Uni.lu HPC School 2021

PS4: HPC Management of Sequential and Embarrassingly Parallel Jobs

Uni.lu High Performance Computing (HPC) Team

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Latest versions available on Github:

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

UL HPC School: hpc.uni.lu/education/hpcschool

PS4 tutorial sources: ulhpc-tutorials.rtfd.io/en/latest/sequential/basics

Summary

Main Objectives of this Session

- Understanding the **jobs and tasks concepts**
- Recognizing **embarrassingly parallel tasks**
  - ↪ Understanding scheduling challenges induced by their execution even on an HPC facility
- Guidelines to the **optimized** design of HPC job campaign in such case
  - ↪ prepare `run_*` task script
  - ↪ `launcher.*` **design** for tasklist management, exploiting Slurm & HW characteristics
  - ↪ **interactive** tests and performance analysis
  - ↪ **passive runs** and speedup analysis compared to seq. executions **up to 92% improvement**
- Discovering GNU Parallel
  - ↪ usage and exploitation of ULHPC Generic launcher for GNU parallel

Test Case for the session

- Sample "Stress Me!" parameter exploration job campaign
  - ↪ `run_stressme <N>` imposes configurable amount of *stress* on 1 core for `<N>` seconds

Jobs, Tasks & Local Execution

```
$> ./myprog
```

Jobs, Tasks & Local Execution

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Jobs, Tasks & Local Execution

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

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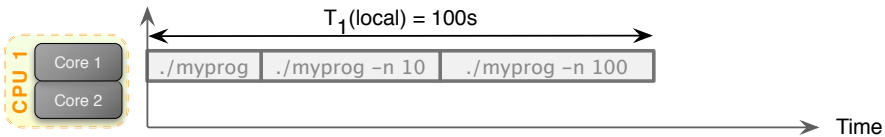


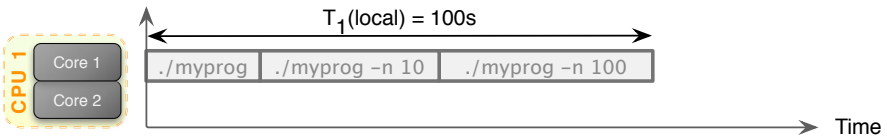
Jobs, Tasks & Local Execution

Job(s)

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

3

Task(s) 3



Jobs, Tasks & Local Execution

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# launcher

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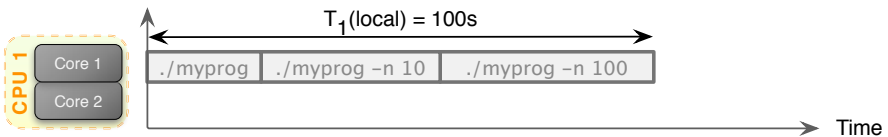

Jobs, Tasks & Local Execution

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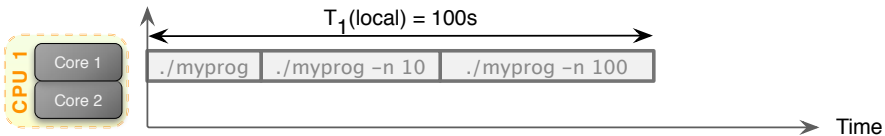
Job(s) 1

Task(s) 3



Jobs, Tasks & Local Execution

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Jobs, Tasks & Local Execution

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# launcher2
"Run in //:"
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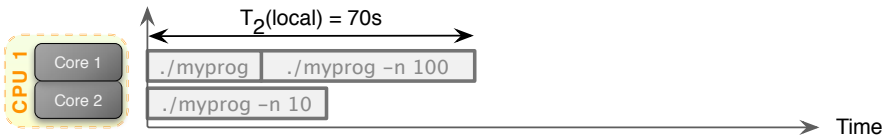

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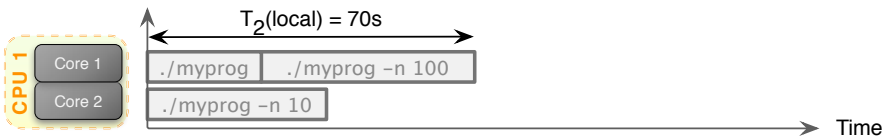

