



Introduction to HPC

2nd RSG Luxembourg National Congress 2017

UL High Performance Computing (HPC) Team

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<http://hpc.uni.lu>

Summary

1 Introduction

2 High Performance Computing (HPC) @ UL

Overview

UL HPC Cluster Organisation

3 Hands-on



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Why High Performance Computing ?

“The country that out-computes will be the one that out-competes”. *Council on Competitiveness*

- **Accelerates** research by accelerating **computation**



$\simeq 64$ GFlops

(Dual-core i5 2GHz)

198.172 TFlops

(594 computing nodes, 8228 cores)

- Increases **storage** capacity and velocity for Big Data processing



4 TB

(1 disk, 250 MB/s)

6856.4TB

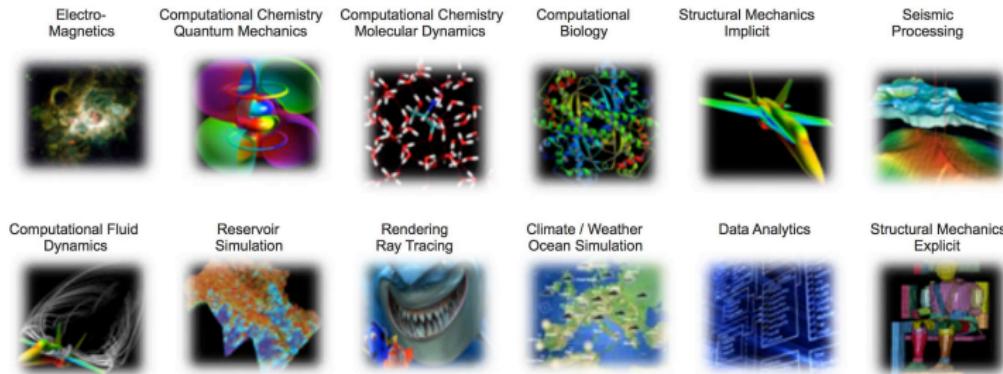
(1558 disks, 10 GB/s)

- **Communicates faster**

1 GbE (1 Gb/s) vs Infiniband EDR (100 Gb/s) ~ The logo for Infiniband EDR, consisting of four vertical bars of increasing height in red, orange, yellow, and green, followed by the letters 'i' and 'L'.

HPC at the Heart of our Daily Life

- **Today:** Research, Industry, Local Collectivities



- ... **Tomorrow:** applied research, digital health, nano/bio tech.



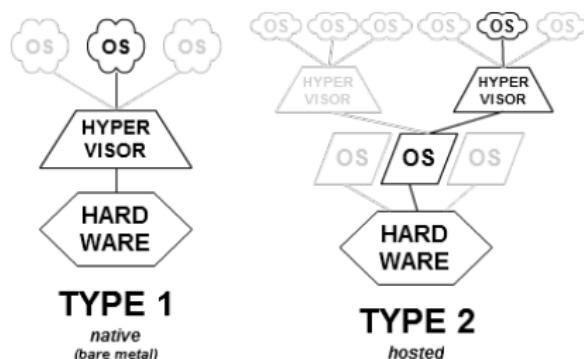
Computing for Researchers: Laptop

- Regular PC / Local Laptop / Workstation
 - ↪ Native OS (Windows, Linux, Mac etc.)



Computing for Researchers: Laptop

- Regular PC / Local Laptop / Workstation
 - ↪ Native OS (Windows, Linux, Mac etc.)
 - ↪ Virtualized OS through an **hypervisor**
 - ✓ Hypervisor: core virtualization engine / environment
 - ✓ **Performance loss:** $\geq 20\%$



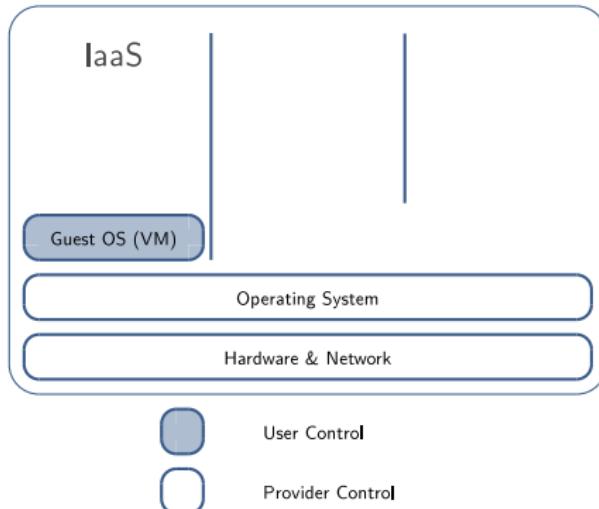
Xen, VMWare ESXi, KVM, VirtualBox

Computing for Researchers: Cloud



- Cloud Computing

- access to shared (*generally virtualized*) resources in a pay-per-use manner
- **Infrastructure as a Service (IaaS)**

