Optimizing the utilization of C2: time, memory and cost

Shyam Gopalakrishnan

18th February 2021

Opt tion
# of C ory

Why is it important to optimize?

Saving money by optimization

C2 pricing model - quantized per node

- *You pay per node - not how many cores or CPUs you used*
    - *Remember C2 architecture -
CPUs are distributed 40 per node*

Saving money by optimization

C2 pricing model - quantized per node

- *You pay per node - not how many cores or CPUs you used*
  - *Remember C2 architecture - CPUs are distributed 40 per node*

C2 is like a bar of chocolate

- *You pay per bar, not how many pieces you have eaten*

My mama always said
"Life is like a box of
chocolates. You never
know what you're
gonna get."
Forrest Gump

Saving time by optimization

Time savings

- Parallelization: More threads used usually means faster execution

Not parallelized

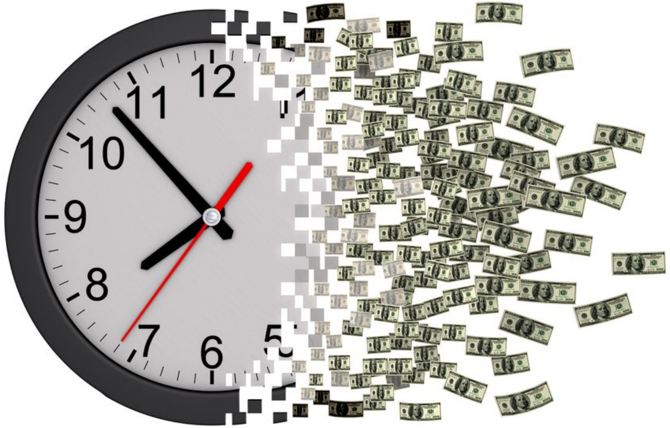
Parallelized

Saving time by optimization

Time savings

- Parallelization: More threads used usually means faster execution

Not parallelized



ized

Memory optimization

How much memory does my job need?

- Again, remember C2 architecture
  - Thin compute node: **696** total thin nodes
    40 cores (2 CPUs with 20 cores each), **192 GB RAM**

  - Fat compute node: **55** total fat nodes
    40 cores (2 CPUs with 20 cores each), **1536 GB RAM (1.5 TB)**

- More thin nodes => job is launched faster
  - Only use fat node if your job needs more than ~ 192 GB RAM

Core/CPU usage optimization

- If your program is not multi-threaded (or cannot use the full 40 threads), run multiple commands in the background, thus utilizing CPU bandwidth

Core/CPU usage optimization

- If your program is not multi-threaded (or cannot use the full 40 threads), run multiple commands in the background, thus utilizing CPU bandwidth

```
#!/bin/sh
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=120gb,walltime=12:00:00

module load bwa/0.7.15

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 10 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 10 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
bwa mem -t 10 canFam31.fasta Batch4.R1.fastq.gz Batch4.R2.fastq.gz > Batch4.out &
wait
```

Core/CPU usage optimization

- If your program is not multi-threaded (or cannot use the full 40 threads), run multiple commands in the background - using forking, thus utilizing CPU bandwidth

```
#!/bin/sh
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=120gb,walltime=12:00:00

module load bwa/0.7.15

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 10 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 10 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
bwa mem -t 10 canFam31.fasta Batch4.R1.fastq.gz Batch4.R2.fastq.gz > Batch4.out &
wait
```

