

Parallelization and Responsible Resource Use on Sedna

SEDNA Computational Roundtable Series
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Why parallelize?

- Speed
- Necessity
- Break up a task into multiple smaller jobs, may run quicker on a busy cluster (small jobs will likely start running before resources for one big job become available)

Discussion: What types of analyses are good for parallelization

- When the overall job consists of many small jobs or discrete tasks that are independent
 - Examples:
 - Bootstrapped phylogenetics
 - Phylogenetic gene tree inference
 - Differential gene expression
 - BLAST
 - Trimming and mapping reads
 - Replicate MCMCs
 - Sliding genomic window analyses
 - Genome repeat masking

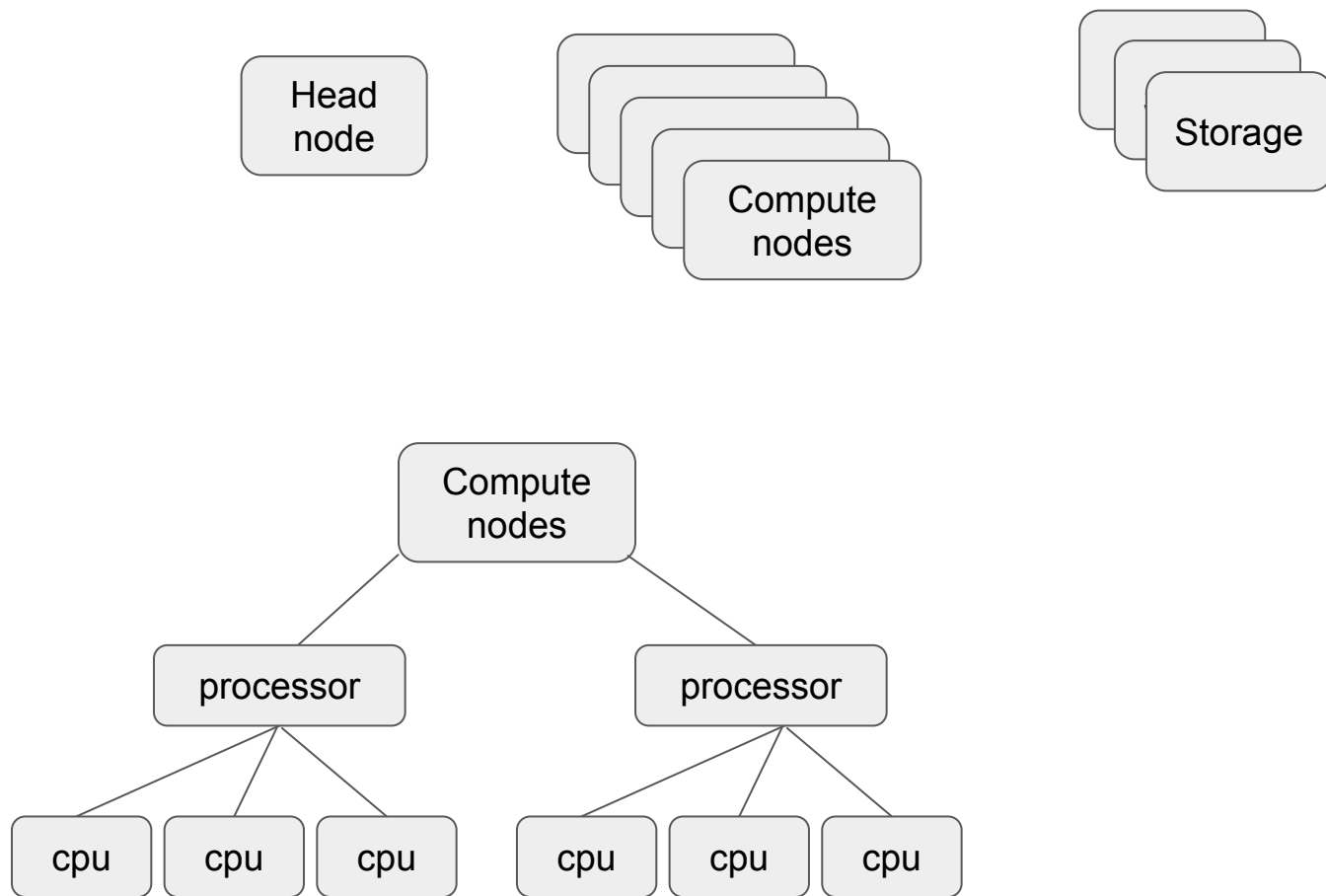
How much to parallelize?

Ideally as much as possible. But...

Consider Sedna resources...

- Partitions, node, core, etc.

General HPC architecture



Sedna hardware

Sedna hardware

/home

/share

/scratch1

/scratch2

Storage:

197 tb

197 tb

43 tb

91 tb

Compute Nodes

standard

medmem

highmem

Number:

28

7

4

CPUs/node:

20

20

24

Memory/node:

96 gb

192 gb

1.5 tb

How much of Sedna can I use?