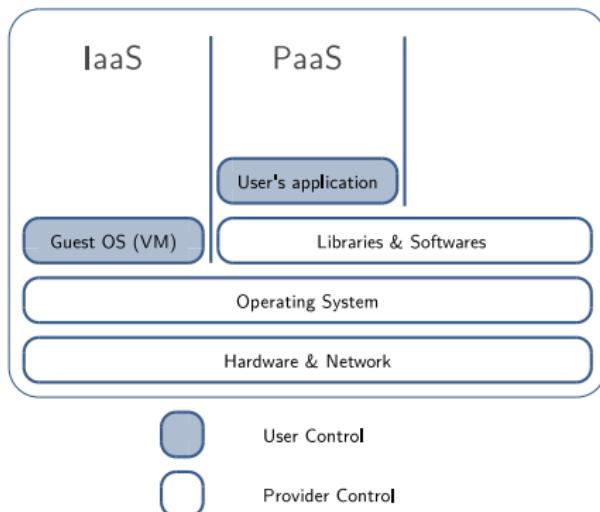


Computing for Researchers: Cloud



- Cloud Computing

- access to shared (*generally virtualized*) resources in a pay-per-use manner
- **Platform as a Service (PaaS)**

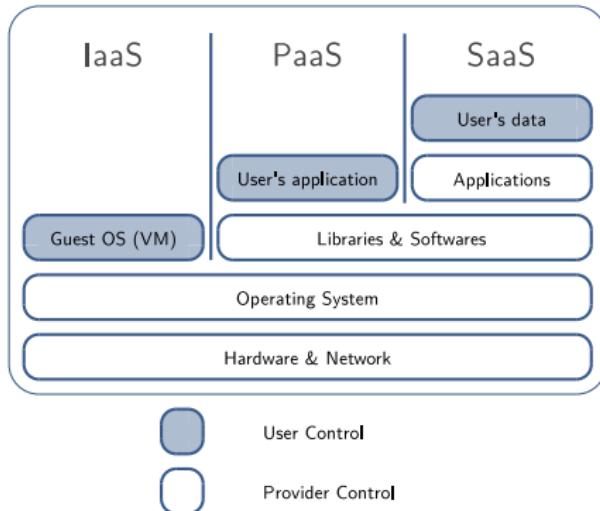


Computing for Researchers: Cloud



- Cloud Computing

- access to shared (*generally virtualized*) resources in a pay-per-use manner
- **Software as a Service (SaaS)**



Computing for Researchers: HPC

- High Performance Computing (HPC) platforms
 - ↪ For **Speedup**, **Scalability** and **Faster Time to Solution**



Computing for Researchers: HPC

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YET...

PC ≠ Cloud ≠ HPC

Computing for Researchers: HPC

- High Performance Computing (HPC) platforms
 - ↪ For **Speedup**, **Scalability** and **Faster Time to Solution**



YET...

PC ≠ Cloud ≠ HPC

- $\text{HPC} \simeq \text{Formula 1}$
 - ↪ relies on ultra efficient hardware / interconnect (IB EDR...)
 - ↪ ... when Cloud has to stay standard ([10] GbE etc...)
- **Does not mean the 3 approaches cannot work together**



Jobs, Tasks & Local Execution



```
$> ./myprog
```



Jobs, Tasks & Local Execution



```
$> ./myprog
```



Jobs, Tasks & Local Execution



```
$> ./myprog  
$> ./myprog -n 10
```



Jobs, Tasks & Local Execution



```
$> ./myprog  
$> ./myprog -n 10
```



Jobs, Tasks & Local Execution



```
$> ./myprog  
$> ./myprog -n 10  
$> ./myprog -n 100
```



Jobs, Tasks & Local Execution



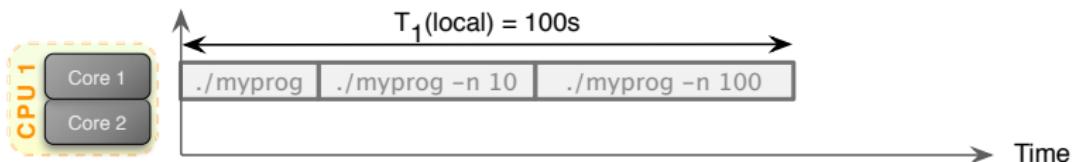
```
$> ./myprog  
$> ./myprog -n 10  
$> ./myprog -n 100
```



