Running programs on HARDAC

Goals of this Class

- **Understand**
  - A cluster provides CPU, RAM, and Disk space.
  - Terms: Cluster, Partition, Node, Job, and Job Step
  - Job life-cycle
- **Be able to**
  - Run a job on the cluster
  - Run batch and **batch array jobs**
  - Monitor/cancel jobs

Laptop Not Powerful Enough

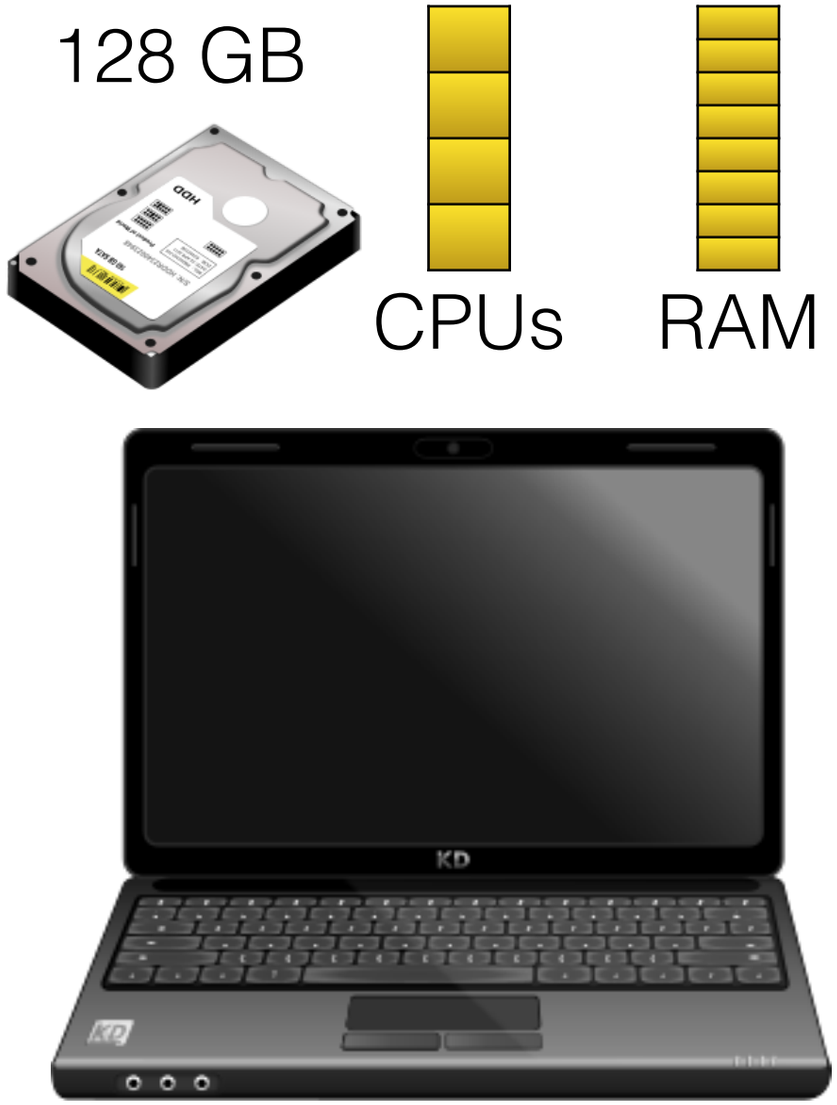
Symptoms

projects **TOO BIG** for your hard drive

processing many files takes **FOREVER**

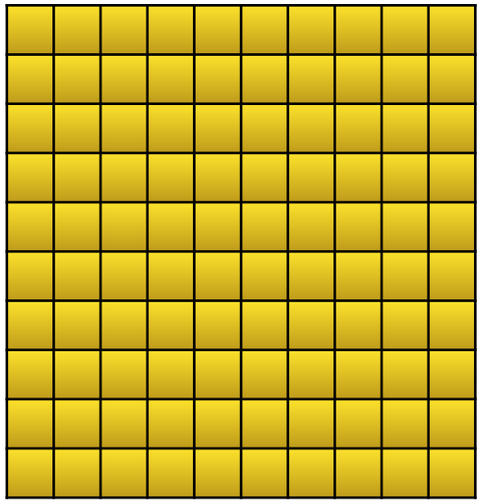
high RAM commands **CRASH**

The Problem

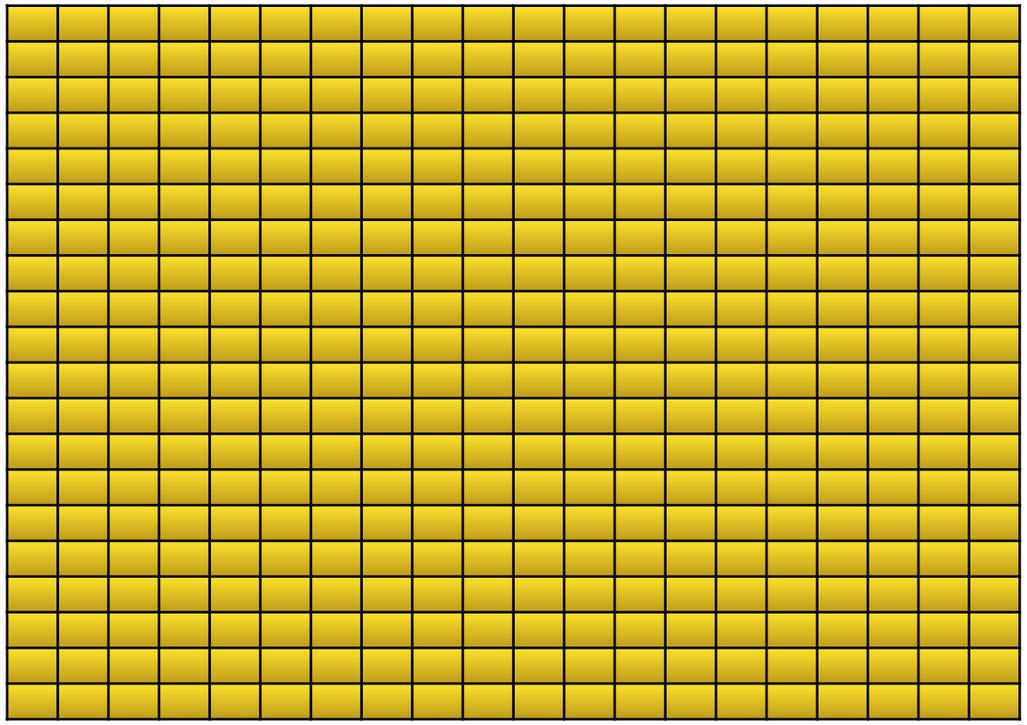


Cluster Has More Power

500,000 GB



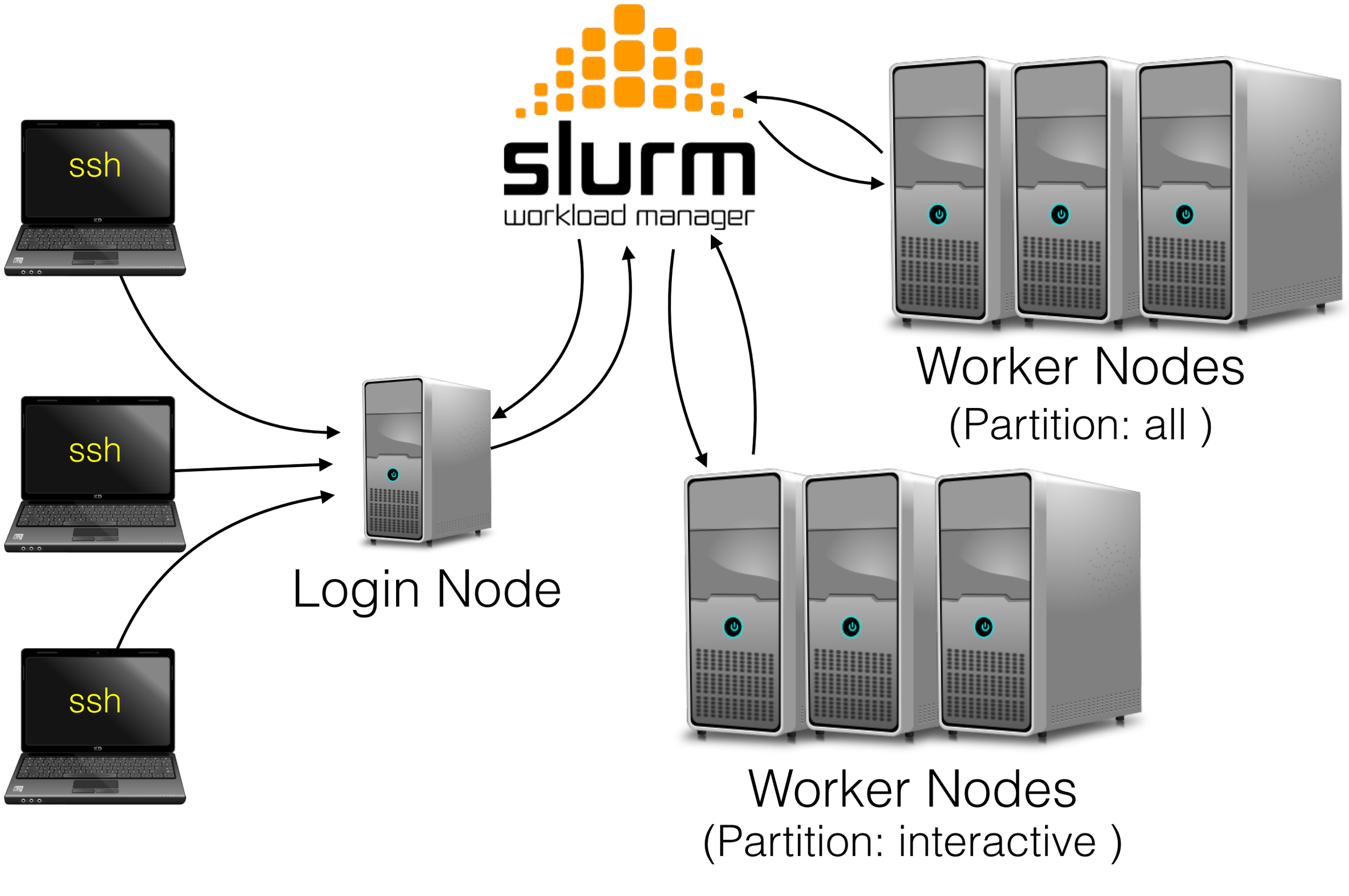