- Not all of it!
- Request the minimum resources you need for your job
 - You can check how much prior jobs have used with ``seff``
- What if I have a really big job?
 - You still shouldn't use all of Sedna.
 - But you can use more over the weekend or at night
 - Less of an impact if your jobs are short (so you can run more at once).
 - Check with other users for their plans in the SEDNA user G-chat
- Apply limits to how many jobs run at once

How to parallelize while limiting resource use

Run multiple task / processes in one slurm job:

Gnu parallel

Parallelize with multiple jobs for each task:

Array

Snakemake

Nextflow

Link to GitHub demo

Find the following examples on our [github page](#)

GNU parallel

Determine number of
“jobs” to run at time
(match cpu request in
header)

```
#!/bin/bash
#SBATCH --job-name=fastp_trim
#SBATCH -c 10
#SBATCH --mem=100G
#SBATCH --partition=medmem
#SBATCH -t 1-0:0:0
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err
```

Memory is divided by
processors (# jobs
indicated in script)

Feed parallel a list of
file / sample names

```
cat Parallel_samplenames.txt | parallel -j 10 \
```

Can test setup with:
parallel --dry-run

Indicate your
standard input with
{ } in code

```
fastp \
--in1 $READS/{ }_R1.fastq.gz \
--in2 $READS/{ }_R2.fastq.gz \
--out1 $OUTDIR/{ }_R1_trimmed.fastq.gz \
--out2 $OUTDIR/{ }_R2_trimmed.fastq.gz \
--json $OUTDIR/{ }_fastp.json \
--html $OUTDIR/{ }_fastp.html
```

Slurm arrays

```
#!/bin/bash
#SBATCH --job-name=fastp_array
#SBATCH -c 1
#SBATCH -t 1-0:0:0
#SBATCH --mem=10G
#SBATCH -p medmem
#SBATCH -o %x_%A_%a.out
#SBATCH -e %x_%A_%a.err
#SBATCH --array=[0-12]%13
```

Each job gets memory and cpu indicated

Indicate how many slurm array tasks will be completed

Important: %13 means run 13 at a time. In this case all jobs but good to limit

Create a list of files and then assign each file to a slurm task id (0-12)

```
#Create Array
FILES=$(find $READS/*_R1.fastq.gz -type f -exec basename {} _R1.fastq.gz \; )
FILES_ARRAY=(${FILES})
SAMPLE=${FILES_ARRAY[${SLURM_ARRAY_TASK_ID}]}
```

Indicate sample with variable

```
fastp \
  --in1 $READS/${SAMPLE}_R1.fastq.gz \
  --in2 $READS/${SAMPLE}_R2.fastq.gz \
  --out1 $OUTDIR/${SAMPLE}_R1_trimmed.fastq.gz \
  --out2 $OUTDIR/${SAMPLE}_R2_trimmed.fastq.gz \
  --json $OUTDIR/${SAMPLE}_fastp.json \
  --html $OUTDIR/${SAMPLE}_fastp.html
```

snakemake

Command Line Launch

```
snakemake --executor slurm --default-resources slurm_account=nfsc slurm_partition=standard --jobs 10  
--use-conda --config config.yaml
```

Specify configuration
file

Important: defines how
many simultaneous
jobs snakemake can
run at a time

Snakemake Rule

```
rule pre_fastqc:  
    output:  
        "log/pre_fastqc_{sample}.done"  
    conda:  
        "envs/fastp-0.24.0.yaml"  
    resources:  
        runtime=10000,  
        cpus_per_task=1,  
        mem_mb=1000  
    shell:  
        ""  
    ...  
    ""
```

Default runtime,
memory usage, and #
cores defined in config
file (yaml format)

Configuration

runtime: 100
cpus_per_task: 1
mem_mb: 1000

Customized resources
for each job detailing
runtime, memory
usage, and # cores

nextflow

Nextflow tips for HPC users:

https://sequera.io/blog/5_tips_for_hpc_users/

Command line launch

```
nextflow -c "/path/to/my/config.txt"
```

Usually best to specify resources in a config file rather than at the command line

Configuration file

```
executor {  
  name = 'slurm'  
  queueSize = 10  
}
```

Important: maximum number of jobs to submit simultaneously

```
process {  
  queue = 'standard'  
  cpus = 8  
  memory = '24 GB'  
  time = '2h'  
  clusterOption = "OTHER SLURM OPTIONS"
```

Default queue, # CPUs, RAM, and runtime per job

Use this for other SLURM options

```
withLabel: big_mem {  
  memory = '64 GB'  
  executor.queueSize = 2  
}
```

Can use labels for processes that require more/less than the default resources

Check on resource usage

- Seff

- Check job efficiency with seff <jobid>
 - CPU utilized: cpu hours used by job
 - Wall clock time: time span that job ran
 - CPU efficiency: average rate of CPU usage
 - Peak memory usage / memory requested

- Sacct

- sacct -o jobid,jobname,nodelist,partition,state,ReqMem,MaxRSS,ReqCPUS,elapsed,Timelimit,submit -j <job id>

- Re-adjust scripts if your requests aren't efficient

- How do I find the <jobid> for a job that already finished?

- sacct --state=CD --starttime=2025-06-01 --endtime=now
 - “--state=CD” → only show completed jobs, can use [other state codes](#)
 - “--starttime=2025-06-01 --endtime=now” → show jobs that completed between 6/1/25 and now, can adjust the date

Planning for a cloudy computing future...

- In cloud computing, our shared resource is \$\$\$, not hardware
- Resource monitoring may be even more important if we are paying per CPU hour (time-based or usage-based pricing)
- Optimizing CPU, memory, and walltime will help minimize computing costs
- Workflow managers will be critical; Snakemake and Nextflow have built-in support for parallelization in cloud computing environments