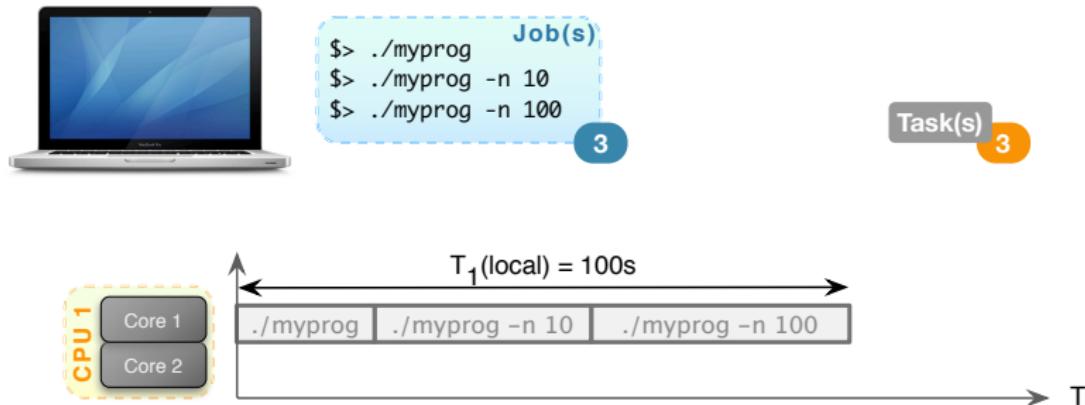
Jobs, Tasks & Local Execution



```
$> ./myprog  
$> ./myprog -n 10  
$> ./myprog -n 100
```



Jobs, Tasks & Local Execution



Jobs, Tasks & Local Execution



```
# launcher  
./myprog  
./myprog -n 10  
./myprog -n 100
```



Jobs, Tasks & Local Execution



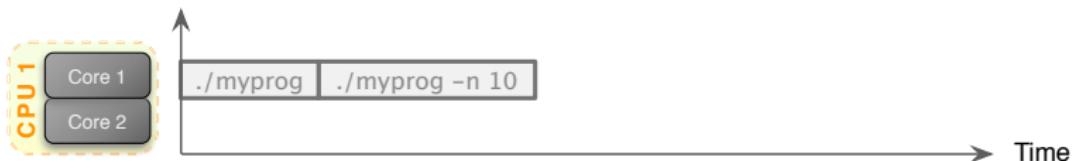
```
# launcher  
./myprog  
./myprog -n 10  
./myprog -n 100
```

A green rectangular box containing a text file named "launcher". The file contains three lines of code: "./myprog", "./myprog -n 10", and "./myprog -n 100".

Jobs, Tasks & Local Execution



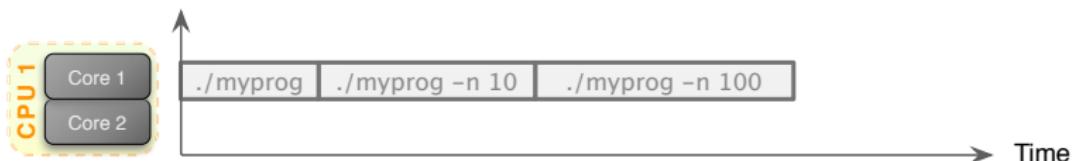
```
# launcher
./myprog
./myprog -n 10
./myprog -n 100
```



Jobs, Tasks & Local Execution



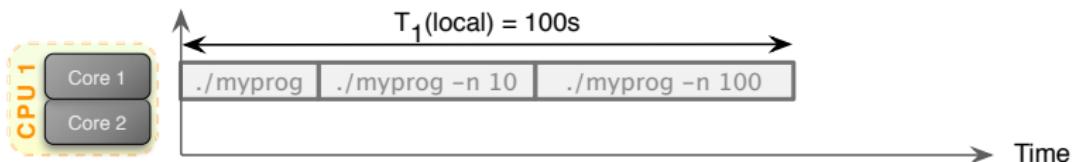
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# launcher  
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./myprog -n 10  
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```