CPUs



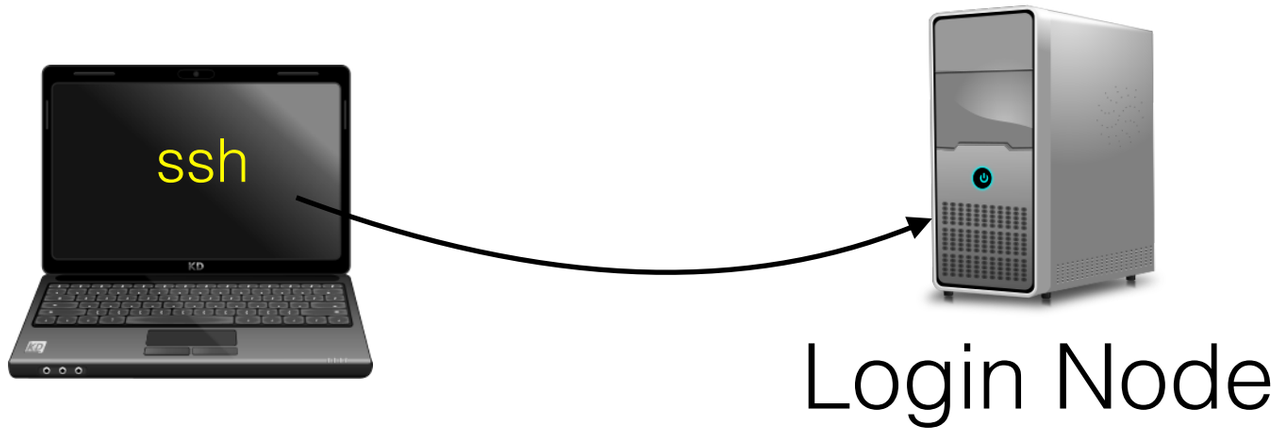
RAM

Cluster
Just a bunch of computers (nodes)

Slurm manages our cluster



ssh to the Login Node




```
$ ssh <netid>@hardac-login.genome.duke.edu
...
...password:XXXXX
...
...hardac-login ~]$
```

⚠ You must be on medicine network to connect to HARDAC

hostname

what machine am I on?

