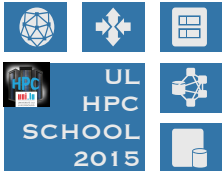# UL HPC School June 2015
Opening Session

Sebastien Varrette

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University of Luxembourg (UL), Luxembourg

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Welcome to the UL HPC School

- **Third edition** after successful 2014 and March 2015 editions
    - ↪ main event of 2015 with basic + advanced tutorials
    - ↪ following the newcomer edition of March
    - ↪ 46 registered participants
    - ↪ 7 distinct speakers
        - ✓ supported by some of the leading UL computational scientists
    - ↪ Open and public access – content on GitHub

UL HPC School Overview

- **6 keynotes** (including user's session)
- **15 practical sessions across 3 tracks**
  - ↪ focusing on observed daily usage of the platform
  - ↪ basics, sequential & parallel jobs, specific applications targeted (Matlab, R, bioinfo, engineering, physics, chemistry)

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Agenda - Day 1 (June 25th)

June 25th	Main Track (BS 3.03 Auditorium)	Track 1 (BS 1.04)	Track 2 (BS 3.04)
09h00-09h15	HPC School opening session – S. Varrette		
09h15-10h00	*Keynote 1*: High Performance Computing at UL and abroad – S. Varrette		
10h00-10h30	*Keynote 2*: UL HPC in practice: why, what, how, where to look – X. Besseron		
10h30-10h45	**Coffee break**		
10h45-12h30	*Keynote 3 / PS 1A*: Complementary yet key IT Survival Guide: Git, Vagrant, Puppet – S. Varrette	*PS 1B*: Getting Started on the UL HPC platform (SSH, data transfer, OAR, modules, monitoring) – S. Diehl	
12h30-13h45	**LUNCH**	**LUNCH**	
13h45-14h00	*Keynote 4*: XCS Portal – V. Plugaru		
14h00-15h45	*PS 2A*: HPC workflow with sequential jobs (test cases on GROMACS, Python and Java) – S. Varrette	*PS 2B*: MATLAB 1 (interactive, passive, sequential, XCS) – V. Plugaru	*PS 2C*: Virtualization on Grid'5000 platform (KVM, Xen) – H. Cartiaux
15h45-16h00	**Coffee break**	**Coffee break**	**Coffee break**
16h00-17h30	*PS 3A*: HPC workflow with Parallel/Distributed jobs: application on MPI software (test cases on OSU/HPL) – S. Varrette	*PS 3B*: MATLAB 2 (checkpointing, parallel) – V. Plugaru	*PS 3C*: R - statistical computing – J. Emeras

Agenda – Day 2 (June 26th)

June 26th	Main Track (BS 3.03 Auditorium)	Track 1 (BCE 0.12)	Track 2 (BCE 2.08)
09h15-09h30	Second day opening session – S. Varrette		
09h30-10h30	Keynote 5: Users' session: UL HPC experiences		
10h30-10h45	**Coffee break**		
10h45-12h30	PS 4A: Software environment generation: RESIF/Easybuild – M. Schmitt		
12h30-13h45	**LUNCH**		
13h45-14h15	Keynote 6: Data management – S. Varrette		
14h15-15h45	PS 5A: Bioinformatics workflows using the Galaxy portal – S. Diehl	PS 5B: Running parallel software: test cases on CFD / MD / Chemistry applications (OpenFOAM, NAMD, ASE, ABINIT, Quantum Espresso) – V. Plugaru	PS 5C: GPGPU and shared memory programming (CUDA, OpenMP and Intel TBB) – S. Varrette
15h45-16h00	**Coffee break**	**Coffee break**	**Coffee break**
16h00-17h30	PS 6A: Running bioinformatics software: test cases on Abyss, GROMACS, Bowtie2/TopHat, mpiBLAST – S. Diehl	PS 6B: Graphical Sessions and Visualization: Paraview and Rstudio under XCS – V. Plugaru	PS 6C: Advanced workflows on parametric jobs management (best-effort, containers, checkpointing) – H. Cartiaux

http://hpc.uni.lu/hpc-school

Github Tutorials: `https://github.com/ULHPC/tutorials`

UL HPC website `https://hpc.uni.lu`

The UL HPC Team

Pascal Bouvry is a full professor of the FSTC and the head of the ILIAS research unit and the DS-CSCE doctoral school. His team (PCOG) is composed of 25 researchers working on Parallel computing and Optimization applied to Cloud Computing and HPC (scheduling, energy-efficiency, security), Ad-Hoc Networks (Vanets simulation and service optimization) and Biology (gene sequencing, regulatory networks, protein folding).