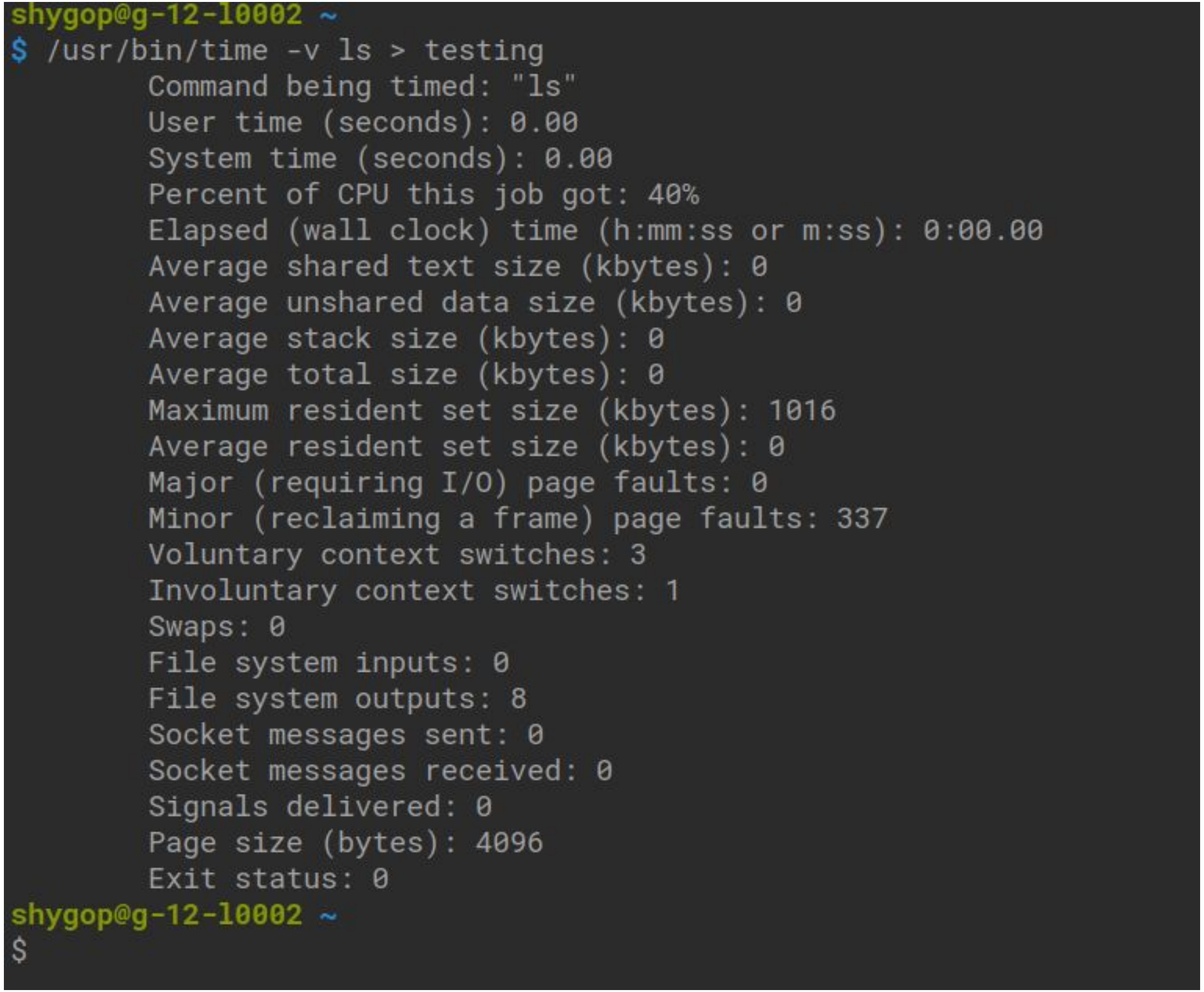
Estimating resource requirements

- How much time to execute program?
    - Run a single job first to estimate time and use this as a guide to figure out how much time other similar jobs might require.
    - Use the `/usr/bin/time` command OR use `qstat`

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=120gb,walltime=12:00:00

module load bwa/0.7.15

/usr/bin/time -v bwa mem -t 40 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out
```



```
shygop@g-12-10002 ~
$ /usr/bin/time -v ls > testing
        Command being timed: "ls"
        User time (seconds): 0.00
        System time (seconds): 0.00
        Percent of CPU this job got: 40%
        Elapsed (wall clock) time (h:mm:ss or m:ss): 0:00.00
        Average shared text size (kbytes): 0
        Average unshared data size (kbytes): 0
        Average stack size (kbytes): 0
        Average total size (kbytes): 0
        Maximum resident set size (kbytes): 1016
        Average resident set size (kbytes): 0
        Major (requiring I/O) page faults: 0
        Minor (reclaiming a frame) page faults: 337
        Voluntary context switches: 3
        Involuntary context switches: 1
        Swaps: 0
        File system inputs: 0
        File system outputs: 8
        Socket messages sent: 0
        Socket messages received: 0
        Signals delivered: 0
        Page size (bytes): 4096
        Exit status: 0
shygop@g-12-10002 ~
$
```

QUIZ on running jobs on C2

Only one question every time: Is this job optimized to launch on computerome?
Yes, no, what is the problem?

JOB 1

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=10,mem=120gb,walltime=12:00:00

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 10 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 10 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
bwa mem -t 10 canFam31.fasta Batch4.R1.fastq.gz Batch4.R2.fastq.gz > Batch4.out &
wait
```

