

# Changing and growing HPC @ UL

---



**Valentin Plugaru**

Parallel Computing & Optimisation Group  
University of Luxembourg, Luxembourg

**PCOG Team Meeting**

**Dec. 5, 2016**



## Background

- **Economics degree** - Computer Science for Business Management - Romanian-American University (Bucharest, Romania)
- **Masters degree** - Information and Computer Sciences - University of Luxembourg (Luxembourg)
  - ↪ dual specialization: **Adaptive Computing & Network Systems**
- **High Performance Computing**
  - **since 2016**: Permanent researcher in PCOG, main duties for UL HPC
  - **since 2012**: PCOG collaborator, work linked to the HPC facility
  - **previously**: Research Assistant at the Laboratory for Molecular Nanotechnology, National Institute for R&D in Microtechnologies working in partnership with:
    - the Institute of Physical Chemistry of the Romanian Academy and
    - the National Institute for Materials Physics (Bucharest, Romania)



## Experience

17 years of Linux systems and networks

11 years of Cluster and HPC technologies



## Experience

17 years of Linux systems and networks

11 years of Cluster and HPC technologies

1.5 years as CEO of a Junior Enterprise

2 years as IT consultant for the pharmaceutical industry



## Experience

17 years of Linux systems and networks

11 years of Cluster and HPC technologies

1.5 years as CEO of a Junior Enterprise

2 years as IT consultant for the pharmaceutical industry

As a result of my background and previous experience, I am ...

**result-oriented** with a strong focus on **applied** sciences



## Work highlights of 2016 (I)

### International level

- Drafting UL membership for **ETP4HPC**
  - European Technology Platform for High Performance Computing
- Work on LU **PRACE** pre-membership documents
  - Partnership for Advanced Computing in Europe
- LU expert (through **ILNAS**) within **ISO/IEC JTC 1/SC 39**
  - Sustainability for and by Information Technology
- Promoting UL & its HPC for **international delegations**
  - Spain, Czech Republic
- **CloudCom 2016** conference - Workshops Co-chair
  - 5 workshops! - 4 returning/1 new
- UL HPC delegate visiting supercomputing facilities - **Cyfronet**
- ... and supercomputing conferences - **ISC 2016**



## Work highlights of 2016 (II)

### National / UL level - UL HPC

- Planning UL HPC renewal (2016) and extension (to 2020)
  - ↪ Discussions with top HPC vendors for **insight into new tech.**
  - ↪ Drafting and analyzing **RFPs worth 1.4M €**
  - ↪ Close **collaboration with SIU** for HPC integration in CDC
- Enabling new and amazing research though:
  - ↪ New and updated HW/SW HPC facilities
  - ↪ Interaction with user workflows and user training
- Meetings for collaboration - **LIH & LIST**
  - ↪ Requirements analysis
  - ↪ Trial utilization of our platform



The year past

---

So..

**How did we enable and accelerate scientific discovery and innovation?**





The year past

---

So..

**Now let's focus on this year's results.**



## ETP4HPC - WP 2018-20

- UL part of ETP4HPC since May 2016
- ETP4HPC now tasked by EC to prepare a draft of the next 2018-2020 HPC Work Programme (based on SRA-2)

### Contact point for UL, member of WG:

- HPC System Architecture and Components
- System Software and Management
- Programming Environment
- Balance Compute, I/O and Storage Performance
- Big Data and HPC usage Models



## The here and now in 2016

### New computing systems

- **Doubled** Gaia's performance through GPUs Hello ML!
  - ↪ 4 new nodes – **16 Nvidia Tesla K80 (46.56 TFlops)**
  - ↪ Upgraded 5 older nodes – **10 Nvidia Tesla K40 (14.3 TFlops)**
- Extended our low power, high performance systems
  - ↪ 60 new single socket systems – **HP Moonshot (10.6 TFlops)**
- Also 2 new *bigmem* nodes – **64 core, 2 TB RAM each**



## The here and now in 2016

### New computing systems

- **Doubled** Gaia's performance through GPUs Hello ML!
  - ↪ 4 new nodes – **16 Nvidia Tesla K80 (46.56 TFlops)**
  - ↪ Upgraded 5 older nodes – **10 Nvidia Tesla K40 (14.3 TFlops)**
- Extended our low power, high performance systems
  - ↪ 60 new single socket systems – **HP Moonshot (10.6 TFlops)**
- Also 2 new *bigmem* nodes – **64 core, 2 TB RAM each**

