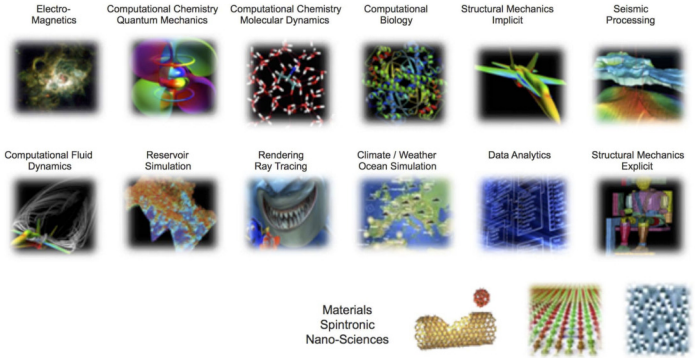
Dr. Sébastien Varrette

International Supercomputing Conference (ISC'18)
2nd Workshop on HPC Collaboration Between Europe and Latin America

Thursday, June 28th, 2018

UNIVERSITÉ DU LUXEMBOURG

Why HPC & BD ?



- **HPC**: **H**igh **P**erformance **C**omputing
- **BD**: **B**ig **D**ata
- Essential tool for **Science**, **Society and Industry**

- All scientific disciplines are becoming **computational** today
  - modern scientific discovery requires very high computing power and handles huge volumes of data
  - cf. J. Rifkin report: "3rd Industrial Revolution Strategy for the Grand Duchy of Luxembourg"

- **Industry and SMEs** are increasingly relying on the power of supercomputers...
  - ... to invent innovative solutions while reducing cost and decreasing time to market

- HPC is part of a **global race** (recognized as a strategic priority) - EU is taking up the challenge
  - Ambitious plans from many countries (USA, China, Japan, **Brazil & South america**, India...) around HPC

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

To out-compete you must out-compute

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

Science & Technology Facilities Council

Prof Tony Hey CBE FREng, STFC Chief Data Scientist & Joint Chair, UK E-infrastructure Leadership Council

Excellent research requires excellent research infrastructure

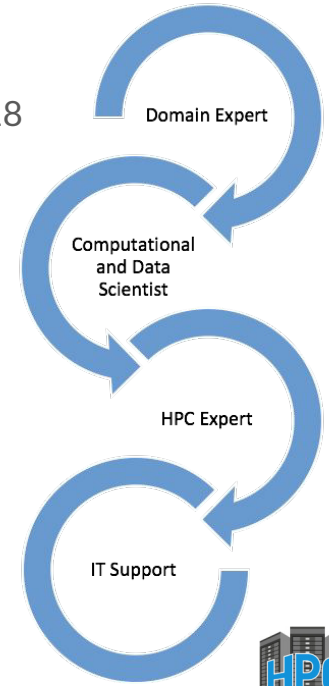
European HPC strategy and its implementation

- EU HPC strategy initiated in 2012
  - implementation within H2020 program
- Latest advances:
  - **IPCEI on HPC and Big Data (BD) Applications** (IPCEI-HPC-BDA) (Nov. 2015)
    - Luxembourg (leader), France, Italy & Spain
    - Testbed around Personalized Medicine, Smart Space, Industry 4.0 and Smart Manufacturing, New Advanced Materials, FinTech, Smart City...

  - **PRACE** (Partnership for Advanced Computing in Europe) transitioning to PRACE2.
    - Luxembourg: 25th country to join in Oct. 17th, 2017
      - Official Delegate/Advisor (P. Bouvry/S. Varrette) from Uni.lu
  - EU Member States sign the **EuroHPC initiative** and prepare its implementation (Mar. 2017)
    - A common effort to create and grow the European supercomputing ecosystem
    - Federation of national and regional HPC centers (see also PRACE/PRACE2)
      - Funding next-generation Peta-scale / Pre-exascale / Exascale systems
    - EuroHPC Joint Undertaking (JU) effective starting Jan. 2019

University of Luxembourg as a Jewel

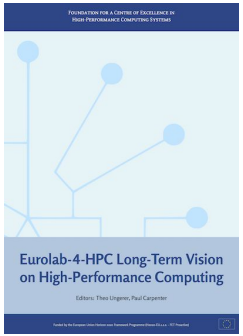
- **Created in 2003**, moved to Belval in 2015
  - An international university serving its country
- **Ranked 12** among the young universities for the Times Higher Education Ranking in 2018
- *With regards to HPC*, University of Luxembourg offers:
  - **People**
    - Domain experts
    - Computational and data scientists
    - Specialists in parallel algorithmics
  - **Services**
    - HPC clusters and management team
    - IT team (IT department)
    - Infrastructure team (IT department) in collaboration with Fonds Belval
  - **Infrastructure**
    - Data center and a set high-end clusters
  - **Education & Training**



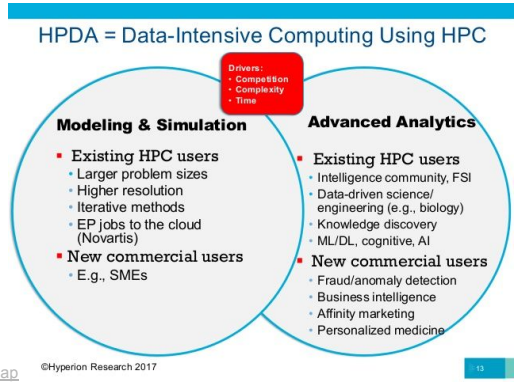
New Trends in HPC

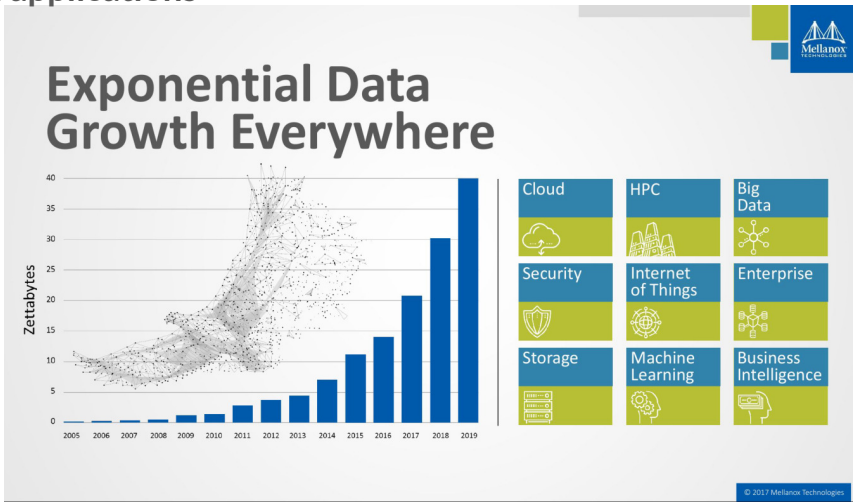
Source : IDC report: RIKEN (2016)

