Raxml on HPC cluster:

What is Raxml?

Raxml is a phylogenetic tree inference tool which uses maximum-likelihood (ML) optimality criterion. Its search heuristic is based on iteratively performing a series of Subtree Pruning and Regrafting (SPR) moves, which allows to quickly navigate to the best-know ML tree.

RAxML-NG offers improvement in speed, flexibility, and user-friendliness over the previous versions.

The documentation for the Raxml is found on:

https://github.com/amkozlov/raxml-ng

https://github.com/amkozlov/raxml-ng/wiki/Tutorial#preparing-the-alignment

Versions Available:

RAxML-8.2.4

RAxML-8.2.12

RAxML-ng

How to load a version of Raxml?

To load a version of Raxml on the HPC on current terminal session, use the following command:

module avail bio/raxml

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

module load bio/raxml/ng

Verify by using this command:

module list

The loaded software and dependencies will be shown.

How to use Raxml on the cluster?

Here is one example of how to use the Raxml on the cluster. To get a test file to process through Raxml, use the following commands

```
# Make a test directory on home folder
cd ~ && mkdir raxml_test && cd raxml_test
# download test file
curl -L -o test.phy https://adelaide.figshare.com/ndownloader/files/14243024
# Now after you loaded your module and downloaded test files, we can make a script to
```

The Script:

run Raxml

```
#!/bin/bash
$SBATCH -J Jobname # Jobname
#SBATCH -n 1  # Nodes per task
#SBATCH -mem=56  # Must need to allocate memory to run raxml - at least 4G
#SBATCH -p main  # Partition
#SBATCH --qos main  # Quality of service
#SBATCH -o Raxml_sim_out-%J.txt # STDOUT Out file
#SBATCH -e Raxml_sim_out-%J.txt # Error file
#SBATCH -t 25  # time in minuets
```

```
module load bio/raxml/ng  # load the module
cd $SLURM_SUBMIT_DIR  # Moving to the test directory
#runs raxml command on test.phy
raxml-ng --msa test.phy --model GTR+G --prefix first --seed 2 --threads 3
```

Schedule the job with following sbatch command.

sbatch myscript.sh

All the processed file will be written in a same directory as the script. The required file will be generated there.

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

Resources:

https://github.com/amkozlov/raxml-ng/wiki/Tutorial#preparing-the-alignment

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