Jobs, Tasks & HPC Execution

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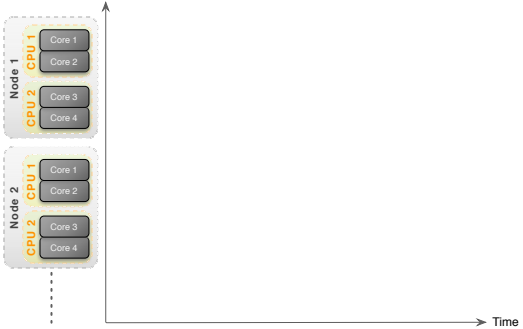

- **Note**: Simplified example! in practice:
  - ↪ `iris` nodes (28c): 2 CPUs of 14 cores each
  - ↪ `aion` nodes (128c): (virtual) 8 CPUs of 16 cores each

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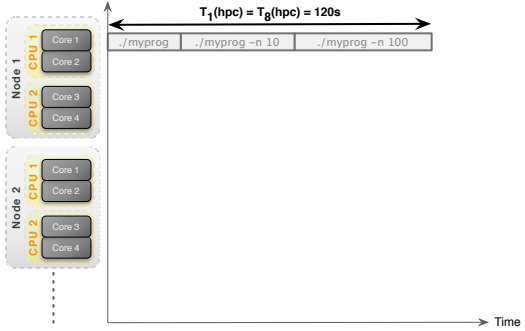

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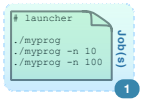

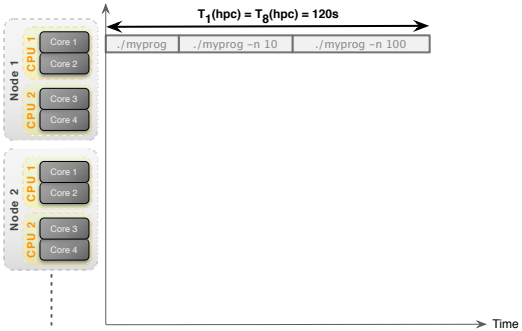

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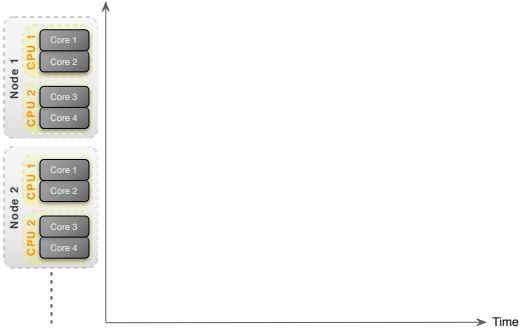

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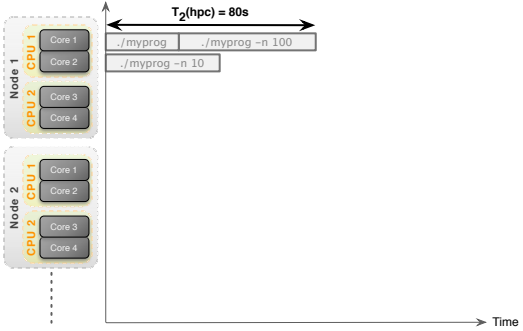

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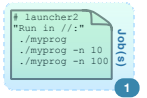

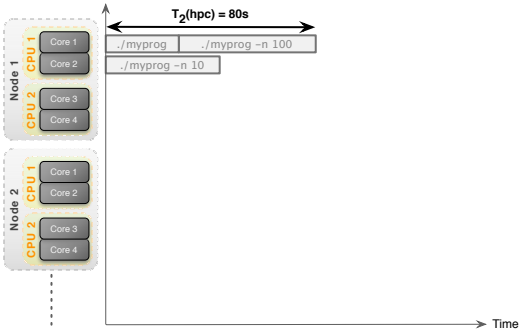

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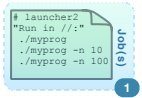