- **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: EU Eurolab-4-HPC Long-Term roadmap (to 2030) for High Performance Computing (2017)

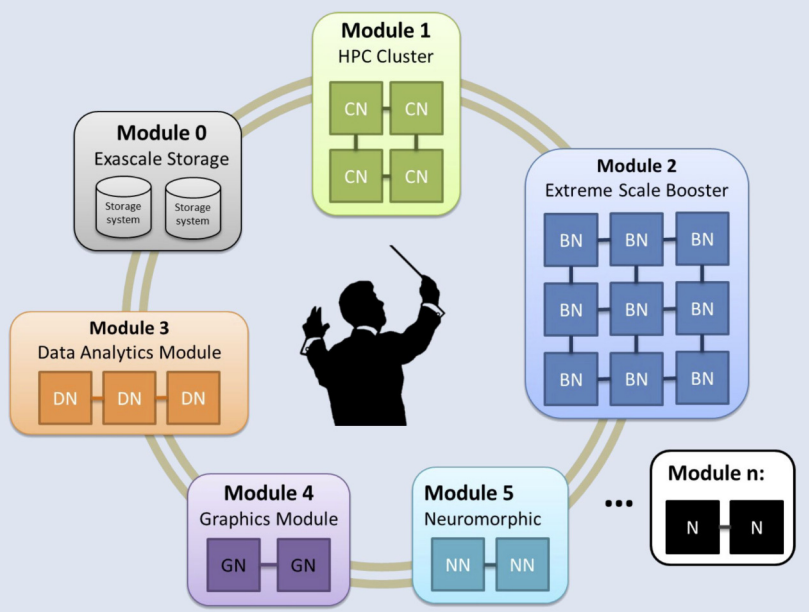




Source : 2017 Mellanox Corporate Deck

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
- 88%* of stakeholders will have multiple architectures
- Creates new adopters, targets also SME market



Source: "Towards Modular Supercomputing: The DEEP and DEEP-ER take on Heterogeneous Cluster Architectures", Norbert Eicker, SC'16 (Nov. 2016)

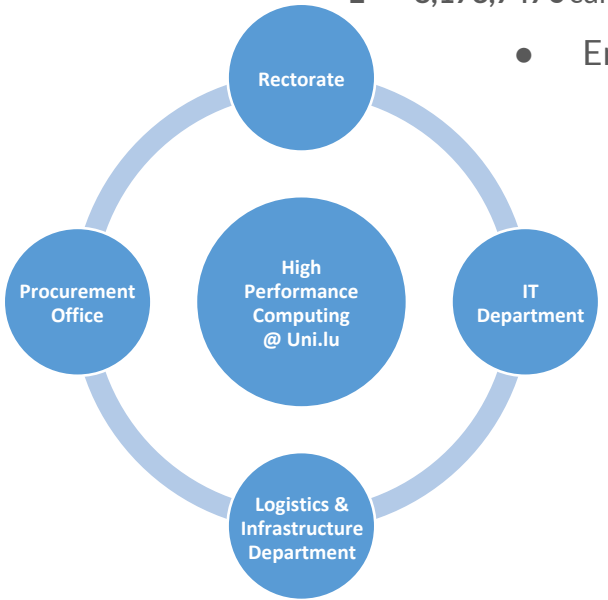
Next-generation HPC-BD platforms expected to increase modularity … and thus flexibility

* Source: Addison Snell, Intersect 360

hpc.uni.lu

HPC Facility @ Uni.lu

- **Started in 2007**, under responsibility of Prof. P. Bouvry & Dr. S. Varrette
  - expert UL HPC team
    - S. Varrette, V. Plugaru, S. Peter, H. Cartiaux, C. Parisot, among others
    - **8,173,747€** cumulative investment hardware (excl. Server rooms)
- Enables & accelerates scientific discovery & innovation
  - Largest HPC facility in Luxembourg w. GoodYear



HPC/Computing Capacity

423 TFlops → 1035,8 TFlops by eoy

HTC/Storage Capacity

9,8 PB shared

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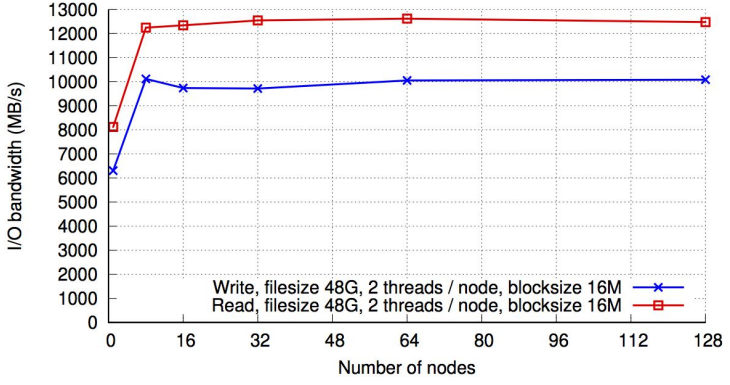
HPC Facility @ Uni.lu / Computing

- 5 clusters, 2 sites
- **Total computing capacity: 423 TFlops**
  - 10,130 CPU cores + 120,704 GPU cores
  - Planned extension to **1035,8 TFlops** by Q4 2018 (RFP 180027)
  - Fast interconnect based on Infiniband
    - … typically over a non-blocking Fat-tree network topology

HPC Facility @ Uni.lu / Storage

Total shared storage capacity: 9.8 PB

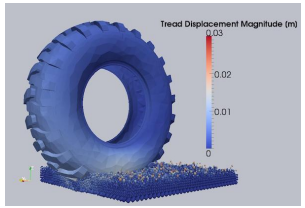
- 3.24 PB on GPFS/SpectrumScale
- 1.94 PB on Lustre
- 4.67 PB on other FS (OneFS…)
  - incl. backups



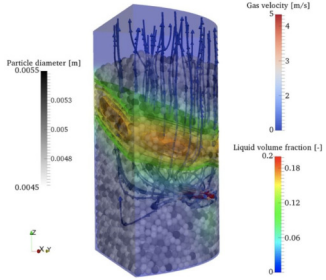
Lustre IOR performance on the iris cluster, 2018

Case Study 1: Material Science & Engineering

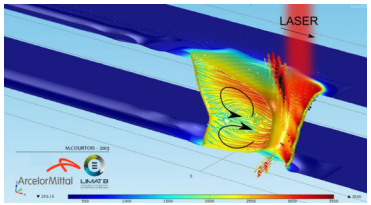
- **Companies & Research centers in Luxembourg**
  - GoodYear, IEE, Delphi, ArcelorMittal, ProNewTech, Prosciens, CrmClouder.com, UL, LIST...
- **Application domains**
  - Physics and Chemistry (materials design, new insights), Finite Element Analysis (FEA), Computational Fluid Dynamics (CFD), Optimization, Visualisation...
- **Computing infrastructure answering these needs**
  - Traditional (CPU only) or Hybrid (CPU + Accelerators)