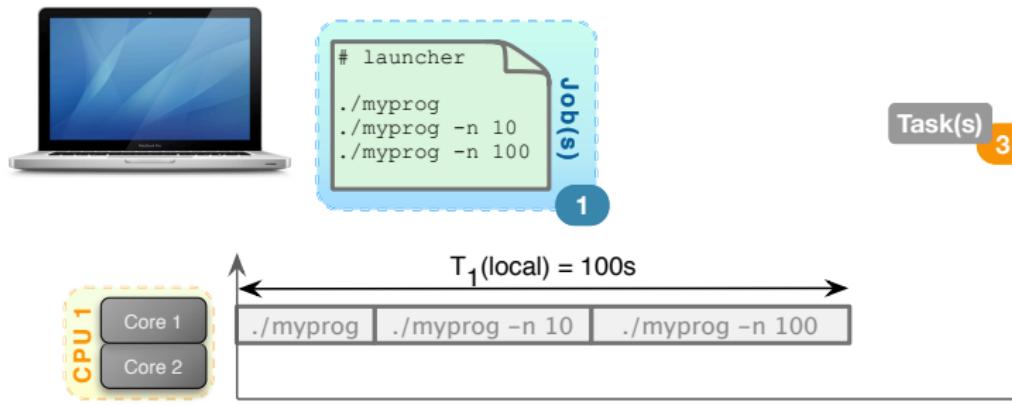
Jobs, Tasks & Local Execution



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# launcher  
./myprog  
./myprog -n 10  
./myprog -n 100
```



Jobs, Tasks & Local Execution



Jobs, Tasks & Local Execution



```
# launcher  
./myprog  
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```



Jobs, Tasks & Local Execution



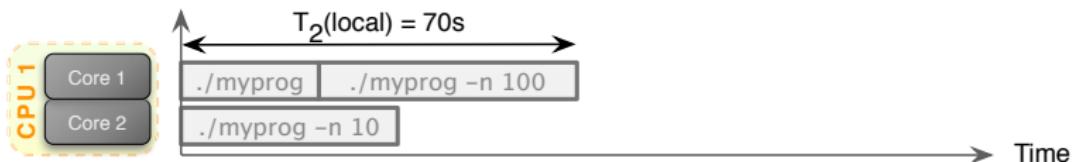
```
# launcher2
"Run in //:""
./myprog
./myprog -n 10
./myprog -n 100
```