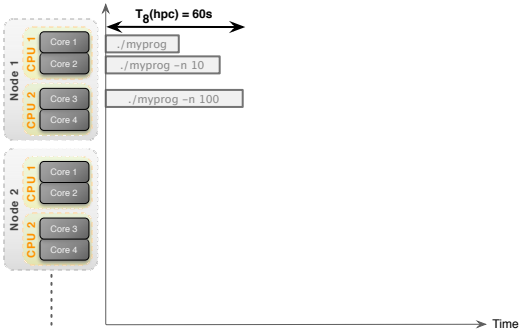

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Local vs. HPC Executions

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

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

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

- **Parallel/Distributed** runs **DO NOT COME FOR FREE**
  - ↪ runs **will be sequential** even if you reserve $\geq$ 2 cores/nodes
  - ↪ you have to **explicitly** adapt your jobs to benefit from the multi-cores/nodes

Serial Task script Launcher

```
#!/bin/bash -l      # <--- DO NOT FORGET '-l'
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH -c 1
#SBATCH --time=0-01:00:00
#SBATCH -p batch
print_error_and_exit() { echo "***ERROR*** $*"; exit 1; }
module purge || print_error_and_exit "No 'module' command"
# C/C++: module load toolchain/intel # OR: module load toolchain/foss
# Java:  module load lang/Java/1.8
# Ruby/Perl/Rust...:  module load lang/{Ruby,Perl,Rust...}
# /!\ ADAPT TASK variable accordingly - absolute path to the (serial) task to be executed
TASK=${TASK:=${HOME}/bin/app.exe}
OPTS=$*

${TASK} ${OPTS}
```

Serial Python Slurm Launcher

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH -c 1
#SBATCH --time=0-01:00:00
#SBATCH -p batch
print_error_and_exit() { echo "***ERROR*** $*"; exit 1; }
module purge || print_error_and_exit "No 'module' command"
# Python 3.X by default (also on system)
module load lang/Python
# module load lang/SciPy-bundle
# and/or: activate the virtualenv <name> you previously generated with
#     python -m venv <name>
source ./<name>/bin/activate

python [...]
```

R Slurm Launcher

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH -c 28
#SBATCH --time=0-01:00:00
#SBATCH -p batch

print_error_and_exit() { echo "***ERROR*** $*"; exit 1; }
module purge || print_error_and_exit "No 'module' command"
module load lang/R
export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK:-1}

Rscript <script>.R  |& tee job_${SLURM_JOB_NAME}.out
```

MATLAB Slurm Launcher

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH -c 28
#SBATCH --time=0-01:00:00
#SBATCH -p batch

print_error_and_exit() { echo "***ERROR*** $*"; exit 1; }
module purge || print_error_and_exit "No 'module' command"
module load base/MATLAB

matlab -nodisplay -nosplash < INPUTFILE.m > OUTPUTFILE.out
```

Summary

Sample "Stress Me!" parameter exploration

Your Turn!

Hands-on Pre-requisites

▶ url ◀ | github | src

- Access to ULHPC facility `ssh`
- (*eventually*) Open Tmux session (Aion/Iris) `~/.tmux.conf`, `tmux new -s <name>`
  ↪ OR (*eventually*) Open GNU Screen (Iris) `~/.screenrc`, `screen -S <name>`
- Clone/Pull `ULHPC/tutorials` repository `~/git/github.com/ULHPC/tutorials`
- Prepare dedicated directory `~/tutorials/sequential` for this session

```
(access)$> mkdir -p ~/tutorials/sequential
(access)$> cd ~/tutorials/sequential
# create a symbolic link to the reference material
(access)$> ln -s ~/git/github.com/ULHPC/tutorials/sequential/basics ref.d
```

Sample “Stress Me!” parameter exploration

- **Objective**: mimic (integer) parameter exploration in $[1 \dots N]$ for serial (1-core) tasks
  - ↪ each task last different amount time (here ranging ranging from 1 to n seconds)
  - ↪ see `scripts/run_stressme`
    - ✓ stress-based workload generator that imposes a configurable amount of stress on the system