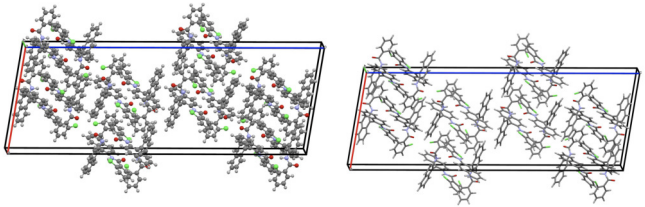
Snow-tyre interaction, LuxDem (UL)



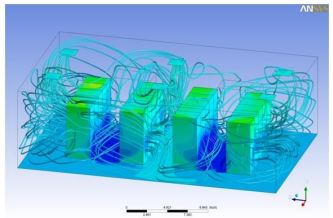
Hydrodynamic study within counter-current packed bed reactor, LuxDem (UL)



Calculated molten pool shape, temperatures and fluid streamlines, ArcelorMittal



Molecular crystal structure prediction with FHI-aims, PMSRU (UL)

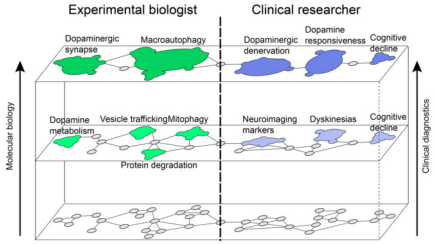


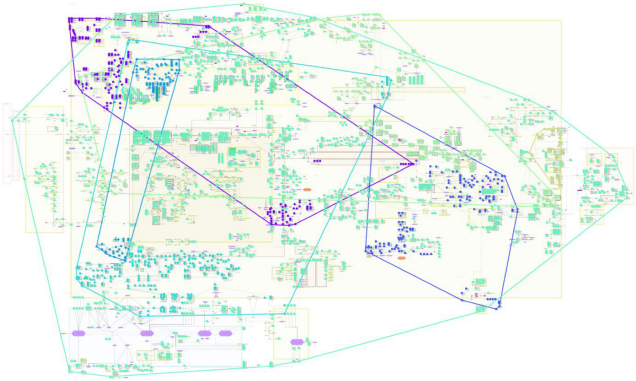
CFD Analysis of Data Center Cooling

Case Study 2: Biomedical Industry

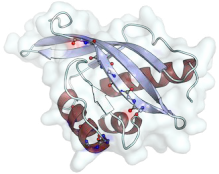
Source: Illumina

- **Companies & Research centers in Luxembourg**
  - ITTM, IBBL, UL, LIH...
- **Potential to attract external companies**
  - Edico Genome (US), Fabric Genomics (US), Swarm64 (DE)...
- **Application domains**
  - System Bio-medicine, BD Analytics, Pharmacology, Personalised Medicine
- **Computing infrastructure answering these needs**
  - Traditional (CPU only), HTC, Hybrid (CPU + Accelerators)
  - [High Performance] Data Storage

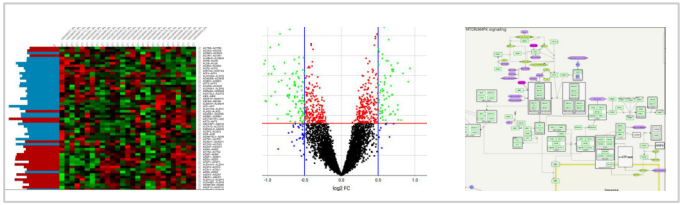




Visualization of biological knowledge: Bi-level optimization/ Parkinson disease map. CSC/LCSB (UL)



Inverse Protein Folding
CSC/LCSB (UL)

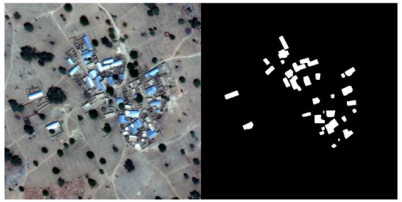


Source: LCSB (UL)

Case Study 3: Deep Learning - Cognitive Computing

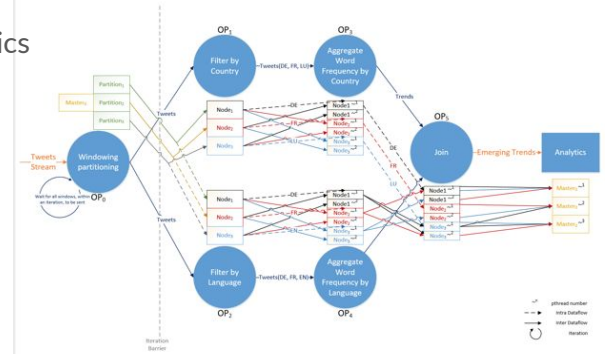
- **Companies & Research centers in Luxembourg**
  - Churchill Frank, SES, Aiva Technologies, IEE, UL...
- **Potential to attract external companies**
  - Amazon (US), Google (US), Uber (US), Tesla (US), Deepsense.AI (US)...
- **Application domains**
  - Data Mining, Self-Driving cars, Satellite & Communications, Big Data Analytics
- **Computing infrastructure answering these needs**
  - Traditional (CPU only), HTC, Hybrid HPC (CPUs + Accelerators)

Source: "Luxembourg strikes deal to create 'driverless car' test zone", Luxembourg Wort, 2017



Satellite imagery via image segmentation from Deep Learning, Deepsense.ai, 2017

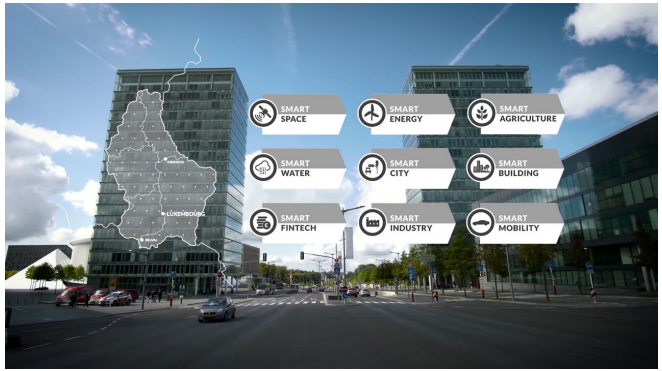
Space Mining, http://www.spaceresources.public.lu/



