Introduction to GNU Parallel - Parallelizing Massive Individual Tasks

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Outline

➢ When and Why to use GNU Parallel?
  – Situations to use it, e.g. 1 million small MD simulations, 10k protein analysis

➢ Basic Usage of GNU Parallel
  – GNU Parallel Syntax and Options
  – Introducing Running 3 Types of jobs using GNU Parallel:
    o Serial Tasks
      ✓ Run each LAMMPS task in serial
    o Multi-Threaded Tasks
      ✓ Run each LAMMPS task using multiple threads
    o Small MPI Jobs
      ✓ Run each LAMMPS task using multiple MPI processes

➢ Proper usage of GNU Parallel
  – Memory consideration
  – Task granularity
What do we want to accomplish?

- Parallize lots of small independent tasks on a multi-core platform (compute nodes)
Background and Distribute

Node 0

Node 1

Core 0

Task 0

Core 1

Task 1

Core 2

Task 2

Core 3

Task 3

Core 0

Task 4

Core 1

Task 5

Core 2

Task 6

Core 3

Task 7
The von Neumann Architecture

Central Processing Unit
- Control Unit
- Arithmetic Logic Unit
- Cache

Core

Input Device

Output Device

Main Memory (code/data)
Changing Times

➢ From 1986 - 2002, microprocessors were speeding like a rocket, increasing in performance an average of 50% per year.
➢ Since then, it’s dropped to about 20% increase per year.

History of Processor Performance

Limitation:
2 GHz Consumer
4 GHz Server

Source:
http://www.cs.columbia.edu/~sedwards/classes/2012/3827-spring/
A Little Physics Problem

- Smaller transistors = faster processors.
- Faster processors = increased power consumption.
- Increased power consumption = increased heat.
- Increased heat = unreliable processors.

Solution:
- Move away from single-core systems to multicore processors.
- “core” = central processing unit (CPU)
- Introducing parallelism
  - What if your problem is also not CPU dominant?
The von Neumann Architecture

Around year 2005

CPU
  core
  cache

CC-interconnect
  Cache

Main Memory
  (code/data)

I/O

Introduction to GNU Parallel
GNU Parallel

- GNU parallel is a shell tool for executing “embarrassingly parallel” tasks using one or more computers (compute nodes).

- Terminology:
  - Task: Each small, independent piece of computation work to be finished, e.g., a single genome computation, a single MD simulation
  - Job: The list of tasks to be completed on a set of nodes (cores)

- A task can be a single command or a small script that must be run for each of the lines in the input.

- The typical input is a list of files, a list of hosts, a list of users, a list of URLs, or a list of tables.

- See more at: https://www.gnu.org/software/parallel/
Introduction to GNU Parallel

GNU Parallel Syntax
Adding GNU Parallel to Environment

➢ On SuperMike3:

[fchen14@mike139 ~]$ module av parallel
---- /usr/local/packages/Modules/default/modulefiles/linux-rhel8-icelake ----
parallel-netcdf/1.12.2/intel-2021.5.0
parallel/20210922/intel-2021.5.0
parallel-netcdf/1.12.2/intel-2021.5.0-intel-mpi-2021.5.1
# load the module to environment
[fchen14@mike139 ~]$ module load parallel/20210922/intel-2021.5.0
[fchen14@mike139 ~]$ which parallel
/usr/local/packages/parallel/20210922/hrsviur/bin/parallel
[fchen14@mike139 ~]$ parallel -version # check GNU parallel version
GNU parallel 20210922
Copyright (C) 2007-2021 Ole Tange, http://ole.tange.dk and Free Software Foundation, Inc.
...

