Pronghorn Homework Module

All personal directories are located: /data/gpfs/assoc/biol\_bids-2/

Setting up

Submission script is located:

/data/gpfs/assoc/biol\_bids-2/atram.slurm.sh

Copy this file to your personal directory.

In your personal directory you will need to create two directories:

mkdir temp

mkdir atram\_out

Below is an example of the submission script and the bold sections within square brackets should be changed accordingly.

*atram.slurm.sh*

#!/usr/bin/bash -l

#SBATCH --job-name=**[give your job a descriptive name]**

#SBATCH --account=cpu-s5-biol\_bids-2

#SBATCH --partition=cpu-core-0

#SBATCH --nodes=1

#SBATCH --ntasks=1

#SBATCH --cpus-per-task=1

#SBATCH --time=14-00:00

#SBATCH --mem-per-cpu=3500M

#SBATCH --output=hostname\_%j.out

#SBATCH --error=hostname\_%j.err

#SBATCH --mail-type=ALL

#SBATCH --mail-user=**[your email]**

singularity exec /apps/atram/aTRAM.sif python3 /aTRAM/atram.py -b /data/gpfs/assoc/biol\_bids-2/Course\_content/atram\_files/AlspHabad/AlspHabad -t /data/gpfs/assoc/biol\_bids-2/**[netID]**/temp -Q /data/gpfs/assoc/biol\_bids-2/Course\_content/atram\_files/query\_files/**[Number of genes]**\_proteins.fasta -a trinity -o /data/gpfs/assoc/biol\_bids-2/**[netID]**/atram\_out/

Target files

All target files are found here: /data/gpfs/assoc/biol\_bids-2/Course\_content/atram\_files/query\_files/

Each file begins with the number of genes it contains. In class you will assemble 2 genes. For your homework you will assemble 20 genes.

Processors

You will need to select the number of processors you want to use per job. You can change the number of tasks and CPUs per task in the SBATCH options in the submission script. Pronghorn has 32 CPUs per node. Pronghorn will allocate the resources you request to aTRAM as it runs. You can start with a single task and CPU per task, measure the gene assembly rate, and change the computational resources from there.

Submitting

Submit the job using:

sbatch atram.slurm.sh

Queue

To check on the status of your job, use squeue in the command line. This will pull up a list of all of the jobs currently running or waiting in the queue. You will see your job by the job name and your user name. If your job is waiting in the queue, the time will say 0:00. Once it starts running the timer will start. You can check on your jobs only with squeue -u <USERNAME>

**For your homework you will assemble 20 genes.**

**Answer the following questions:**

1. What is the purpose of High Performance Computing (HPC) and when might you use an HPC cluster?

HPC allows for greater computing power that is cost effective and can be used simultaneously by many users. By aggregating computing power it can increase performance and reduce time of computation.

2. What is a slurm script? Print the path of your slurm script here (including file name).

/data/gpfs/assoc/biol\_bids-2/leah/atram.slurm.sh

3. What is the path to your gene assemblies on pronghorn (i.e., output files).

/data/gpfs/assoc/biol\_bids-2/leah/atram\_out/

4. How many CPUs per task did you ask for?

I assigned 20 CPU per task (but it only used 8).

5. How many genes assembled?

20 genes were assembled.

6. Did all genes assemble? Why or why not?

Yes, the process was completed successfully and all genes were assembled. We can check the error files and output files to confirm. There are 40 output files when checking ls -1 | wc -l but each gene had 2 files so there were 20 successful genes assembled.

7. How long did it take for them to assemble? What processes might have slowed this down?

It took 00:30:18, or 30 minutes and 18 seconds. We might have increased speeds if we assigned multiple tasks, one for each gene, so that all 20 cores were in use (rather than assigning 20 cores but only 8 being used)