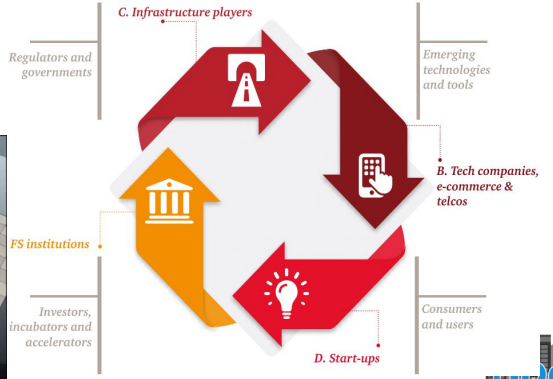
Real-Time Big-Data Analytics: Emerging trends in Twitter streams, UL

Case Study 4: Data science, IoT and FinTech

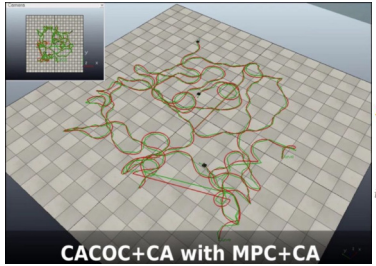
- **Companies & Research centers in Luxembourg**
  - Big Four (E&Y, Deloitte, PwC, KPMG), ExaMotive, AXA, BIL, BCEE, UL…
- **Potential to attract external companies**
  - Amazon (US), NEST (US), Somfy (FR), Google (US)...
- **Application domains**
  - Risk & Asset Management, Data intensive IoT, Smart City
- **Computing infrastructure answering these needs**
  - Cloud Computing, HTC, HPC



A Smart Day in Luxembourg, Luxinnovation

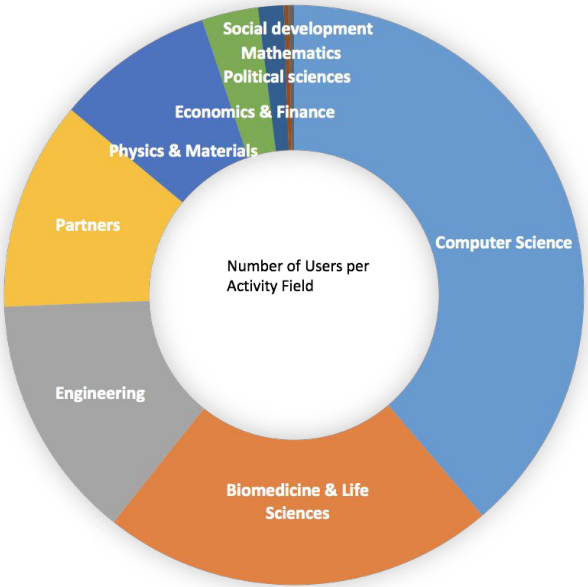


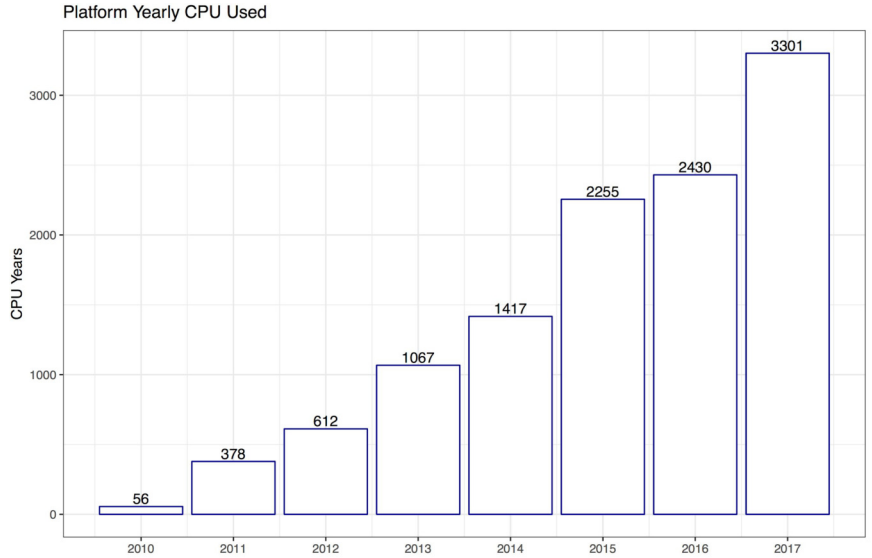
FinTech ecosystem, from 2016 PwC report "How FinTech is shaping Financial Services in Luxembourg"



Chaos-enhanced mobility models for multilevel swarms of UAVs (PCOG)

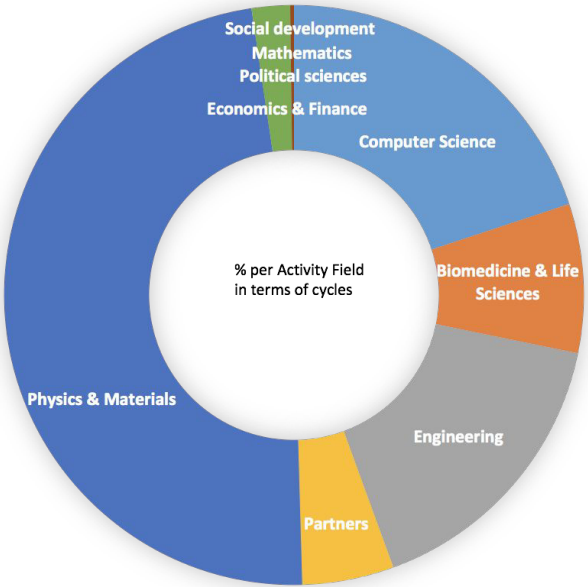
HPC Facility @ Uni.lu usage

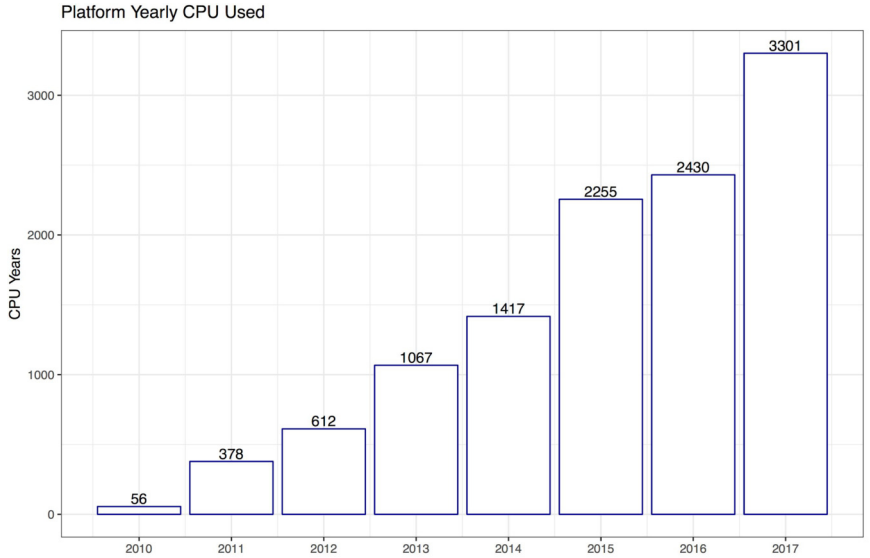




Statistics extracted on HPC **active** users
(submitted at least one job in the last year)