➢ Or add the below line to ~/.modules:

module load parallel/20210922/intel-2021.5.0
GNU Parallel Syntax

➢ Reading commands to be run in parallel from an input file:
  parallel [OPTIONS] < CMDFILE

➢ Reading command arguments on the command line:
  parallel [OPTIONS] COMMAND [ARGUMENTS] :::: ARGLIST

➢ Reading command arguments from an input file:
  parallel [OPTIONS] COMMAND [ARGUMENTS] :::::: ARGFILE
ARGLIST from command line

- `parallel [OPTIONS] COMMAND [ARGUMENTS] :: ARGLIST`

- **Examples:**
  ```
  [fchen14@mike139 ~]$ parallel echo ::: A B C
  A
  B
  C
  [fchen14@mike139 ~]$ parallel echo ::: `seq 1 3`
  1
  2
  3
  [fchen14@mike139 ~]$ parallel echo ::: {A..Z}
  A
  B
  ...
  Z
  [fchen14@mike139 test]$ ls -l | parallel echo
  2013-06-18.tgz
  backups.sh
  bigmem_test.pbs
  ...
  ```
**ARGLIST from file**

- `parallel [OPTIONS] COMMAND [ARGUMENTS] :::: ARGFILE`

[fchen14@mike139 GNU_PARALLEL]$ `pwd`
```
/project/fchen14/GNU_PARALLEL
```
[fchen14@mike139 GNU_PARALLEL]$ `cat input.lst | head`
```
01.lj
02.lj
03.lj
...
```
[fchen14@mike139 GNU_PARALLEL]$ `head input.lst -n 5 | parallel echo`
```
01.lj
02.lj
03.lj
04.lj
05.lj
```
[fchen14@mike139 GNU_PARALLEL]$ `parallel echo :::: input.lst`
```
01.lj
02.lj
...
```
Replacement Strings

➢ ‘{}’ returns a full line read from the input source.
[fchen14@mike139 GNU_PARALLEL]$ parallel echo {} :::: data/in.lj
data/in.lj

➢ ‘{/}’ removes everything up to and including the last forward slash:
[fchen14@mike139 GNU_PARALLEL]$ parallel echo {/} :::: data/in.lj
in.lj

➢ ‘{///}’ returns the directory name of input line.
[fchen14@mike139 GNU_PARALLEL]$ parallel echo {///} :::: data/in.lj
data

➢ ‘{.}’ removes any filename extension:
[fchen14@mike139 GNU_PARALLEL]$ parallel echo {.} :::: data/in.lj
data/in

➢ ‘{/.}’ returns the basename of the input line without extension. It is a combination of {/} and {.}:
[fchen14@mike139 GNU_PARALLEL]$ parallel echo {/.} :::: data/in.lj
in

➢ See “man parallel” for more detailed explanation.
Replacement String Example

- Print the full path of the input file, and then print the desired output file name, e.g.:
  - Input file: data/lj.in
  - Output file name: output/lj.out

# Process data/lj.in and send result to output/lj.out
$ parallel echo {} output/{/.}.out :: data/lj.in
data/lj.in output/lj.out
Parallelize Job Script

- GNU parallel is often called as this:
  ```bash
  cat input_file | parallel command
  parallel command ::: foo bar
  ```

- If command is a script, parallel can be combined into a single file so this will run the script in parallel:
  ```bash
  parallel [OPTIONS] script [ARGUMENTS] ::: ARGLIST
  ```
  - or
  ```bash
  parallel [OPTIONS] script [ARGUMENTS] :::: ARGFILE
  ```

- See next slide for example...
Parallize Script Example

➢ This is the script we want to parallize "cmd_ex.sh":

```bash
#!/bin/bash
# print the input, on which host, which working directory
echo "This script uses input: $1 on $HOSTNAME:$PWD"
```

➢ Parallize the script using **ARGLIST** from command line:

```
[fchen14@mike139 GNU_PARALLEL]$ parallel --wd $PWD ./cmd_ex.sh ::: A B C
This script uses input: A on mike139:/project/fchen14/GNU_PARALLEL
This script uses input: B on mike139:/project/fchen14/GNU_PARALLEL
This script uses input: C on mike139:/project/fchen14/GNU_PARALLEL
```