Sébastien Varrette, PhD, is a Research Associate in Prof. Bouvry's team since 2007. Along with Prof. Bouvry, he defined and set up the global HPC initiative of the UL in 2007. In this context, he is managing the sysadmin team that maintain and extend the platform. In parallel, his research work focuses on Distributed Computing Platforms (clusters, grids or clouds), with a particular interest on the security and performance evaluation of distributed or parallel executions.

Hyacinthe Cartiaux joined the HPC team in 2011 to set up the Grid'5000 Luxembourg site and has since been involved with all the HPC infrastructure of the UL, and other external services such as the Gforge. His interests cover IT automation and devops techniques, HPC & Grid Computing.

Valentin Plugaru is an HPC engineer part of the HPC team since 2014. Beginning with 2012 he has collaborated with Prof. Bouvry's team on research in Energy Efficiency and Performance Evaluation of HPC/Cloud environments. His general interests span R&D in High Performance Computing, Grid and Cloud Computing.

Sarah Diehl is a bioinformatician and joined the LCSB BioCore in 2015 as an HPC systems administrator. Her goal is to bridge the gap between researchers and IT specialists. She is experienced in data management, next-generation sequencing analysis and development of analysis pipelines.

Top 2014 User reports

- Total **used** resources in 2014: **1417 years**
- **Up 33%** compared with 2013
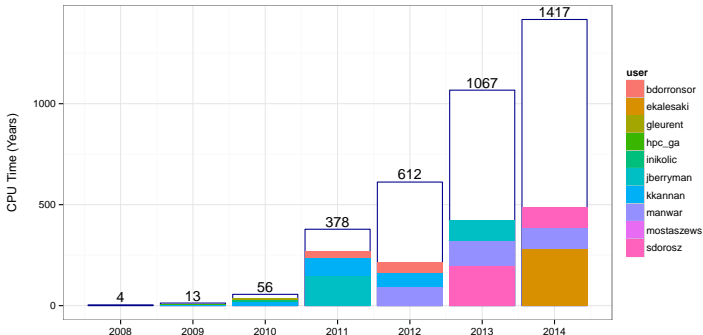
Top 2014 User reports

```
    login          total_asked  total_used CPUHour used
--  ---------      -----------  ---------- ----------------------------
1   ekalesaki      51975866400  8970447983 0285 years 096 days 15:06:23
2   manwar         7847452800   3179608677 0101 years 278 days 00:37:57
3   sdorosz        6205410000   3162397174 0110 years 078 days 19:39:34
4   amolinasanchez 24369418958  2207770186 0070 years 351 days 21:29:46
5   jberryman      9067514400   1913896245 0061 years 237 days 13:50:45
6   hmiranda       35220902400  1662562243 0053 years 250 days 14:50:43
7   sokawa         7206109200   1086009034 0035 years 152 days 13:10:34
8   pmay           3734942400   1064860651 0034 years 272 days 18:37:31
9   akalantari     7572693600   1058740031 0034 years 201 days 22:27:11
10  snielsen       5725191600   1030758605 0033 years 243 days 01:50:05
11  mdiarra        164418453000 1028947965 0033 years 222 days 02:52:45
12  ahunegnaw      1557208800   976436531  0031 years 345 days 08:22:11
13  jmuszynski     2814051551   951645828  0031 years 058 days 10:03:48
14  dkim           125761759200 858230347  0028 years 073 days 05:19:07
15  skillcoyne     13590576000  853731503  0028 years 021 days 03:38:23
```

```
## Function to convert cpuhour (in s) into a readable time formating
getTime <- function(x) {
  str = format(as.POSIXct('0001-01-01 00:00:00') + x, "%Y years %j days %H:%M:%S")
  return(str)
}
```