UL HPC School 2017

PS2: HPC workflow with sequential jobs (test cases on GROMACS, Java and Python)

UL High Performance Computing (HPC) Team

H. Cartiaux

University of Luxembourg (UL), Luxembourg

http://hpc.uni.lu

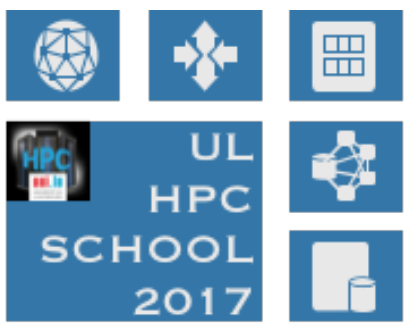
Latest versions available on Github:

UL HPC tutorials: https://github.com/ULHPC/tutorials

UL HPC School: http://hpc.uni.lu/hpc-school/

PS2 tutorial sources:

http://ulhpc-tutorials.readthedocs.io/en/latest/basic/sequential_jobs/



Summary

1 Introduction

2 Pre-requisites

3 Exercise 1: Parametric execution of Gromacs

4 Exercise 2: Watermarking images in Python

5 Exercise 3: Advanced use case, using a Java program: "JCell"

6 Conclusion

Main Objectives of this Session

- Run sequential, parametric programs on the clusters
- Learn how-to use our set of launcher scripts
- Submit jobs
- use the cluster monitoring tools
  - ↪ Ganglia
  - ↪ Monika & Drawgantt

Read the full subject of this PS here

- http://git.io/5cYmPw

Summary

1 Introduction

2 Pre-requisites

3 Exercise 1: Parametric execution of Gromacs

4 Exercise 2: Watermarking images in Python

5 Exercise 3: Advanced use case, using a Java program: "JCell"

6 Conclusion

Getting started

1. Connect to the cluster(s)

```
(laptop)$> ssh {iris,gaia,chaos}-cluster
```

2. Send files

```
(laptop)$> rsync -avz local_directory {iris,gaia,chaos}-cluster:
```

3. Retrieve files

```
(laptop)$> rsync -avz {iris,gaia,chaos}-cluster:path/to/files
local_directory
```

4. Submit jobs

OAR on Chaos/Gaia	Slurm on Iris
oarsub -I	srun -p interactive –qos qos-interactive –pty bash
oarsub ./program	sbatch program

Tutorial link

This tutorial is available on github !

- https://git.io/vHyh3

Summary

1 Introduction

2 Pre-requisites

3 **Exercise 1: Parametric execution of Gromacs**

4 Exercise 2: Watermarking images in Python

5 Exercise 3: Advanced use case, using a Java program: "JCell"

6 Conclusion

Gromacs

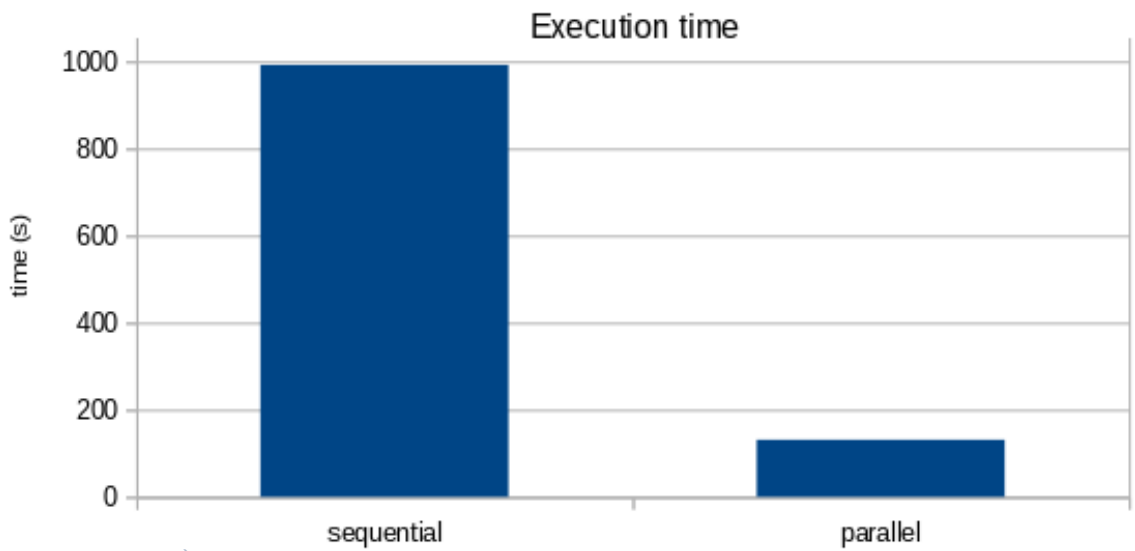
GROMACS: GROningen MAchine for Chemical Simulations
versatile package for molecular dynamics, primarily designed for biochemical molecules