Run hostname command

```
..login ~]$ hostname
hardac-login.genome.duke.edu
```

This command prints out the name of the machine we are running it on. In this case the login node.

NOTE: Do not run intensive commands on the login node

srun

Slurm run a command in the foreground

Ask slurm to run the hostname command on a worker node

```
..login ~]$ srun hostname
srun: job 51 queued and waiting for resources
srun: job 51 has been allocated resources
c1-10-4.genome.duke.edu
..login ~]$
```

srun

Specify memory requirements

By default HARDAC allocates 2G memory per job.
Run hostname command specifying 4G of RAM (memory)

```
..login ~]$ srun --mem=4G hostname
srun: job 51 queued and waiting for resources
srun: job 51 has been allocated resources
c1-10-3.genome.duke.edu
..login ~]$
```

- Slurm will stop your job if you use more than the requested memory
- If you allocate too much memory it can take longer to get your job scheduled and wastes resources

partitions

Cluster nodes are grouped into partitions based.
To specify a partition with **srun** use the **-p** flag.
The default partition is named all.

Explicitly run hostname on a node in the all partition:

```
..login ~]$ srun -p all hostname
```

Worker Nodes
(Partition: interactive)

Worker Nodes
(Partition: all)

Interactive Job

typing srun and waiting is tedious

Steps

1. Connect to Login Node
2. Start interactive job using **srun** on the interactive partition
3. Run whatever commands you want
4. type **exit** to quit interactive job

```
...login ~]$ srun -p interactive --pty bash
<workernode> ~]$ hostname
```

Getting code onto the Cluster

Works just like on your laptop!

```
$ git clone https://github.com/Duke-GCB/scicomp-hpc.git
```

Change into this directory

```
$ cd scicomp-hpc
```

See the files we downloaded

```
$ ls
```

Foreground vs Background Jobs

Foreground Job - srun

- Useful for testing but not for long running commands
- Actively monitored through terminal output
- Canceled by pressing Ctrl-C or closing your terminal window

Background Job

- Useful for long running commands
- Monitored via log files, slurm commands, and email messages
- Canceled by using a slurm command

sbatch

Run command(s) in the background

Make a file called countgc.sh using nano:

```
#!/bin/bash
echo "Starting GC counter"
python fasta_gc.py data/E2f1_dna.fasta
```

Run it by using the **sbatch** command:

```
$ sbatch countgc.sh
Submitted batch job 26651766
```

When done Slurm will create an output file(s) based on jobid.

```
$ cat slurm-*.out
```

Slurm Job Lifecycle

1. Slurm creates a Job in the Job Queue with status Pending when a user submits a request.

2. When resources are available Slurm will run Pending jobs. The job state is changed to Running.

3. When a job is finished Slurm removes it from the Job Queue. Slurm records the job in the Accounting List with the final state.

Job Queue - squeue

User	Cmd	State	Job ID
Bob	Star Aligner	Running	123
John	**fastqc…**	**Running**	**411**

Accounting List - sacct

User	Cmd	State	Job ID
Dan	kalign…	Error	112
John	**fastqc…**	**Complete**	**411**

squeue

shows active job status

Look at your active jobs.

```
$ squeue -u <netid>

JOBID PARTITION     NAME     USER  ST       TIME ...
6335778       all long_ru...  jpb67  R       0:05 …
...
```

Job Status Column

R - Running

P - Pending

Start a long running job the repeat the above command.

```
$ sbatch long_running.sh
```

scancel

Terminate a running Job

Find the job id of that long_running job.

```
$ squeue -u <netid>
```

Stop a single job

```
$ scancel <JOBID>
```

Or stop all jobs for your user

```
$ scancel -u <netid>
```

will cancel interactive jobs

sacct

historical job status

```
$ sacct
       JobID    JobName  ...      State ExitCode
------------ ---------- ... ---------- --------
26705496     countgc.sh ...  COMPLETED      0:0
26705496.ba+      batch ...  COMPLETED      0:0
26705566     countgc.sh ...     FAILED      1:0
26705566.ba+      batch ...     FAILED      1:0
26706541     countgc.sh ...  CANCELED      0:0
26706541.ba+      batch ...  CANCELED     0:15
```