HPC Facility @ Uni.lu usage





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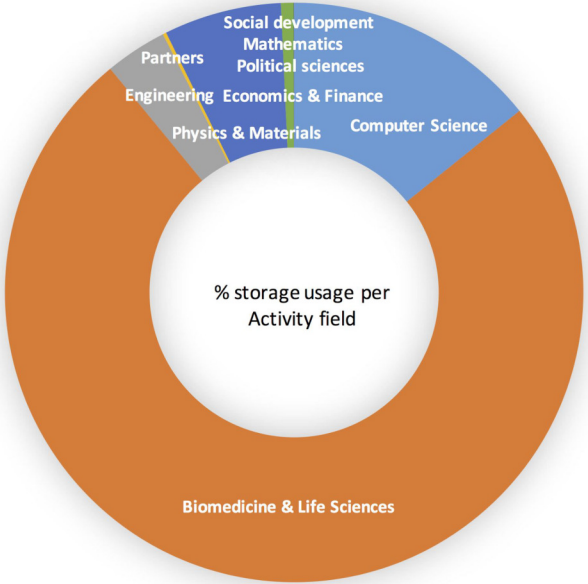
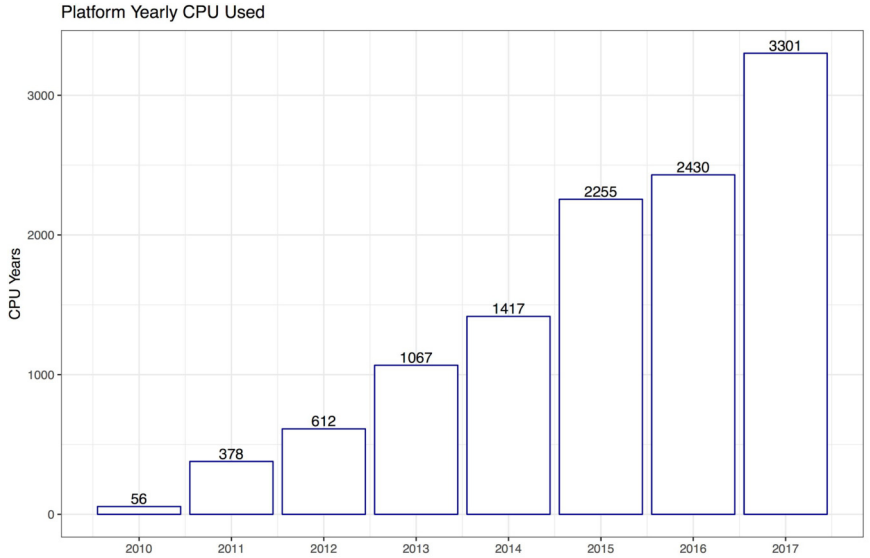
HPC Facility @ Uni.lu usage





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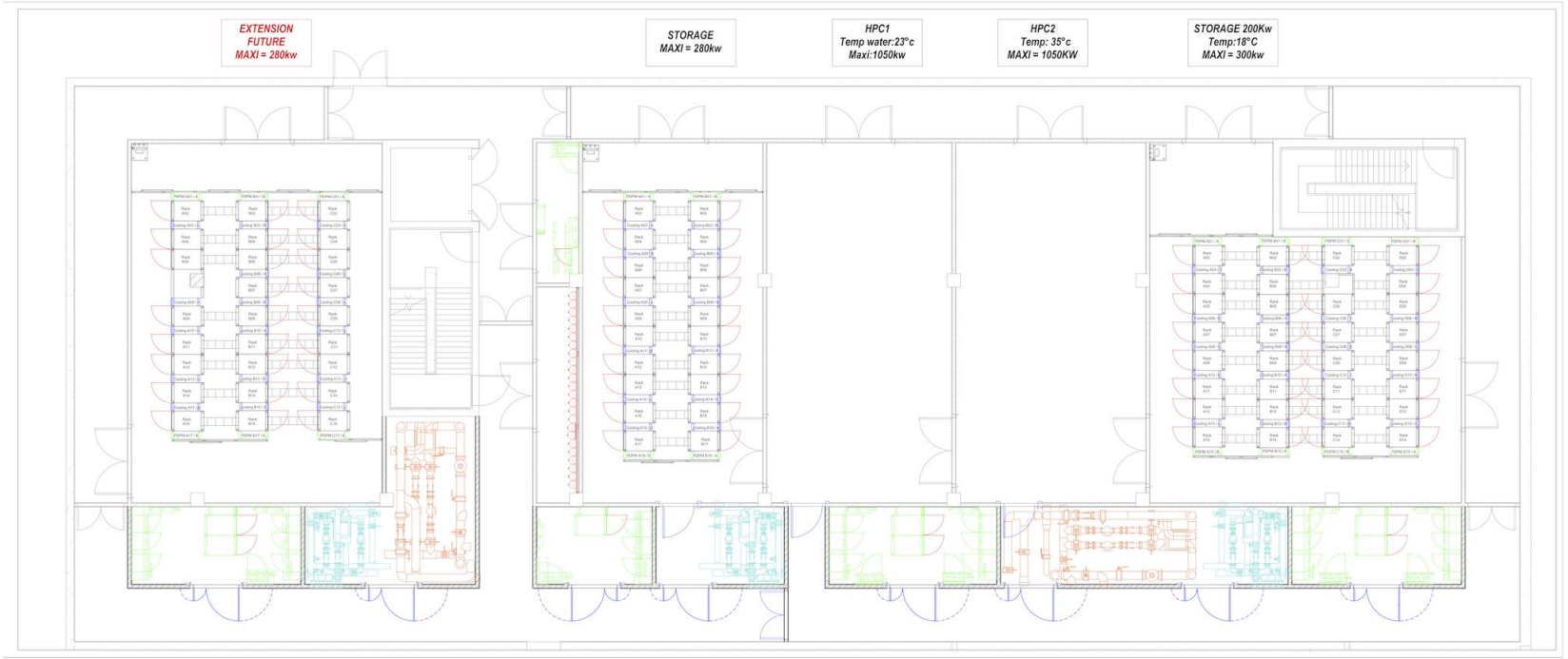
Uni.lu CDC (Centre de Calcul):
Toward Energy-Efficient HPC enabling DLC