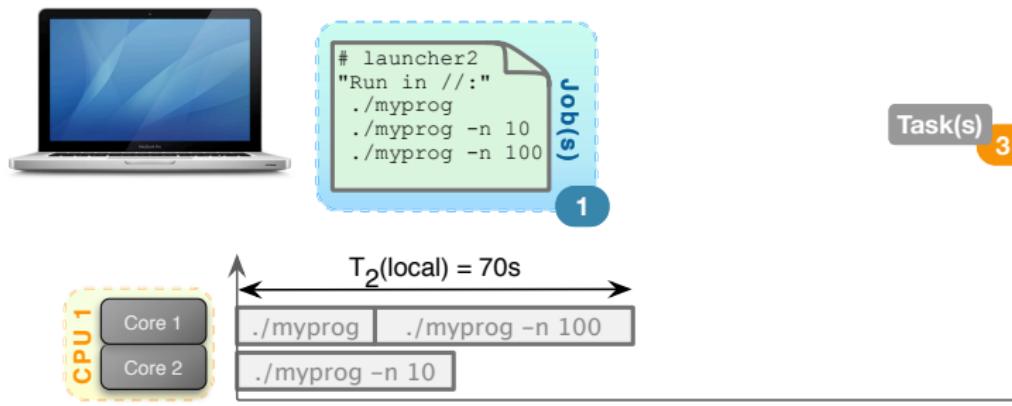
Jobs, Tasks & Local Execution



```
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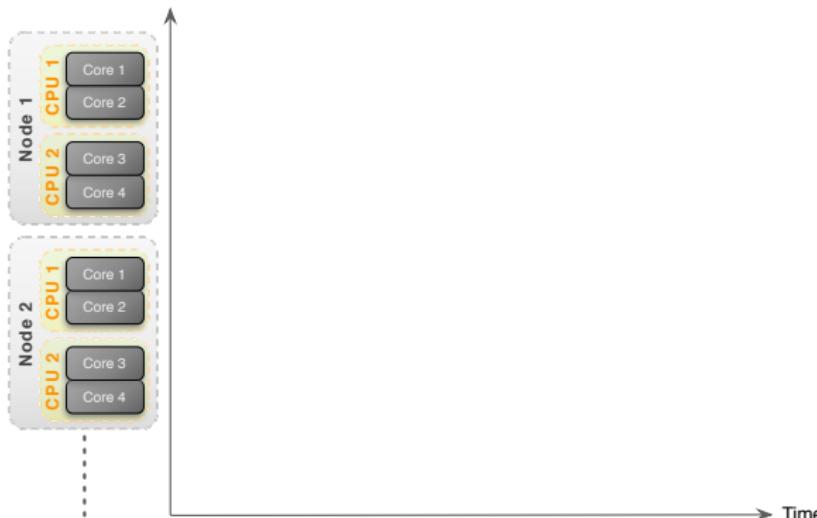
Jobs, Tasks & Local Execution



Jobs, Tasks & HPC Execution



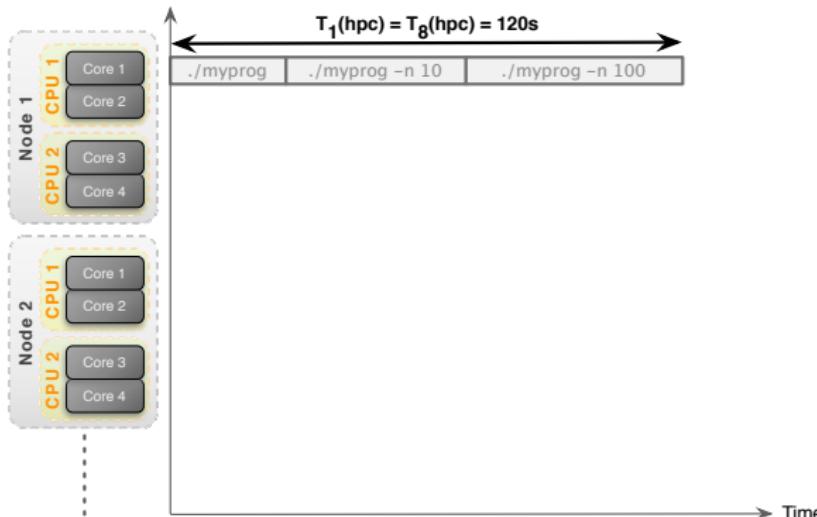
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```



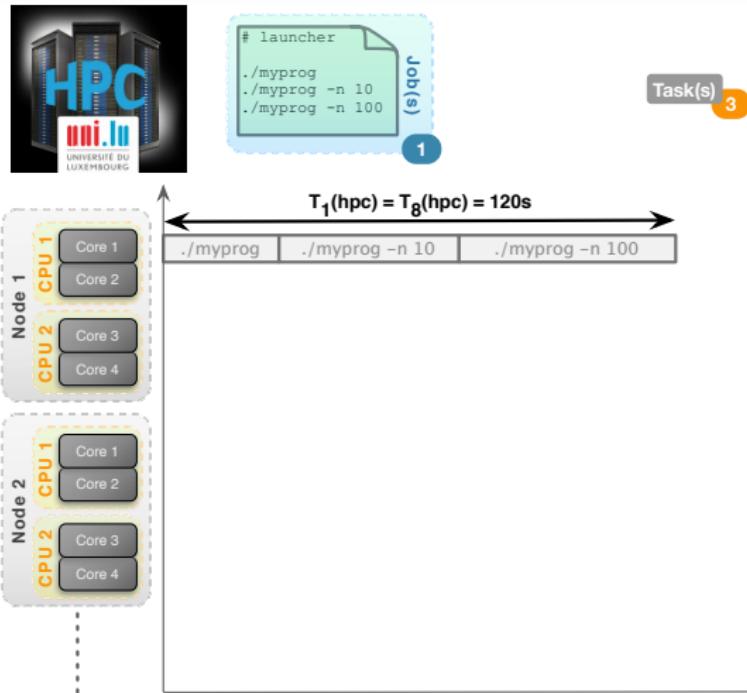
Jobs, Tasks & HPC Execution