```
./scripts/run_stressme -h
NAME
  run_stressme: A sample workload generator that imposes a stress on the
     computing node using the 'stress' command.
USAGE
  ./scripts/run_stressme [-n] [N]:  run serial stress during N second (Default: 20)
OPTIONS
  -n --noop --dry-run:      Dry run mode
```

Sample “Stress Me!” parameter exploration

N=#tasks	Expected Seq. time (T_1)	Optimal time (T_∞)
1	1s	1s
10	55s (~1 min)	10s
30 (default)	**465s (7 min 45s)**	**30s**
100	5050s (1h 24 min 10s)	100s

Hands-on: Single task run (interactive)

► url ◄ | github | src

- Get an interactive job — `si`
- Open another terminal (or another screen tab/windows)
  - ↪ connect to your running job — `sjoin <JOBID>`
  - ↪ monitor it's load with `htop` — `htop`
- Execute `run_stressme` tasks for various parameters
  - ↪ monitor its effect on second window in `htop`

Sample "Stress Me!" parameter exploration

Hands-on: A First launcher (1 job, 1 task on one core)

▶ url ◀ | github | src

- Copy and adapt ULHPC Generic serial launcher `launcher.stressme-serial.sh`
- Get an **interactive** job `si`
  - ↪ dry-run vs real execution
- Test **passive** job execution `sbatch`

Sample "Stress Me!" parameter exploration

- Previous approach works but will **induces an non-necessary overload of the scheduler** when scaling the number of tasks (Ex: job campaign to 1000 or 10000 test cases)
  - ↪ **To complete `N` (serial) tasks, you need to submit `N` jobs**
    - ✓ **DO NOT make a for loop!!!**: better efficient alternatives **MUST** be used
    - ✓ You will likely wait (sometimes very long time) to have all your jobs completed
  - ↪ Node coverage is sub-optimal
    - ✓ **your serial jobs can be spread on up to N different nodes**
  - ↪ Very often (90% of the cases), your serial tasks are short-lived (couple of seconds)
    - ✓ You loose more time to schedule jobs than actually running them

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- You **SHOULD** restrict to 1 node **YET** exploit at best the many cores available
  - ↪ Recall: 128 cores per Aion nodes, 28 cores per Iris nodes
  - ↪ Make 1 jobs (for a full nodes) and use it to schedule **inside** your tasks
    - ✓ From scheduler point of view: **only 1 job to schedule** (faster)
    - ✓ **Efficient**: exploit at best the available cores

Embarrassingly Parallel Jobs

(1 node, 1 job, #cores tasks per node)

- **VERY BAD / To avoid**: **Fork [bomb]** `for` **loop of** `sbatch/srun`
  - ↪ (**dangerous**) ampersand & to spawns the command in the background
  - ↪ optimize `wait` synchronization barrier YET prefer GNU Parallel

```
TASK=run_stressme
ncores=${SLURM_NTASKS_PER_NODE:-$(nproc --all)}  # Number of cores per node
for i in {1..1000}; do   # DON'T DO THAT - just to illustrate
    srun -n1 --exclusive -c 1 --cpu-bind=cores ${TASK} $i &  # NO!! Fork 1000 sub-processes
done
wait
```

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for i in {1..1000}; do   # DON'T DO THAT - just to illustrate
    srun -n1 --exclusive -c 1 --cpu-bind=cores ${TASK} $i &
    [[ $((i%ncores)) -eq 0 ]] && wait     # Better but suboptimal
done
wait
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- **BAD / To avoid**: Job arrays `sbatch --array 1-1000%128 [...]`
  - ↪ in all cases, job array capabilities are drastically reduced (on purpose)
    - ✓ `scontrol show config | grep -i maxarray`

Job Array Variable	Description
`$SLURM_ARRAY_JOB_ID`	first job ID of the array
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```
${TASK} ${SLURM_ARRAY_TASK_ID} # Simpler syntax YET induce same (worse) load on scheduler
```

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- **Always prefer GNU Parallel for Embarrassingly Parallel Serial Tasks!**
  - ↪ **Good, efficient and Optimized**
  - ↪ Transparent through the provided ULHPC launcher

Summary

GNU Parallel

- A shell tool to execute **independent** tasks in parallel using one or more nodes
  - ↪ A task can be a single command or script
- Typical input could be a list of files, a list of parameters
  - ↪ Recall that in bash, `"{1..10}"` is expanded to `"1 2 3 4 5 6 7 8 9 10"`

Hands-on: GNU Parallel Build and Installation

▶ url ◀ | github | src

- Setup your HOME to support GNU Stow installation
  - ↪ GNU Stow manual - tutorial
- Download, build and install `parallel`
- Use stow to enable/disable the installed version `stow [-D]`