### Software environment

- Incremental software updates to existing stack
- New: **Gurobi Optimizer, STAR, (p)arpack-ng, VisIt, XDEM(XCS), Gazebo, Likwid, IntelPCM**
- Upgraded: **MATLAB, CPLEX, CMake/Boost/netCDF, R, XCS, CUDA, Allinea Forge/P.R.**



# What do researchers want as \$next?

- Designed the 2016 UL HPC user survey
- Goal:

**get necessary insight into users, workflows  
and present/future requirements**



## What do researchers want as \$next?

- Designed the 2016 UL HPC user survey
- Goal:  
**get necessary insight into users, workflows  
and present/future requirements**
- Result: **48** individual responses, **9** on behalf of research teams
- **Highlights:**
  - Striking diversity of fields utilizing HPC (see next slide)
  - Majority of software is parallel (Shared/Distributed memory)



## What do researchers want as \$next?

- Designed the 2016 UL HPC user survey
- Goal:

**get necessary insight into users, workflows  
and present/future requirements**

- Result: **48** individual responses, **9** on behalf of research teams
- **Highlights:**
  - Striking diversity of fields utilizing HPC (see next slide)
  - Majority of software is parallel (Shared/Distributed memory)
  - **70%** researchers using own software on the platform
  - **18%** planning to write software themselves



## What do researchers want as \$next?

- Designed the 2016 UL HPC user survey

- Goal:

**get necessary insight into users, workflows  
and present/future requirements**

- Result: **48** individual responses, **9** on behalf of research teams

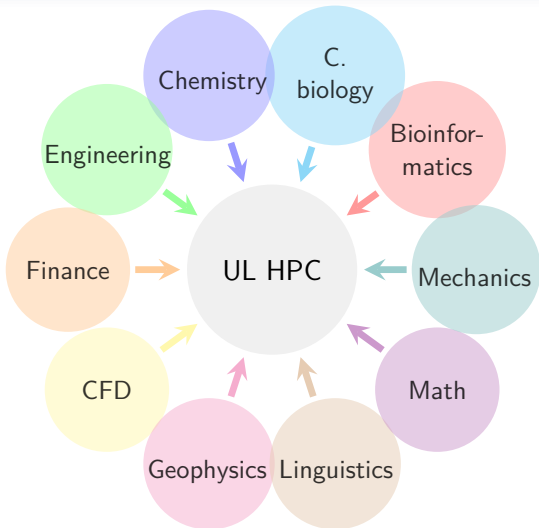
- **Highlights:**

- Striking diversity of fields utilizing HPC (see next slide)
- Majority of software is parallel (Shared/Distributed memory)
- **70%** researchers using own software on the platform
- **18%** planning to write software themselves
- **87%** of work done in batch mode
- Most job executions are **OK with 5 day walltime limit**
- **~41%** of jobs can be resumed with minimal/no loss