```
# launcher  
./myprog  
./myprog -n 10  
./myprog -n 100
```



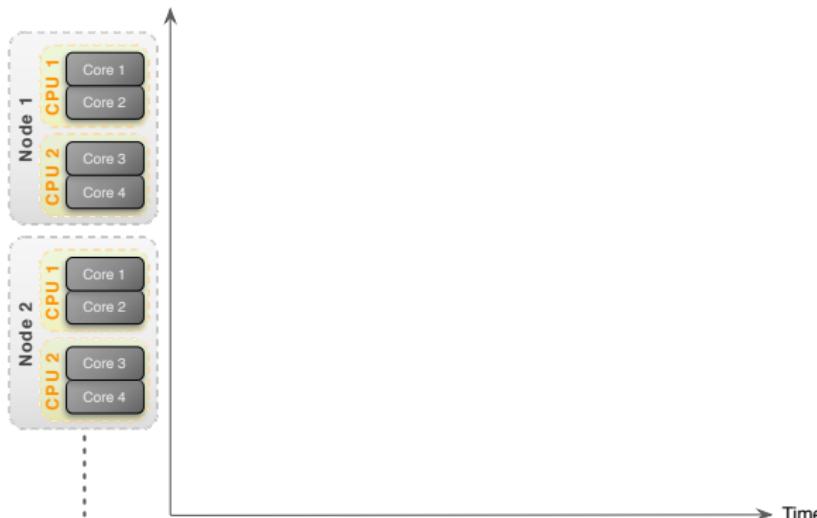
Jobs, Tasks & HPC Execution



Jobs, Tasks & HPC Execution



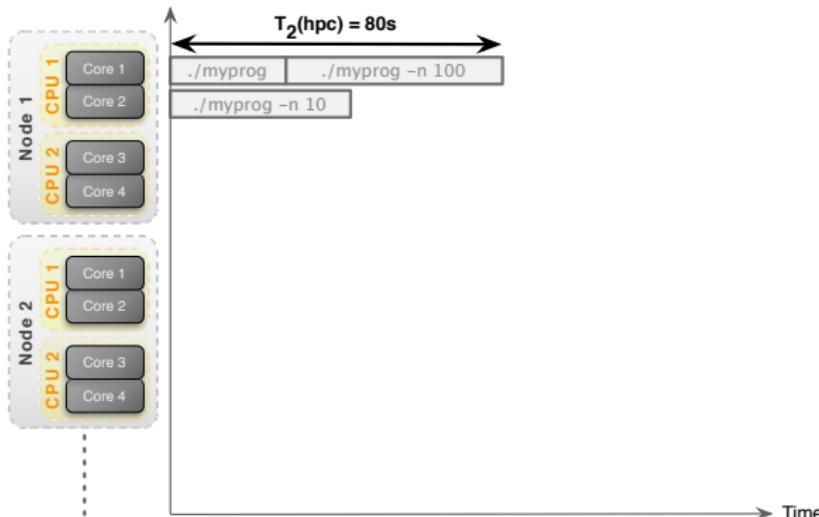
```
# launcher2
"Run in //:""
./myprog
./myprog -n 10
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```