slido

Is job 1 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 2

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=30,mem=120gb,walltime=12:00:00

module load bwa/0.7.15

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 10 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 10 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
wait
```

Is job 2 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 3

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=200gb,walltime=12:00:00

module load bwa/0.7.15

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 10 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 10 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
bwa mem -t 10 canFam31.fasta Batch4.R1.fastq.gz Batch4.R2.fastq.gz > Batch4.out &
wait
```

slido

Is job 3 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 4

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=48,mem=160gb,walltime=12:00:00

module load bwa/0.7.15

bwa mem -t 12 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 12 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 12 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
bwa mem -t 12 canFam31.fasta Batch4.R1.fastq.gz Batch4.R2.fastq.gz > Batch4.out &
wait
```

slido

Is job 4 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 5

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=120gb,walltime=12:00:00

module load bwa/0.7.15

bwa mem -t 40 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out
```

slido

Is job 5 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 6

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=120gb,walltime=12:00:00

module load bwa/0.7.15

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out
bwa mem -t 10 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out
bwa mem -t 10 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out
bwa mem -t 10 canFam31.fasta Batch4.R1.fastq.gz Batch4.R2.fastq.gz > Batch4.out
wait
```

slido

Is job 6 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 7

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=150gb,walltime=12:00:00

module load bwa/0.7.15

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 10 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 10 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
bwa mem -t 10 canFam31.fasta Batch4.R1.fastq.gz Batch4.R2.fastq.gz > Batch4.out &
wait
bwa mem -t 10 canFam31.fasta Batch5.R1.fastq.gz Batch5.R2.fastq.gz > Batch5.out &
bwa mem -t 10 canFam31.fasta Batch6.R1.fastq.gz Batch6.R2.fastq.gz > Batch6.out &
bwa mem -t 10 canFam31.fasta Batch7.R1.fastq.gz Batch7.R2.fastq.gz > Batch7.out &
bwa mem -t 10 canFam31.fasta Batch8.R1.fastq.gz Batch8.R2.fastq.gz > Batch8.out &
wait
```

slido

Is job 7 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 8

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=500gb,walltime=60:00:00:00

module load bwa/0.7.15

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 14 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 16 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
wait
```

slido

Is job 8 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 9

```
#!/bin/bash
#PBS -W group_list=ku_fa -A ku_fa
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=120gb,walltime=12:00:00

module load bwa/0.7.15

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 10 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 10 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
bwa mem -t 5 canFam31.fasta Batch4.R1.fastq.gz Batch4.R2.fastq.gz > Batch4.out &
bwa mem -t 5 canFam31.fasta Batch5.R1.fastq.gz Batch5.R2.fastq.gz > Batch5.out &

wait
```

slido

Is job 9 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 10

```
#!/bin/bash
#PBS -N test
#PBS -e test.err
#PBS -o test.log
#PBS -l nodes=1:ppn=40,mem=500gb,walltime=60:00:00:00

module load bwa/0.7.15

bwa mem -t 10 canFam31.fasta Batch1.R1.fastq.gz Batch1.R2.fastq.gz > Batch1.out &
bwa mem -t 14 canFam31.fasta Batch2.R1.fastq.gz Batch2.R2.fastq.gz > Batch2.out &
bwa mem -t 16 canFam31.fasta Batch3.R1.fastq.gz Batch3.R2.fastq.gz > Batch3.out &
wait
```

slido

Is job 10 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

JOB 11!

```
#! /bin/bash

#PBS -W group_list=ku_fa -A ku_fa
#PBS -N canid1Map
#PBS -e canid1.err
#PBS -o canid1.log
#PBS -l nodes=1:ppn=40,mem=50gb,walltime=1:00:00
#PBS -d /home/projects/C2_test

### Load modules
module load bwa/0.7.15
module load samtools/1.9
module load htslib/1.9

### Run your jobs
bwa mem -t 40 refgenome/canFam31.fasta Canid1.R1.fastq.gz > Canid1.sam
samtools view -b Canid1.sam > Canid1.bam
samtools index Canid1.bam
```

slido

Is job 11 ok to run on C2?

ⓘ Start presenting to display the poll results on this slide.

That's all Folks!