Only shows results from current day by default.
Checkout **`starttime`** flag to see a better date range.

sacct

How much memory did that use?

```
$ sacct -o JobName,State,MaxRSS,ReqMem,Elapsed
   JobName      State     MaxRSS     ReqMem  ...
---------- ---------- ---------- ----------  ...
countgc.sh  COMPLETED                   2Gc  ...
     batch  COMPLETED      4960K        2Gc  ...
countgc.sh  COMPLETED                   2Gc  ...
     batch  COMPLETED          0        2Gc  ...
countgc.sh  COMPLETED                 400Mn  ...
     batch  COMPLETED      4936K      400Mn  ...
```

- MaxRss / 1024 = MB for use with `sbatch --mem`
- See all options sacct can show: `sacct -e`

sbatch

memory requirements

Change countgc.sh using nano:

```
#!/bin/bash
#SBATCH --mem=400M
python fasta_gc.py data/E2f1_dna.fasta
```

400MB RAM

The #SBATCH comment tells sbatch to pretend that the following flag was passed along the command line. This is preferable to typing the flags again and again.

srun and **sbatch** commands share many of the same arguments**.**

sbatch

email when job completes

Add two lines countgc.sh using nano:

```
#!/bin/bash
#SBATCH --mail-type=END
#SBATCH --mail-user=<your_email_address>
#SBATCH --mem=400M
echo "Starting GC counter"
python fasta_gc.py data/E2f1_dna.fasta
```

Run it with sbatch

```
$ sbatch countgc.sh
```

job steps

break job into steps

Create jobsteps.sh using nano:

```
#!/bin/bash
FILENAME=data/E2f1_dna.fasta
srun cksum $FILENAME
srun python fasta_gc.py $FILENAME
```

Run our sbatch script

```
$ sbatch jobsteps.sh
```

Once it finishes look at

```
$ sacct
```

sbatch --array

make a bunch of jobs

Create arraytest.sh using nano:

```
#!/bin/bash
#SBATCH --mem=400M
#SBATCH --array=1-5%2
echo $SLURM_ARRAY_TASK_ID
```

The **1-5** part says to run array_test.sh script 5 times with `SLURM_ARRAY_TASK_ID` filled with a number 1-5.
The **%2** part says to only run 2 at a time.

```
$ sbatch arraytest.sh
```

sbatch --array

use task id to find a filename

Change arraytest.sh using nano:

```
#!/bin/bash
#SBATCH --mem=400M
#SBATCH --array=1-5%2
IDX=$SLURM_ARRAY_TASK_ID
FILENAME=$(ls data/*.fasta | awk NR==$IDX)
echo $FILENAME
```

Run your array job

```
$ sbatch arraytest.sh
```

sbatch --array

run one command on many files

Change arraytest.sh using nano:

```
#!/bin/bash
#SBATCH --mem=400M
#SBATCH --array=1-5%2
IDX=$SLURM_ARRAY_TASK_ID
FILENAME=$(ls data/*.fasta | sed -n ${IDX}p)
python fasta_gc.py $FILENAME
```

This script will determine GC of 5 files in the *data* directory storing result into separate slurm*.out files.

```
$ sbatch arraytest.sh
```

sinfo

How busy is the cluster?

Show status of nodes in the "all" partition

```
$ sinfo -p all
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
all       up     90-00:00:0 2      idle  c1-02-[1-4]
all       up     90-00:00:0 1      down  c1-09-3
all       up     90-00:00:0 1      mix   c1-09-[1-2],c1-10-4
all       up     90-00:00:0 3      alloc x2-01-3,x2-07-3
```

Proper Job Allocations

Only use up to 2 nodes worth of compute resources at a time

Total Memory: 512GB
Total CPUs: 64

Do not run jobs on the login node!

Login Node

your jobs run here **slowly** 😢

other users **can't start their jobs** 😢

Worker Nodes

Instead of here which would be **fast**

Helpful Resources

HARDAC WIKI

https://wiki.duke.edu/display/HAR/

Requesting Software/Help

gcb-help@duke.edu