Fastsimcoal on HPC cluster:

What is Fastsimcoal?

Fastsimcoal is an extremely flexible demographic modelling software developed by the group of Laurent Excoffier at University of Bern. It uses the site frequency spectrum (SFS) to fit model parameters to the observed data by performing coalescent simulations. You can find the manual and more information here and look at the lecture slides.

The full documentation for the Fastsimcoal is found in the following links:

Documentation

Versions Available:

- fastSimcoal2– v2.5.2.21

How to load a version of Fastsimcoal?

To load a version of Fastsimcoal on the HPC, use the following command:

```
module avail bio/fastsimcoal
```

The version will be listed. To use a version of software, use following command:

```
module load bio/fastsimcoal/
```

Verify by using this command:

```
module list
```

The loaded software and dependencies will be shown.

How to use Fastsimcoal on the cluster?

There are two methods to run Fastsimcoal on the cluster.

The Interactive Way:

To run the program interactively, follow the steps:

```
#Open a bash session on compute node
srun -p main --qos main -n 1 -c 12 --mem 10G --pty bash

#Load the module
module load bio/fastsimcoal
# Start your commands here
fsc25 --help

#Follow with commands to execute
```

This method is ideal for a short job run which produces runtime output and to debug the codes.

The Script:

To run a slurm job, the user must prepare input files. For this example, get input files with,

```
#Copy all the required files to the test folder
cp /share/apps/fastsimcoal2/example\ files/1PopDNArand.tpl    ~/test/
cp /share/apps/fastsimcoal2/example\ files/1PopDNArand.est    ~/test/
```

```
# Make a script to run fastsimcoal
touch script.sbatch
```

Use the following template for the script,

```
#!/bin/bash
#SBATCH -J test
#SBATCH -n 1
#SBATCH -mem=16G
#SBATCH -p main
#SBATCH --qos main
#SBATCH -o fast_sim_out-%J.txt
#SBATCH -e fast_sim_out-%J.txt
#SBATCH -t 30

module load bio/fastsimcoal       # load the module


cd $SLURM_SUBMIT_DIR       # Moving to the test directory


#Run Fastsimcoal on the cluster
fsc25 -t 1PopDNArand.tpl -n 1 -e 1PopDNArand.est -E 1000 -q
```

Schedule the job with the following sbatch command.

sbatch script.sbatch

All the processed files will be generated in the same directory as the sbatch script.

Where to find help?

If you are stuck on some part or need help at any point, please contact OIT at the following address.

https://ua-app01.ua.edu/researchComputingPortal/public/oitHelp