➢ Parallize the script using **ARGFILE**:

```
[fchen14@mike139 GNU_PARALLEL]$ cat argfile
A
B
C
[fchen14@mike139 GNU_PARALLEL]$ parallel --wd $PWD ./cmd_ex.sh :::: argfile
This script uses input: A on mike139:/project/fchen14/GNU_PARALLEL
This script uses input: B on mike139:/project/fchen14/GNU_PARALLEL
This script uses input: C on mike139:/project/fchen14/GNU_PARALLEL
```

➢ Can parallize Python/Perl scripts, see “man parallel” for details
Common OPTIONS --jobs (-j)

- **--jobs N (-j N)**
  - Number of jobslots on each machine (node). Run up to N jobs in parallel. 0 means as many as possible. Default is 100% which will run one job per CPU core on each machine.
  - On HPC/LONI clusters, N is number of jobslots per node.
  - Make sure you use GNU Parallel version \texttt{>=20161022} to avoid a "Max jobs to run" bug
    
    ```
    [fchen14@mike139 test]$ parallel --version
    GNU parallel 20210922
    ...
    ```

- **-j +N**
  - Add N to the number of CPU cores. Run this many jobs in parallel.

- **-j -N**
  - Subtract N from the number of CPU cores. Run this many jobs in parallel. If the evaluated number is less than 1 then 1 will be used.
Common OPTIONS --slf (PBS)

- **--slf filename** (-sshloginfile filename)
  - File with sshlogins. The file consists of sshlogins on separate lines. Empty lines and lines starting with '#' are ignored.
  - Look at "man parallel" for more detailed explanation.
  - A typical example on PBS clusters while running batch jobs:
    ```bash
    --slf $PBS_NODEFILE
    ```
  - Recall what is inside $PBS_NODEFILE?
    ```bash
    [fchen14@smic139 laplace]$ cat $PBS_NODEFILE # assume we use SuperMIC
    smic139
    smic139
    ...
    smic139
    smic429
    smic429
    ...
    smic429
    ```
    ```bash
    20 repeats (cores)
    on smic139
    ```
    ```bash
    20 repeats (cores)
    on smic429
    ```

---

**Introduction to GNU Parallel**

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Common OPTIONS --slf (Slurm)

- **--slf filename** (**--sshloginfile filename**)
  - To get the sshloginfile on Slurm job session, use the below command:
    
    ```bash
    scontrol show hostname $SLURM_NODELIST > nodefile
    ```
  - A typical example on HPC/LONI clusters while running batch jobs:
    `--slf nodefile`
  - Look at $SLURM_NODELIST and nodefile

    ```bash
    # start an interactive job requesting 2 nodes (64x2=128 cores)
    [fchen14@mike4 ~]$ srun -N2 -n128 -p workq --cpu-bind none --pty bash
    srun: Job is in held state, pending scheduler release
    srun: job 39474 queued and waiting for resources
    Interactive job 39474 waiting:
    srun: job 39474 has been allocated resources
    # we got mike157 and mike158
    [fchen14@mike157 ~]$ echo $SLURM_NODELIST
    mike[157-158]
    [fchen14@mike157 ~]$ scontrol show hostname $SLURM_NODELIST > nodefile
    [fchen14@mike157 ~]$ cat nodefile
    mike157
    mike158
    ```

*Introduction to GNU Parallel*
Common OPTIONS --sshdelay

- If many tasks are started on the same compute node, sshd can be overloaded. On SuperMike3/QB3, some of the tasks might fail to start, e.g., starting all 64/48 tasks at the same time.