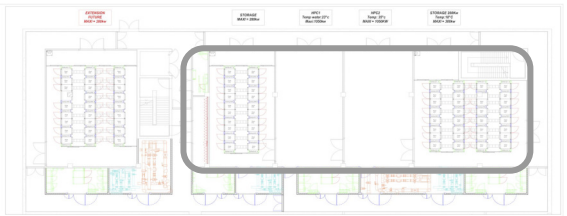


Uni.lu CDC (Centre de Calcul): Toward Energy-Efficient HPC enabling DLC

- 2x500 m^2 deployed since 2015
  - Electric energy , ventilation and chilled water produced by Fonds Belval power plant (located basement MNO)
  - CDC managed by SIU, one *floor* **dedicated to HPC** developments
- 4 server rooms **ready and operational** in 2018
  - One room (CDC S-02-005) holds our (current) flagship HPC facility (`iris`)

Data center ready for DLC with a **dedicated high temperature network** for **energy efficiency**

Location	Cooling	Usage	Max Capacity [kW]
CDC S-02-001	Airflow	*Future extension*	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 m^2)
CDC S-02-004	**DLC**	**High Density/Energy efficient HPC**	**1050 kW** (92 m^2)
CDC S-02-005	Airflow	Storage / Traditional HPC (`iris` cluster)	300 kW (128 m^2)



Education & Training

- **COST NESUS Winter School** on Data Science and Heterogeneous Computing
  - Last edition in January 2018 in Zagreb, Croatia
- **PRACE**
  - Last edition PRACE Days in May 2018 : European HPC Summit Week 2018 in Ljubljana
  - H2020-INFRAEDI-2018-2020 - PRACE-6IP
- **Bachelor degree BICS/BINFO: AI & Middleware**
- **Master degree MICS: Parallel and Grid Computing**
  - **Master in Information and Computer Sciences** - see misc.uni.lu
  - Master 2 courses, lectured since 2008
  - Evaluation based on projects evaluated on the UL HPC platform. *Ex:*
    - Fault Tolerance and Performance of MPI toolchains over HPC Applications
    - Measurement and Optimization of Energy Consumption in HPC Applications
    - Parallelization of the Barnes-Hut N-Body Simulation Algorithm
    - Evaluation of Big Data Framework (Hadoop, Spark…)
    - Evaluation of [Parallel/Distributed] Deep/Machine Learning Framework (Pytorch, Tensorflow, caffee...)
- **Lifelong-learning Smart-ICT for Business Innovation certificate**: Cloud Computing/Big Data/IoT

Education & Training

- **SC-Camp 2017** (Cadiz)
- Bi-annual **HPC School @ Uni.lu** (Part of the doctoral program)
  - 7th edition June 12th - 13th, 2018 in Belval
  - Material publically available: ulhpc-tutorials.rtfd.io
  - Last edition joint event: **UL-NSTDA workshop (EU-ASEAN E-READI)**

Day 1	Main Track (MSA 4.520)	Speaker
9h00	**PS1a**: Getting Started (part I: SSH)	C. Parisot
10h00	**Coffee break**	
10h30	**Overview & Challenges of the UL HPC Facility at the EuroHPC Horizon**	S. Varrette
11h45	**PS1b**: Getting Started (part II)	H. Cartiaux
12h30	**LUNCH**	
13h30	**PS2**: HPC workflow with sequential jobs	H. Cartiaux
14h30	**PS4a**: UL HPC Monitoring in practice	H. Cartiaux
15h30	**Coffee break**	
16h00	**PS5**: Parallel computations with OpenMP/MPI	S. Varrette
17h30	**PS6**: User environment and storage data management	S. Peter

Day 1	Parallel Track (MSA 4.410)	Speaker
10h30	**Keynote in 4.520**	
13h30	**PS3a**: Advanced scheduling (SLURM, OAR)	V. Plugaru
14h30	**PS3b**: Software environment management using Easybuild	S. Peter
15h30	**Coffee break (in 4.520)**	
16h00	**PS4b**: Performance engineering - HPC debugging and profilling	V. Plugaru

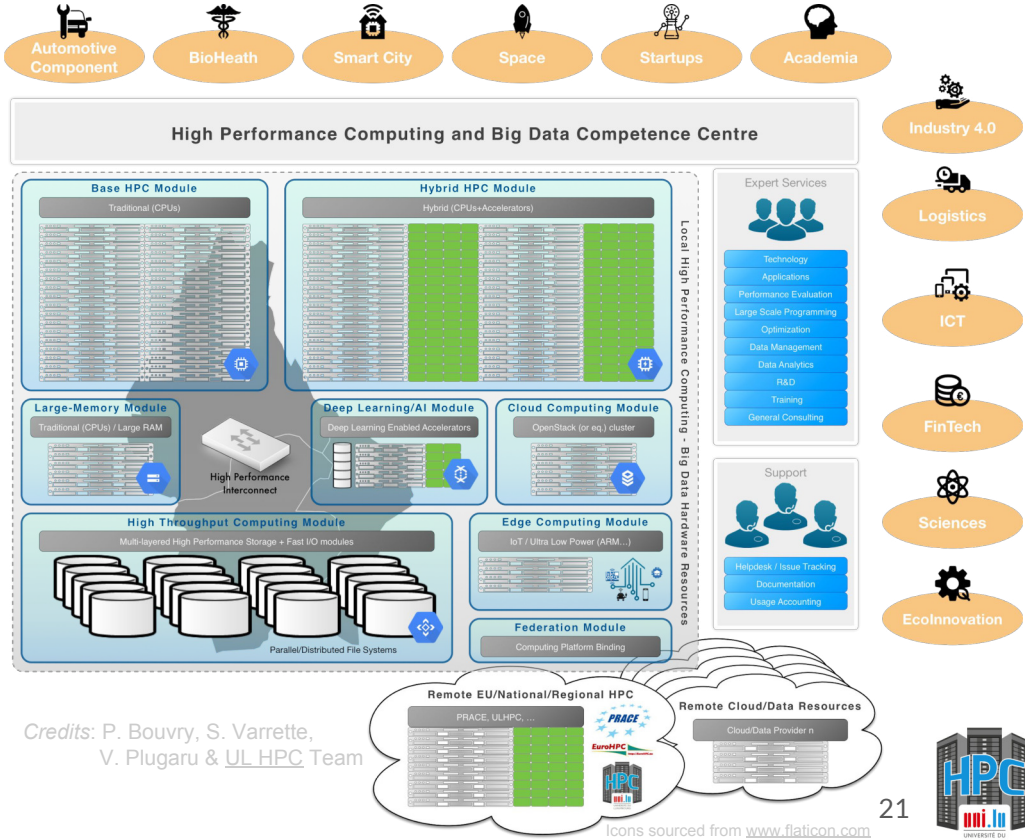
Day 2	Main Track (MSA 4.520)	Speaker
9h00	**PS7**: Multi-Physics workflows: test cases on CFD/MD/Chemistry applications	V. Plugaru
10h30	**Coffee break**	
11h00	**Users' session: UL HPC experiences**	
12h40	**LUNCH**	
13h30	**PS9**: [Basic + Advanced] Prototyping with Python	C. Parisot
15h30	**Coffee break**	
15h45	**PS11**: Big Data Applications	S. Varrette
17h15	**PS13**: Machine / Deep learning (Pytorch, Tensorflow, Caffe2)	S. Varrette
18h15	**Closing Keynote: Take Away Messages**	S. Varrette