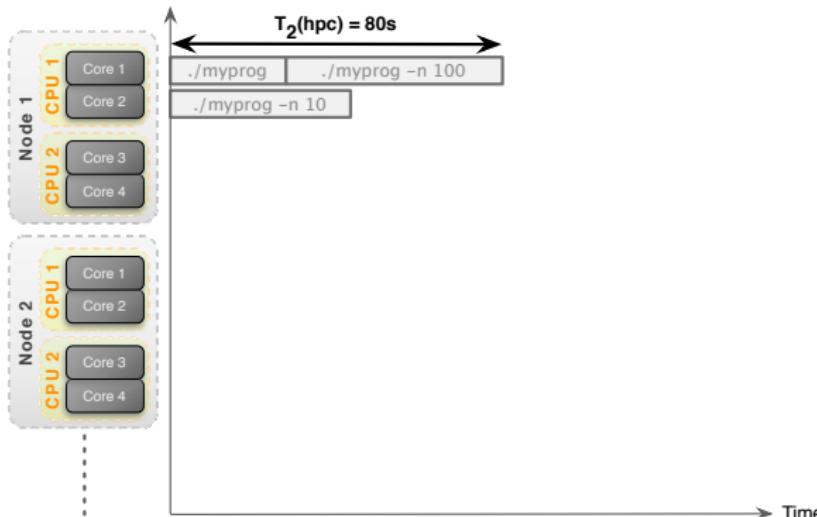
Jobs, Tasks & HPC Execution



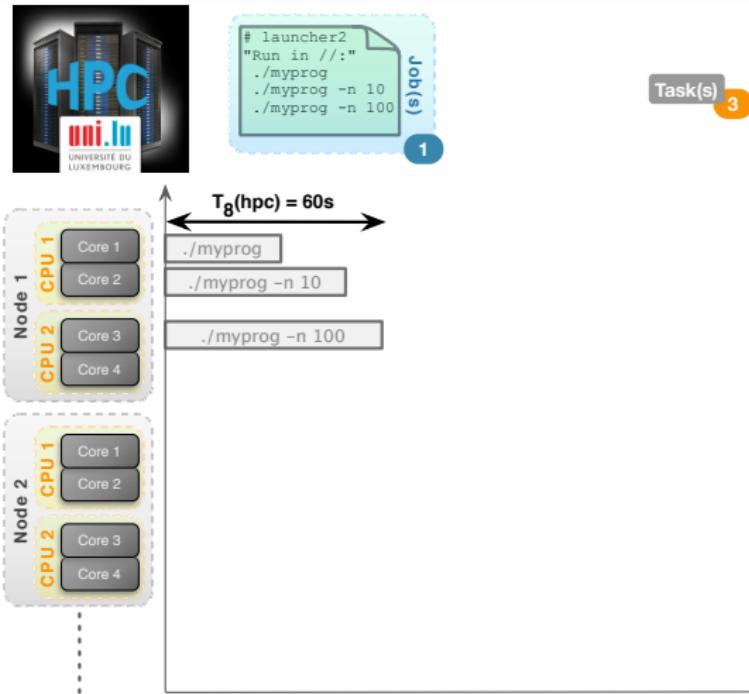
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# launcher2
"Run in //:""
./myprog
./myprog -n 10
./myprog -n 100
```



Jobs, Tasks & HPC Execution



Jobs, Tasks & HPC Execution



Local vs. HPC Executions

Context	Local PC	HPC
Sequential	$T_1(\text{local}) = 100$	$T_1(\text{hpc}) = \text{120s}$
Parallel/Distributed	$T_2(\text{local}) = 70\text{s}$	$T_2(\text{hpc}) = 80\text{s}$ $T_8(\text{hpc}) = \text{60s}$

Local vs. HPC Executions

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- **Sequential** runs **WON'T BE FASTER** on HPC
 - Reason: Processor Frequency (typically $\geq 3\text{GHz}$ vs $\geq 2\text{GHz}$)

Local vs. HPC Executions

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- **Sequential** runs **WON'T BE FASTER** on HPC
 - ↪ Reason: Processor Frequency (typically $\geq 3\text{GHz}$ vs $\geq 2\text{GHz}$)
- **Parallel/Distributed** runs **DO NOT COME FOR FREE**
 - ↪ runs **will be sequential** even if you reserve ≥ 2 cores/nodes
 - ↪ you have to **explicitly** adapt your jobs to benefit from the multi-cores/nodes

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High Performance Computing @ UL

HPC @ Uni.lu

Chaos, Gaia, Nyx and Granduc clusters

Get Updates:

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Welcome to the HPC @ Uni.lu platform !

This is the official website of HPC @ Uni.lu platform, which assemble information about the computing clusters operated by the University of Luxembourg and the organization running them.

The country that out-computes will be the one that out-competes.
— The Council on Competitiveness

This picture corresponds to the server room in the LCSD building @ Belval, hosting the **Gata** cluster. The violet lights come from the Nascent disk enclosures.

Featured Systems
We currently operate a total of 494 computing nodes (540 cores, 90,199 CPU [T]cores) and a shared storage capacity of 4919.4 TB (+ 1916 TB for backup).

Platform Status
Several tools report in live the current status of our systems. Check them out!

Latest News
Get the latest news & advertisements linked to the UL HPC platform in this page.

Recent Posts

- HPC Platform DevTools Army Kravas Tools for the researcher
- Optimizing performance on the Lustre Filesystem
- UL HPC Storage System
- IP2S-HPC R&D Project Released
- UL HPC storage infrastructure upgrade
- HPC as part of the UL Digital Strategy

Github Repos

doftiles qualif tutorials ...

Tweets by [@ulhpc](#)

ulHPC Retweeted [Sébastien Varette](#) (svariete)
Remember to register now for IEEE #CloudCom2016! [https://cloudcom16.github.io/submitting.html...](#) #CloudCom_16 #Belval_LU

ulHPC Retweeted [Sébastien Varette](#) (svariete)
Help us to get your requirements for the next generation UL HPC platform! Contact us to access the UL HPC User Survey