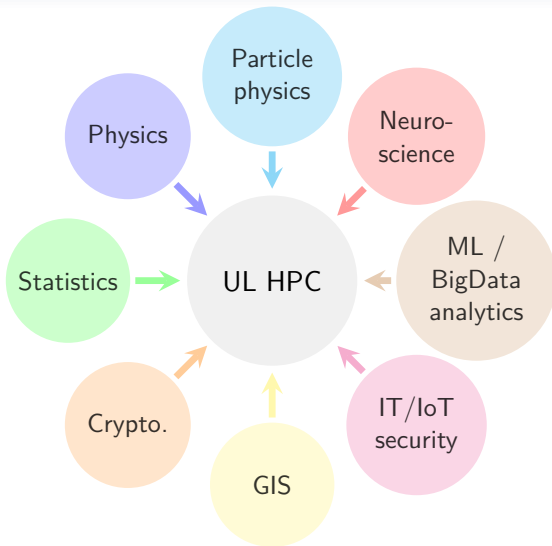




## Survey - Computational domains

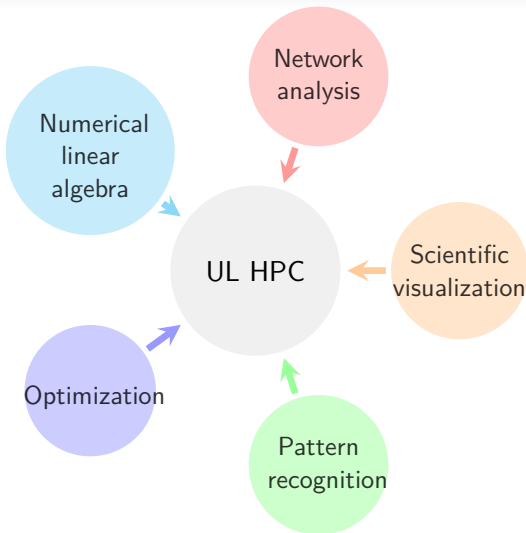


## Survey - Computational domains





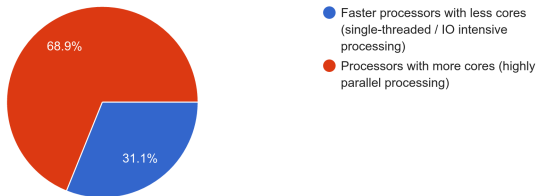
## Survey - Computational domains



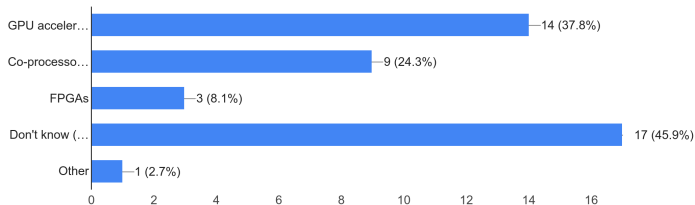


# Survey - looking to the future

Your computing systems preferences: (45 responses)



Do you use or would you use the following accelerators: (37 responses)





## UL HPC Renewal - 2 RFPs in 2016

### It all started..

- March: Visit of Cyfronet (PL) **Prometheus supercomputer**
- June: **ISC 2016** – 10 HPC vendor meetings
- ... and discussions with 5 groups on HPC sw. and technology



## UL HPC Renewal - 2 RFPs in 2016

### It all started..

- March: Visit of Cyfronet (PL) **Prometheus supercomputer**
- June: **ISC 2016** – 10 HPC vendor meetings
- ... and discussions with 5 groups on HPC sw. and technology

### The result?

- 6 vendor offers for our **Storage RFP**  
↔ ~1 PB effective storage ~10GB/s, GPFS-based
- 5 vendor offers for our **Compute RFP**  
↔ ~90 TFlops effective compute 2800 cores, Xeon v4

(btw. it only takes some ~4 months to draft & review RFPs)



## Teaching and training activities

### UL MiCS

- Optimization for CS – project supervision
- Parallel & Grid Computing – lecturing & project supervision
- Presentation of UL HPC at MiCS "Back to the Future"

### HPC training & direct work with UL researchers

- Organization of 2016 HPC school (late November)
  - ↳ 2 sessions on **debugging/perf. analysis** and **parallel workflows**
- enabling and optimization of researcher work on UL HPC
- discussions for integration of different computing methods and algorithms, new high level languages



## What's next - highlights

### 2016 RFPs - fun just now beginning

- Early Q1 2017 deployment of new systems within CDC S-01
  - Update sw. infrastructure with SotA best-practices
- ↪ Use Gaia 2.0 as test-bed for next big system incl. **research**





## What's next - highlights

### 2016 RFPs - fun just now beginning

- Early Q1 2017 deployment of new systems within CDC S-01
  - Update sw. infrastructure with SotA best-practices
- ↪ Use Gaia 2.0 as test-bed for next big system incl. **research**

### 2017 RFP(s) - the next big system

- RFP drafting for Stage 1 to start also Q1 2017
  - **big** for next-gen workloads
  - big but **efficient** – DLC (PUE ~1.001 - as efficient as possible)
- ↪ Stage 1 deployment: Q4 2017 (0.7PFlop Skylake + IB HDR?)



## Thank you

Thank you for your attention!



**Valentin Plugaru**  
valentin.plugin@uni.lu  
hpc.uni.lu  
pcog.uni.lu