Day 2	Parallel Track (MSA 4.510)	Speaker
9h00	**PS8**: Bio-informatics workflows and applications	S. Peter
10h30	**Coffee break (in 4.520)**	
11h00	**Users' session: UL HPC experiences** (in 4.520)	
12h40	**LUNCH**	
13h30	**PS10**: Scientific computing using MATLAB	V. Plugaru
15h30	**Coffee break**	
15h45	**PS12**: R - statistical computing	A. Ginolhac
17h15	**PS14**: HPC Containers: Singularity	V. Plugaru
18h15	**Closing Keynote in 4.520**	S. Varrette

Next steps: National HPC-BD Competence Center

Built by ministerial, academic, industrial stakeholders

- **Comprehensive centre:**
  - HPC *and* data infrastructure
  - Expertise in technology
  - Domain knowledge in applications
- **More than just computing services:**
  - *"Bring HPC and BD to the users"*
- **Creates twofold innovation:**
  - Innovation in applications and
  - Innovation in technology



Credits: P. Bouvry, S. Varrette, V. Plugaru & UL HPC Team

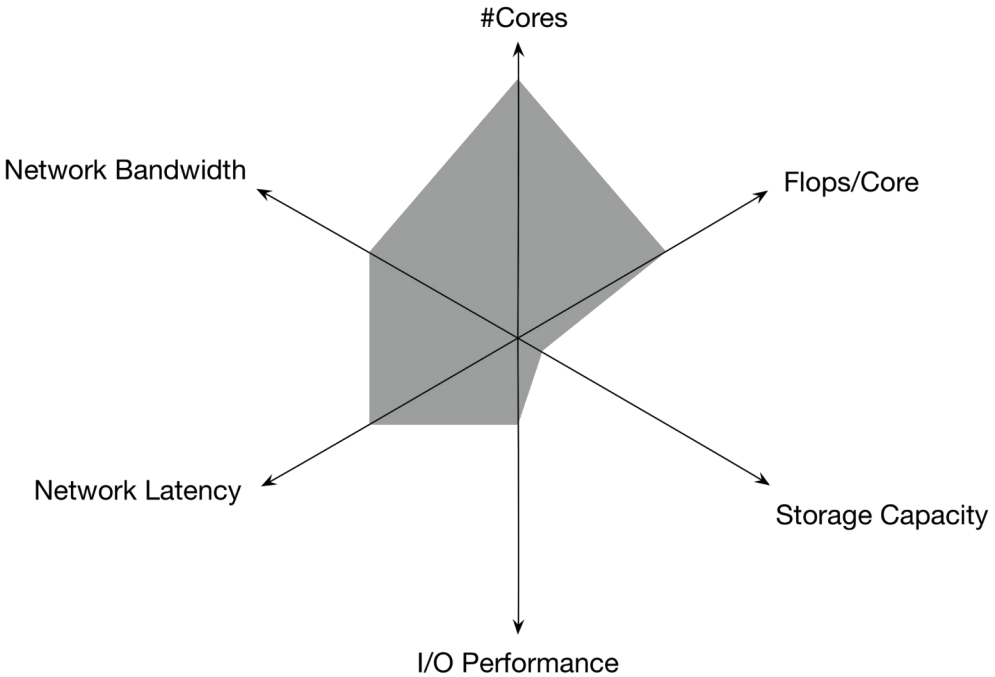
Icons sourced from www.flaticon.com

Appendix

UNIVERSITÉ DU LUXEMBOURG

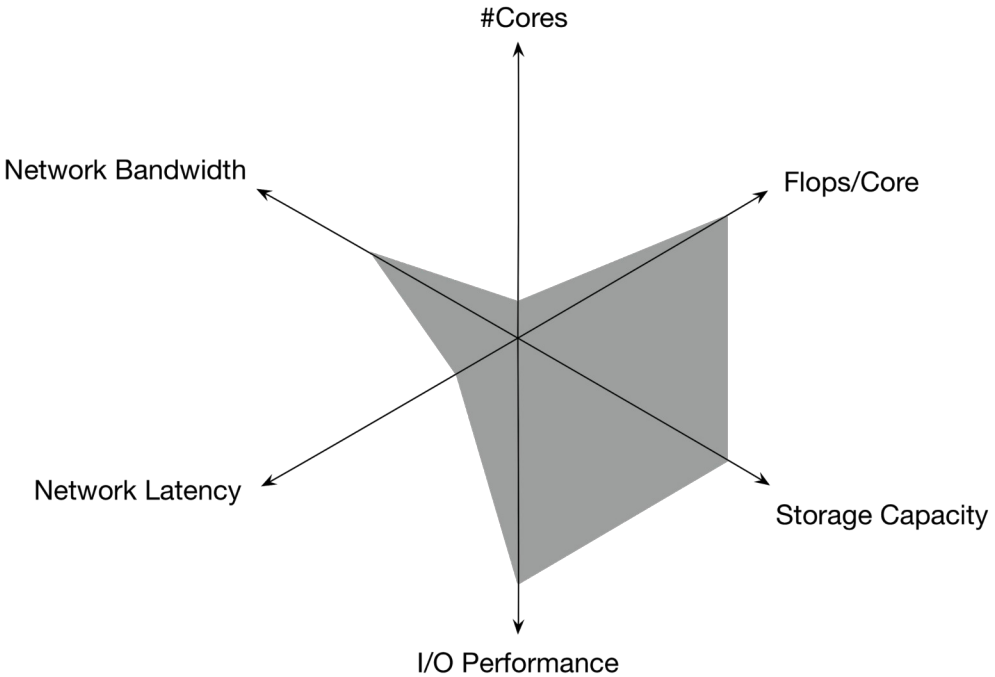
Different Needs for Different Domains

Material Science & Engineering



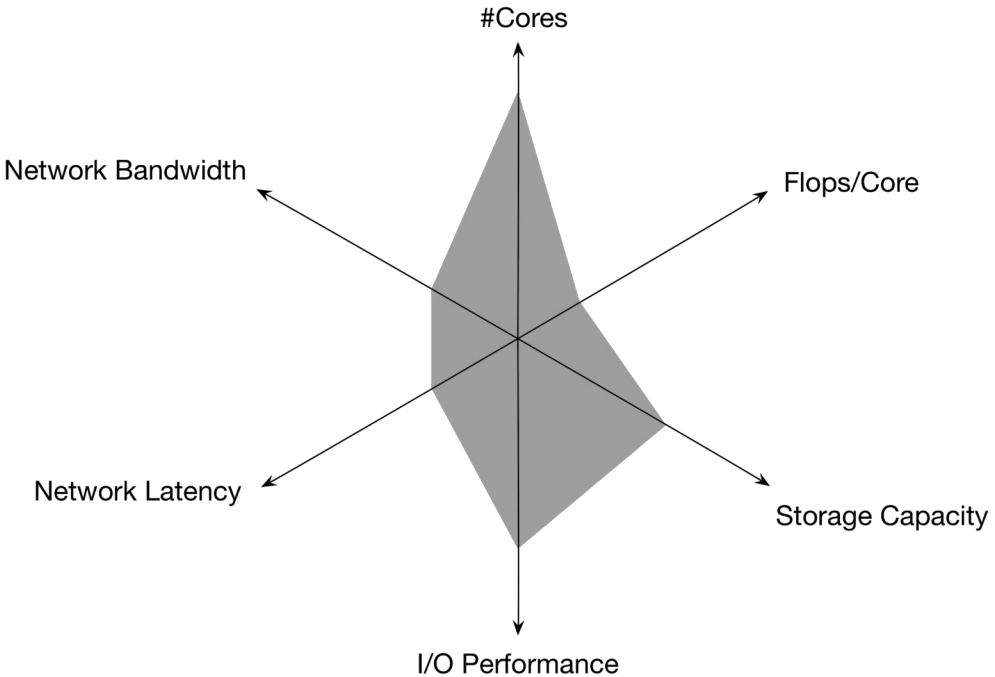
Different Needs for Different Domains

Biomedical Industry / Life Sciences



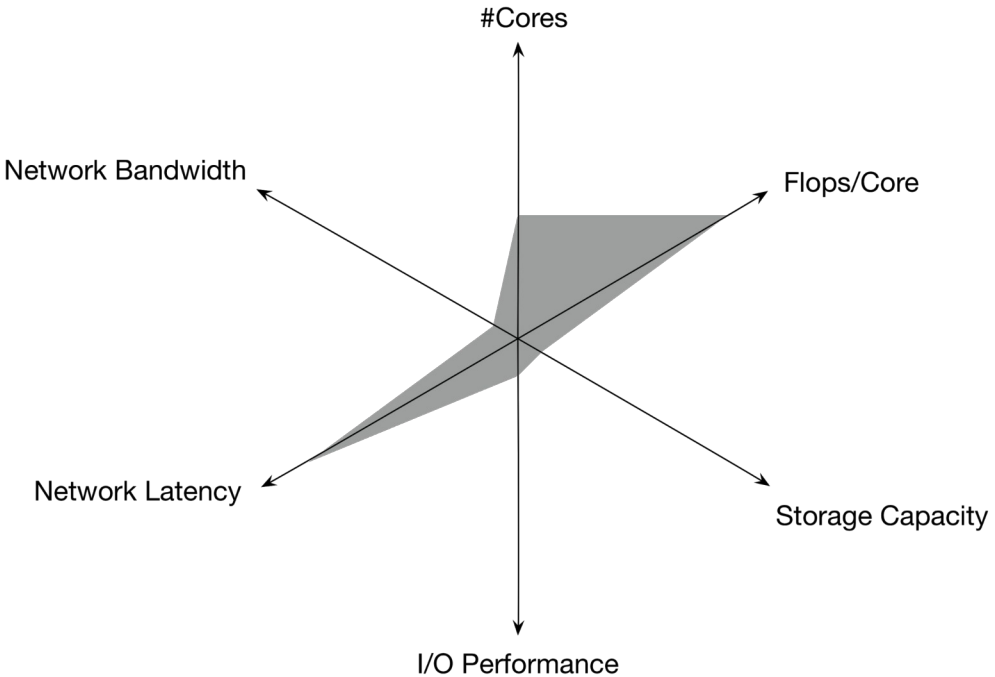
Different Needs for Different Domains

Deep Learning / Cognitive Computing



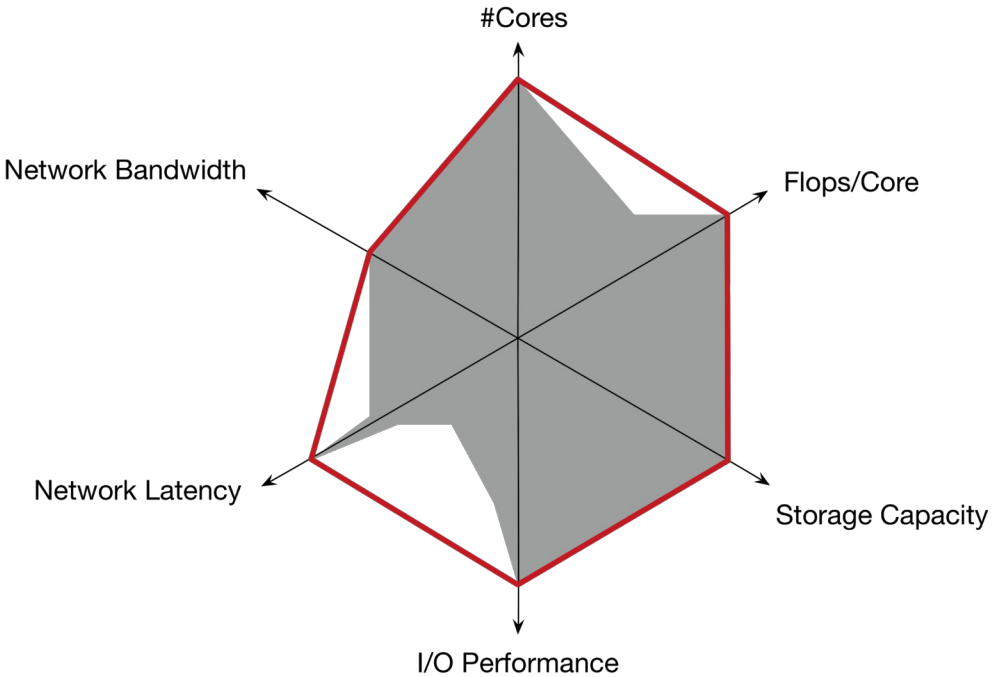
Different Needs for Different Domains

IoT, FinTech



Different Needs for Different Domains

ALL Research Computing Domains



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