- GNU parallel can insert a delay between each task run on the same server:

  ```bash
  [fchen14@mike139 GNU_PARALLEL]$ parallel --sshdelay 0.1 echo ::: A B C
  A
  B
  C
  ```
Common OPTIONS  --wd

- **--wd mydir (--workdir mydir)**
  - Designate the working directory of your commands.
  - A typical value can be:
    - `$PBS_O_WORKDIR` (PBS)
    - `$SLURM_SUBMIT_DIR` (Slurm)
Common OPTIONS --env

- --env ENV_VAR
  - --env to tell GNU parallel to transfer an environment variable to the remote system.
  - A typical usage:
    ```
    export OMP_NUM_THREADS=5
    parallel --env OMP_NUM_THREADS cmd :::: ARGLIST
    ```
Common OPTIONS --progress

- **--progress**
  - Show progress of computations. (*Not recommended for batch jobs*)
  - List the computers involved in the task with number of CPU cores detected and the max number of jobs to run.
  - After that show progress for each node: number of running jobs, number of completed jobs, and percentage of all jobs done by this computer.
  - Example:
    
    ```bash
    [fchen14@mike139 ~]$ parallel --progress echo ::: A B C
    
    Computers / CPU cores / Max jobs to run
    1:local / 64 / 3
    
    Computer:jobs running/jobs completed/%of started jobs/Average seconds to complete
    local:3/0/100%/0.0s A
    local:2/1/100%/1.0s B
    local:1/2/100%/0.5s C
    local:0/3/100%/0.3s
    ```

- See also **--bar**
Common OPTIONS --joblog

➢ **--joblog logfile**
  - Creates a record for each completed subjob (task) to be written to LOGFILE, with info on how long they took, their exit status, etc.
  - Can be used to identify failed jobs, e.g.:

```
[fchen14@mike139 misc]$ parallel --joblog logfile exit :::: 1 2 0 0
[fchen14@mike139 misc]$ cat logfile
```

<table>
<thead>
<tr>
<th>Seq</th>
<th>Host</th>
<th>Starttime</th>
<th>JobRuntime</th>
<th>Send</th>
<th>Receive</th>
<th>Exitval</th>
<th>Signal</th>
<th>Command</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>:</td>
<td>1477514132.358</td>
<td>0.019</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>exit 1</td>
</tr>
<tr>
<td>2</td>
<td>:</td>
<td>1477514132.375</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>exit 2</td>
</tr>
<tr>
<td>3</td>
<td>:</td>
<td>1477514132.376</td>
<td>0.002</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>exit 0</td>
</tr>
<tr>
<td>4</td>
<td>:</td>
<td>1477514132.377</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>exit 0</td>
</tr>
</tbody>
</table>
Common OPTIONS --timeout

- **--timeout secs**
  - Time out for command. If the command runs for longer than secs (seconds) it will get killed.
  - If secs is followed by a % then the timeout will dynamically be computed as a percentage of the median average runtime. Only values > 100% will make sense.

- Useful if you know the command has failed if it runs longer than a threshold.
Introduction to GNU Parallel

Serial Jobs Example
LAMMPS Introduction

- LAMMPS is a classical molecular dynamics code with a focus on materials modeling. [https://www.lammps.org/](https://www.lammps.org/)

- You don’t need any background in molecular dynamics/LAMMPS to understand today’s example.

Typical LAMMPS Syntax

- Serial run
  
  `lmp_serial -in in.script`

- Multi-Threaded run
  
  `env OMP_NUM_THREADS=4 lmp_omp -sf omp -in in.script` # use OMP_NUM_THREADS
  
  `lmp_omp -sf omp -pk omp 5 -in in.script` # use -pk omp to specify threads

- MPI run
  
  `srun --overlap -n 4 lmp_mpi -in in.script` # Slurm version, --overlap only needed for interactive job
  
  `mpirun -n 4 lmp_mpi -in in.script` # PBS version

- Custom command:

  `lmp_serial -var nsteps 200 -in in.script` # we defined a custom variable in the input file to let nsteps control total steps to run,
  