ulHPC Retweeted [Sébastien Varette](#) (svariete)
1 week to go until the submission deadline of IEEE #CloudCom2016! [2016.cloudcom.org](#)

ulHPC Retweeted [Sébastien Varette](#) (svariete)
Today I gave a seminar IT/DevOps/Army Kravas

<http://hpc.uni.lu>

Key numbers

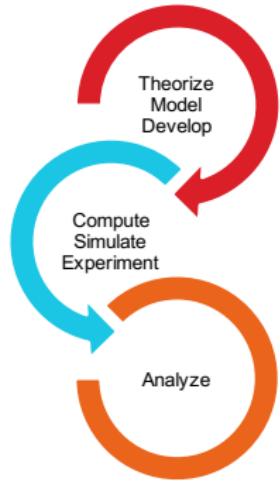
- 416 users
- 110 servers
- 594 nodes
 - 8228 cores
 - **198.172 TFlops**
 - 50 accelerators
 - (+ **76.22 TFlops**)
- **6856.4 TB**
- 5 sysadmins
- 2 sites
 - Kirchberg
 - Belval

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**
 - **BigData analytics & data driven science**: large memory systems
 - ✓ Large SMP systems with 1, 2, 3 & 4 TB RAM
 - **Scale-out workloads**: energy efficient systems
 - ✓ 90 HP Moonshot servers + 96 viridis ARM-based systems

Accelerating UL Research



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

- >140 software packages available for researchers
 - ↪ General purpose, statistics, optimization:
 - ✓ Matlab, Mathematica, R, Stata, CPLEX, Gurobi Optimizer...
 - ↪ Bioinformatics
 - ✓ BioPython, STAR, TopHat, Bowtie, mpiHMMER...
 - ↪ Computer aided engineering:
 - ✓ ANSYS, ABAQUS, OpenFOAM...
 - ↪ Molecular dynamics:
 - ✓ NAMD, ABINIT, Q.ESPRESSO, GROMACS...
 - ↪ Visualisation: ParaView, VisIt, VMD, XCS portal
 - ↪ Compilers, libraries, performance modeling tools
 - ↪ [Parallel] debugging tools aiding development

UL HPC Team



Prof. Pascal Bouvry

Director of DS-CSCE, Leader of PCO Group
Senior advisor for the president as regards the HPC strategy



Sébastien Varrette, PhD

CDI, Research Scientist (CSC, FSTC)



Valentin Plugaru, MSc.

CDI, Research Associate (CSC, FSTC)



Sarah Peter, MSc.

CDD, Research Associate (LCSB)



Hyacinthe Cartiaux

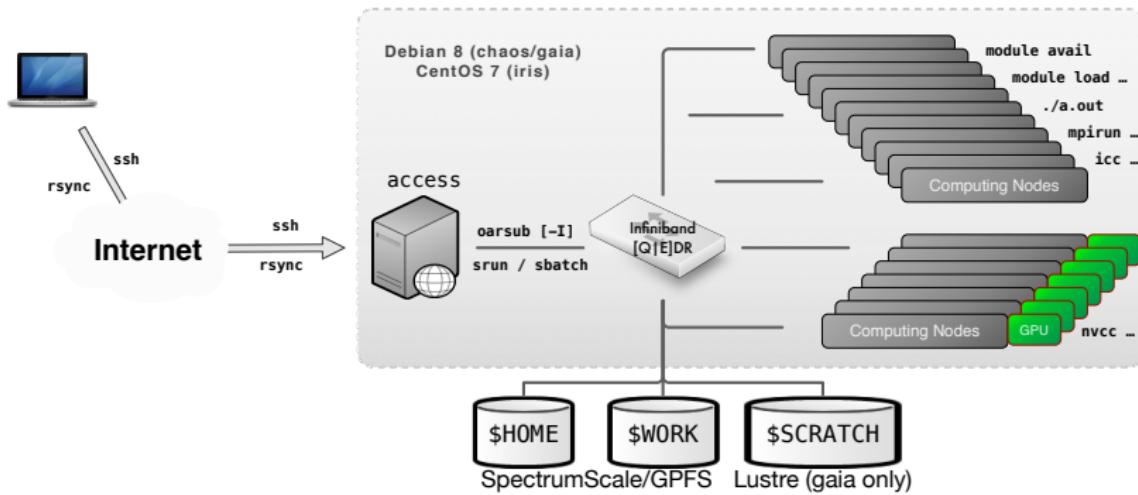
CDI, Support (SIU)



Clément Parisot

CDI, Support (CSC, FSTC)

UL HPC: General cluster organization



Software/Modules Management

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

- Based on Environment Modules / LMod
 - ↪ convenient way to dynamically change the users' environment \$PATH
 - ↪ permits to easily load software through module command
- Currently on UL HPC:
 - ↪ > **140 software packages**, in *multiple* versions, within **18 categ.**
 - ↪ reworked software set for iris cluster and now deployed everywhere
 - ✓ RESIF v2.0, allowing [real] semantic versioning of released builds
 - ↪ hierarchical organization Ex: toolchain/{foss,intel}

```
$> module avail                                                          # List available modules
```

```
$> module load <category>/<software>[/<version>]
```

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Hands-on

Tutorial

<https://github.com/sarah-peter/hpc-tutorial>

Questions?

<http://hpc.uni.lu>



Sarah Peter & The UL HPC Team

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mail: hpc-sysadmins@uni.lu

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