- very large codebase: 1.836.917 SLOC
- many applications in the package, several parallelization modes
- **mdrun**: computational chemistry engine, performing:
  - ↪ molecular dynamics simulations
  - ↪ Brownian Dynamics, Langevin Dynamics
  - ↪ Conjugate Gradient
  - ↪ L-BFGS
  - ↪ Steepest Descents energy minimization
  - ↪ Normal Mode Analysis
- **mdrun** - parallelized using MPI, OpenMP, pthreads and with support for GPU acceleration

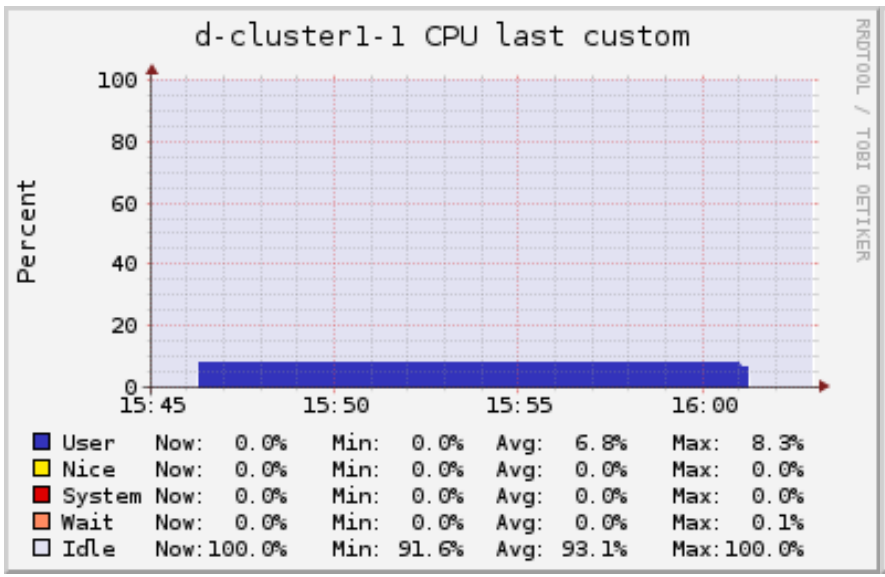
Comparison

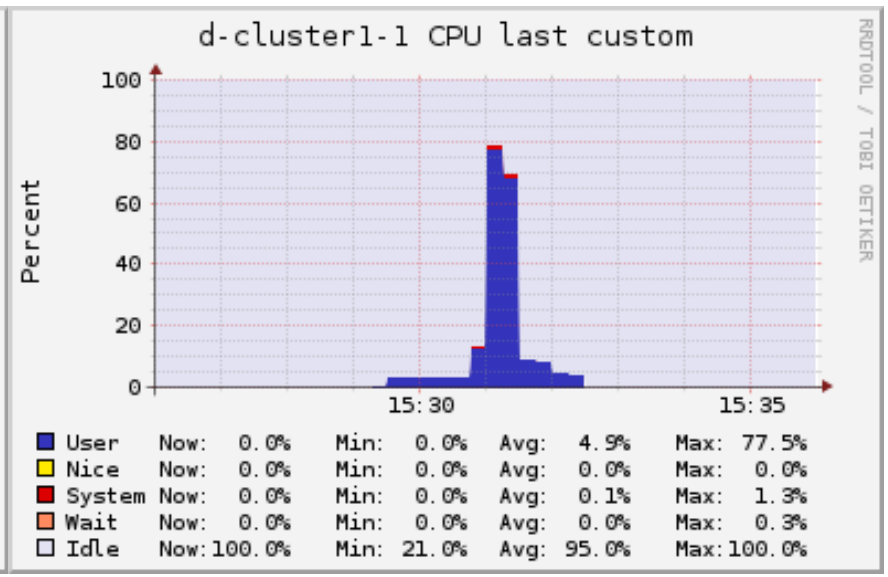
2 approaches

- Sequential (loop)
- Parallized (with GNU parallel)



Comparison - Ganglia





Summary

1 Introduction

2 Pre-requisites

3 Exercise 1: Parametric execution of Gromacs

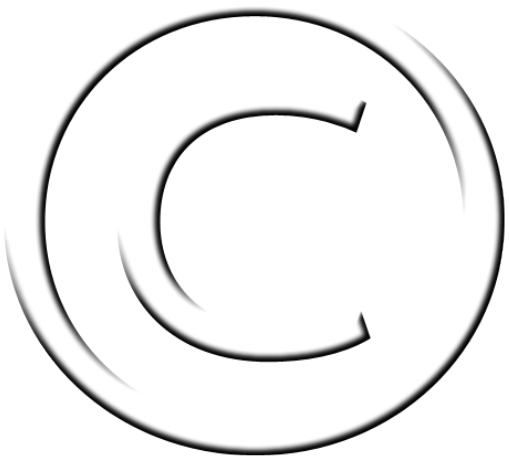
4 **Exercise 2: Watermarking images in Python**

5 Exercise 3: Advanced use case, using a Java program: "JCell"

6 Conclusion

Apply a watermark to a given set of pictures

- Simple Python script
- Generic parallel launcher
- Distribute the work on several nodes



Source image

Watermarked image

Summary

1 Introduction

2 Pre-requisites

3 Exercise 1: Parametric execution of Gromacs

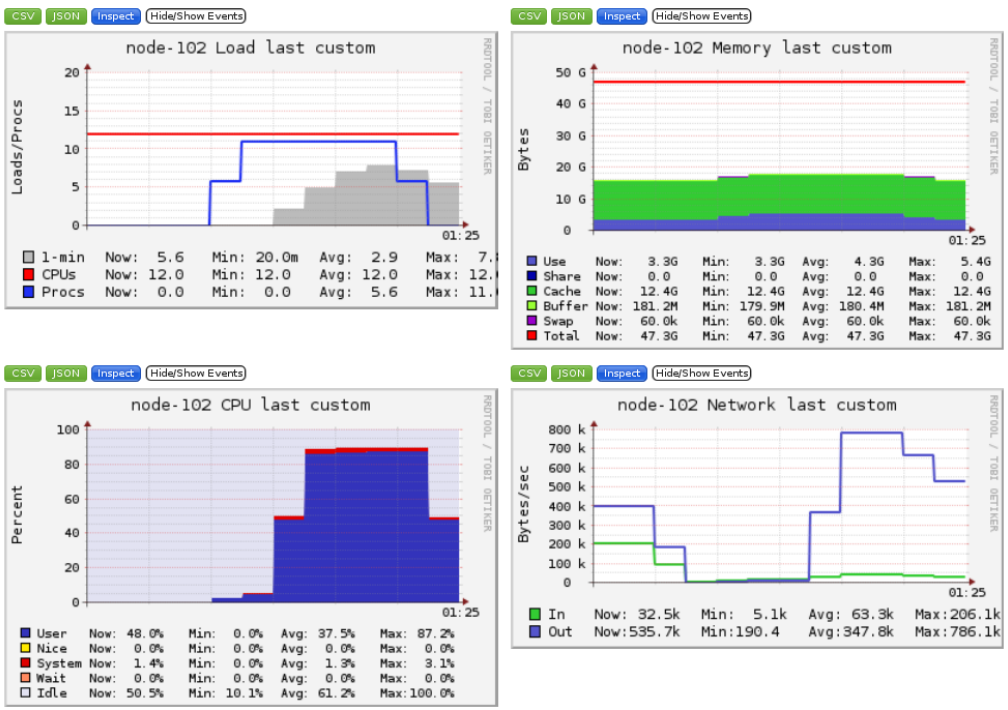
4 Exercise 2: Watermarking images in Python

5 **Exercise 3: Advanced use case, using a Java program: "JCell"**

6 Conclusion

Jcell

- **JCell**: a Java framework for working with genetic algorithms
- Example: Generational algorithm for the Combinatorial ECC problem
- Test the variations of these parameters: *Mutation probability* and *Crossover probability*



Summary

1 Introduction

2 Pre-requisites

3 Exercise 1: Parametric execution of Gromacs

4 Exercise 2: Watermarking images in Python

5 Exercise 3: Advanced use case, using a Java program: "JCell"

6 Conclusion

Conclusion

- We have covered one of the most common workflow:
  - ↪ **parametric jobs**
- Our launchers can be improved!

Perspectives

- Array jobs
- Best effort jobs
- Checkpoint/Restart mechanism

Questions?

http://hpc.uni.lu

The UL High Performance Computing (HPC) Team
University of Luxembourg, Belval Campus:
Maison du Nombre, 4th floor
2, avenue de l'Université
L-4365 Esch-sur-Alzette
mail: hpc@uni.lu

1 **Introduction**
2 **Pre-requisites**
3 **Exercise 1: Parametric execution of Gromacs**
4 **Exercise 2: Watermarking images in Python**
5 **Exercise 3: Advanced use case, using a Java program: "JCell"**
6 **Conclusion**