  The above command will run our input for 200 steps
LAMMPS Input File Used Today

# 3d Lennard-Jones melt
variable x index 1
variable y index 1
variable z index 1
variable xx equal 80*$x
variable yy equal 80*$y
variable zz equal 80*$z
units lj
atom_style atomic
lattice fcc 0.8442
region box block 0 ${xx} 0 ${yy} 0 ${zz}
create_box 1 box
create_atoms 1 box
mass 1 1.0
velocity all create 1.44 87287 loop geom
pair_style lj/cut 2.5
pair_coeff 1 1 1.0 1.0 2.5
neighbor 0.3 bin
neighbor_modify delay 0 every 20 check no
fix 1 all nve

# ${nsteps} is the parameter passing from LAMMPS command line "-var nsteps 200"
run ${nsteps}
Distribute Serial Jobs LAMMPS (Slurm)

#!/bin/bash
#SBATCH -N 2 # request two nodes
#SBATCH -n 128 # specify 128 process
#SBATCH -t 2:00:00
#SBATCH -p checkpt
#SBATCH -A hpc_hpcadmin8
#SBATCH -o gp-serial.out

TASKS_PER_NODE=16
SECONDS=0

scontrol show hostname $SLURM_NODELIST > nodefile
parallel --joblog lmp.serial.log \ 
  -j $TASKS_PER_NODE \ 
  --slf nodefile \ 
  --workdir $SLURM_SUBMIT_DIR \ 
  --sshdelay 0.1 \ 
  `which lmp_serial` -in {} -var nsteps 200 ::::: input.lst

echo "took $SECONDS sec"
In case the task command is too long (complex)

➢ Use a script for each task to be distributed, example here (call_lmp.sh)
➢ GNU Parallel will distribute each task script

```bash
TASKS_PER_NODE=16

scontrol show hostname $SLURM_NODELIST > nodefile
parallel --joblog lmp.serial.log \
  -j $TASKS_PER_NODE \
  --slf nodefile \
  --workdir $SLURM_SUBMIT_DIR \
  --sshdelay 0.1 \
  ./call_lmp.sh \{\} 200 :::: input.lst
```

```bash
#!/bin/bash

echo "\$1=$1, \$2=$2"
lmp_serial -in $1 -var nsteps $2
```

$1 is the input from input.lst, e.g. data/01.lj.in

$2 is the input parameter 200
Distribute Serial Jobs LAMMPS (PBS)

```
#!/bin/bash
#PBS -l nodes=2:ppn=20
#PBS -l walltime=1:00:00
#PBS -q checkpt
#PBS -A hpc_hpcadmin8
#PBS -j oe
#PBS -o gp-serial-pbs.out

module load parallel
module load lammps
TASKS_PER_NODE=20
SECONDS=0

cd $PBS_O_WORKDIR
parallel --joblog lmp.serial.log \
  -j $TASKS_PER_NODE \
  --slf $PBS_NODEFILE \
  --workdir $PBS_O_WORKDIR \
  --sshdelay 0.1 \
  `which lmp_mpi` -in {} -var nsteps 200 ::::: input.lst

echo "took $SECONDS sec"
```

[fchen14@smic1 GNU_PARALLEL]$ head input.lst
data/01.lj.in
data/02.lj.in
data/03.lj.in
data/04.lj.in
data/05.lj.in
data/06.lj.in
...

Introduction to GNU Parallel
Multi-Threaded Example
Distribute Multi-Threaded Jobs

➢ Distribute Multi-Threaded jobs is very similar to the pure serial job example, the only difference is `TASKS_PER_NODE`:
  - `TASKS_PER_NODE=CPU_CORES_PER_NODE / NUM_THREADS_PER_TASK`

➢ If each job uses 4 threads, each node on SuperMike3 has 64 cores, then
  - `TASKS_PER_NODE=64/4=16`