On `stow -D`, you can ignore the '`BUG in find_stowed_path?`' message due to recent Issues #65

GNU Parallel Syntax

GNU Parallel syntax can be a little distributing, but basically it supports two modes:

1. Reading command arguments **on the command line**:

```
parallel    [-j N] [OPTIONS]    COMMAND {} ::: TASKLIST
```

2. Reading command arguments **from an input file**:

```
parallel    -a  TASKLIST.LST    [-j N] [OPTIONS]    COMMAND {}
parallel    [-j N] [OPTIONS]    COMMAND {} :::: TASKLIST.LST
```

- **Tips & Tricks**:
  - ↪ If your COMMAND embed a pipe stage, you have to escape the pipe symbol as follows \|
  - ↪ **ALWAYS** `echo` your commands until you're satisfied

GNU Parallel Syntax

Hands-on: Discovering the parallel command ▶ url ◀ | github | src

- play with a TASKLIST from the command line
- play now with a TASKLIST from an input file.

GNU Parallel Syntax

```
# Default string {}   --> path/to/filename.ext
parallel echo {} :::  path/to/filename.ext
# Remove extension {.} --> path/to/filename
parallel echo {.} ::: path/to/filename.ext
# Remove path {/}      --> filename.ext
parallel echo {/} ::: path/to/filename.ext
# Remove path and extension {/.} --> filename
parallel echo {/.} ::: path/to/filename.ext
# Change extension and path  --> output/filename.out
parallel echo output/{/.}.out ::: path/to/filename.ext
```

Back to "Stress Me!" parameter exploration

Hands-on: Best launcher based on GNU Parallel

▶ url ◀ | github | src

- Copy and adapt ULHPC Generic GNU Parallel launcher
  - ↪ `launcher.stressme.${ULHPC_CLUSTER}.sh`
  - ↪ only difference optimized default `--ntasks-per-node` for aion/iris
  - ↪ convenient symlink `launcher.stressme.sh`
- Get an **exclusive** **interactive** job `si --exclusive`
  - ↪ dry-run vs test vs real execution
- Test **passive** job execution `sbatch`
- Embarrassingly [GNU] parallel tasks across multiples nodes
  - ↪ Concepts and Safeguards
  - ↪ Slurm dependency mechanism `--dependency=singleton`
  - ↪ sample submission script `scripts/submit_stressme_multinode`

Back to "Stress Me!" parameter exploration

```
(access)$> ./scripts/submit_stressme_multinode -h
Usage: submit_stressme_multinode [-x] [-N MAXNODES]
    Sample submision script across multiple nodes
    Execution won t spread on more than 4 nodes (singleton dependency)
      -x --execute         really submit the jobs with sbatch
      -N --nodes MAXNODES  set max. nodes
# Target restriction to 2 running nodes max
(access)$> ./scripts/submit_stressme_multinode -N 2
(access)$> ./scripts/submit_stressme_multinode -N 2 -x
# squeue -u $(whoami)
   JOBID PARTIT    QOS        NAME  NODE  CPUS ST  TIME TIME_LEFT NODELIST(REASON)
 2175780  batch normal  StressMe_0     1    28 PD  0:00   1:00:00 (Dependency)
 2175781  batch normal  StressMe_1     1    28 PD  0:00   1:00:00 (Dependency)
 2175782  batch normal  StressMe_0     1    28 PD  0:00   1:00:00 (Dependency)
 2175779  batch normal  StressMe_1     1    28  R  0:02     59:58 iris-064
 2175778  batch normal  StressMe_0     1    28  R  0:05     59:55 iris-047
```

Thank you for your attention...

Questions?

ulhpc-tutorials.rtfd.io/en/latest/sequential/basics

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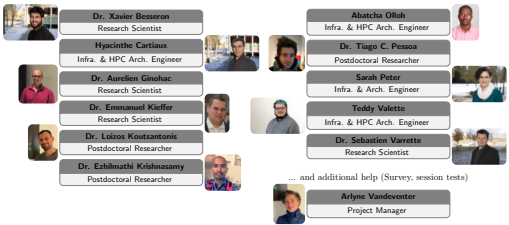

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