➢ **Slurm script (#SBATCH comments omitted):**

```bash
TASKS_PER_NODE=16
export OMP_NUM_THREADS=4
SECONDS=0
scontrol show hostname $SLURM_NODELIST > nodefile
parallel -j $TASKS_PER_NODE \ 
  --slf nodefile \ 
  --workdir $WDIR \ 
  --sshdelay 0.1 \ 
  --env OMP_NUM_THREADS \ 
  `which lmp_omp` -sf omp -in {} -var nsteps 200 ::::: input.lst
echo "took $SECONDS sec"
```

- Put 64/4=16 tasks per node
- Pass the environmental variable OMP_NUM_THREADS to each task
- OpenMP switch in lammps

Introduction to GNU Parallel
Multi-Threaded LAMMPS (Slurm)

#!/bin/bash
#SBATCH -N 2 # request two nodes
#SBATCH -n 128 # specify 128 process
#SBATCH -t 2:00:00
#SBATCH -p checkpt
#SBATCH -A hpc_hpcadmin8
#SBATCH -o gp-omp.out

TASKS_PER_NODE=16
export OMP_NUM_THREADS=4
SECONDS=0
scontrol show hostname $SLURM_NODELIST > nodefile

parallel --joblog lmp.omp.log \
  -j $TASKS_PER_NODE \
  --slf nodefile \
  --workdir $SLURM_SUBMIT_DIR \
  --sshdelay 0.1 \
  --env OMP_NUM_THREADS \
  `which lmp_omp`-sf omp-in {} -var nsteps 200 :::: input.lst

echo "took $SECONDS sec"

This script is on SuperMike3, 64 cores per node, so TASKS_PER_NODE=64/4=16

Use 4 OMP threads per task

OpenMP switch in lammps

Introduction to GNU Parallel
Multi-Threaded LAMMPS (PBS)

#!/bin/bash

#PBS -l nodes=2:ppn=20
#PBS -l walltime=1:00:00
#PBS -q checkpt
#PBS -A hpc_hpcadmin8
#PBS -j oe
#PBS -o gp-omp-pbs.out

module purge
module load parallel
module load lammps

TASKS_PER_NODE=4
SECONDS=0

cd $PBS_O_WORKDIR

parallel --joblog lmp.omp.pbs.log \
  -j $TASKS_PER_NODE \n  --slf $PBS_NODEFILE \n  --workdir $PBS_O_WORKDIR \n  --sshdelay 0.1 \n  `which lmp` -sf omp -pk omp -in {} -var nsteps 200 ::::: input.lst

echo "took $SECONDS sec"

This script is on SuperMIC, 20 cores per node, so TASKS_PER_NODE=20/5=4

Use 5 OpenMP threads per task
Distribute MPI Jobs - LAMMPS

- This section describes how to distribute small MPI jobs.
- Example problem - LAMMPS MPI
  - Using the same input file, but with multiple MPI processes for each task.
  - For simplicity, each MPI process will use only one thread
#!/bin/bash

#SBATCH
-N 2        # request two nodes
-n 128      # specify 128 process
-t 2:00:00  #SBATCH
-p checkpt
-A hpc_hpcadmin8
-o gp-mpi.out

TASKS_PER_NODE=16
PROC_PER_TASK=4
SECONDS=0

scontrol show hostname $SLURM_NODELIST > nodefile

parallel --joblog lmp.mpi.log \
  -j $TASKS_PER_NODE \ 
  --slf nodefile \
  --workdir $SLURM_SUBMIT_DIR \
  --sshdelay 0.1 \ 
  srun --overlap -n $PROC_PER_TASK `which lmp` -in {} -var nsteps 200 \\
  input.lst

echo "took $SECONDS sec"

This script is on SuperMike3, 64 cores per node, so TASKS_PER_NODE=64/4=16

Use 4 MPI processes per task
#! /bin/bash
#PBS -l nodes=2:ppn=20
#PBS -l walltime=1:00:00
#PBS -q checkpt
#PBS -A hpc_hpcadmin8
#PBS -j oe
#PBS -o gp-omp-pbs.out

module purge
module load parallel
module load lammps

TASKS_PER_NODE=4
SECONDS=0

cd $PBS_O_WORKDIR
parallel --joblog lmp.mpi.pbs.log \
  -j $TASKS_PER_NODE \ 
  --slf $PBS_NODEFILE \ 
  --workdir $PBS_O_WORKDIR \ 
  --sshdelay 0.1 \ 
  mpirun -np `which lmp` -in {} -var nsteps 200 :::: input.lst

echo  "took $SECONDS sec"
Proper Usage of GNU Parallel

Introduction to GNU Parallel
Common Rules

➢ Don’t use more than one node when you are debugging/testing your code
➢ Know the performance of single task
➢ Start with only a few tasks in your input.1st
➢ After you are comfortable with one node job, start with two node job first before jumping to more than three nodes
➢ Typically use no more than 5 nodes.
Memory Consideration

- **Relationship between node memory and cores**
  - Rule of Thumb: cannot exceed the available memory on a node

  - **Available node memory 256 GB**
    - **4 GB mem per task,** How many tasks per node?
    - **8 GB mem per task,** How many tasks per node?

  - **Avoid this situation, hard to calculate/predict memory usage**
GNU Parallel spawns the next job when one finishes - keeping the CPUs active and thus saving time.

**Without Load Balancing**

<table>
<thead>
<tr>
<th>Cpu0</th>
<th>Cpu1</th>
<th>Cpu2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Job 1</td>
<td>Job 5</td>
<td>Job 8</td>
</tr>
<tr>
<td>Job 2</td>
<td>Job 6</td>
<td>Job 9</td>
</tr>
<tr>
<td>Job 3</td>
<td>Job 7</td>
<td>Waste</td>
</tr>
<tr>
<td>Job 4</td>
<td>Waste</td>
<td>Waste</td>
</tr>
</tbody>
</table>

**With Load Balancing**

<table>
<thead>
<tr>
<th>Cpu0</th>
<th>Cpu1</th>
<th>Cpu2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Job 1</td>
<td>Job 2</td>
<td>Job 3</td>
</tr>
<tr>
<td>Job 6</td>
<td>Job 5</td>
<td>Job 4</td>
</tr>
<tr>
<td>Job 8</td>
<td>Job 9</td>
<td>Job 7</td>
</tr>
<tr>
<td>Job 10</td>
<td>Waste</td>
<td>Waste</td>
</tr>
</tbody>
</table>

Execution Time
Task Granularity

➢ In parallel computing, granularity (or grain size) of a task is a measure of the amount of work (or computation) which is performed by that task.

➢ Impact of granularity on performance
  – Using fine grains or small tasks results in more parallelism and hence increases the speedup. However, synchronization overhead, scheduling strategies etc. can negatively impact the performance of fine-grained tasks.
  – Simply increasing parallelism alone cannot give the best performance.
  – In order to reduce the communication overhead, granularity can be increased. Coarse grained tasks have less communication overhead but they often cause load imbalance. Hence optimal performance is achieved between the two extremes of fine-grained and coarse-grained parallelism.

Ref: https://en.wikipedia.org/wiki/Granularity_(parallel_computing)
Components of a Task (Process)

- Load program instructions
- Allocate memory space
- Load program data
- Perform Computation on CPU cores
- Release memory, data, other resources

Process start
Overhead

Real computation work

Process end overhead
Typical Misuse - Tiny grain size case

- Tiny grain size
  - E.g., each task takes little time (e.g., less than a second)
  - Most time will be spent on overhead

An extreme case - Cores are just idling
Typical Misuse - Large grain size case

- **Large grain size**
  - Some tasks are much longer than the rest
  - Load balancing can never be achieved

An extreme case - Load imbalancing
Summary

➢ Why need GNU Parallel?
➢ Basic syntax of GNU Parallel and examples
➢ How to use it wisely

➢ For more information about GNU Parallel, refer to: