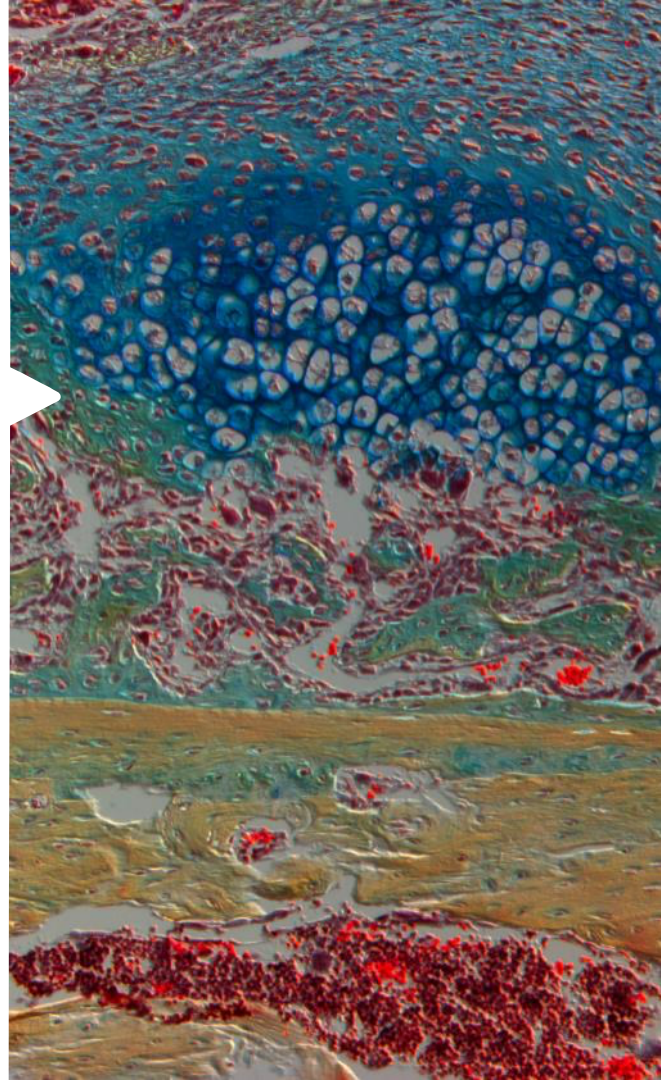




Working on Big Purple

Mark Grivainis

08 October 2020

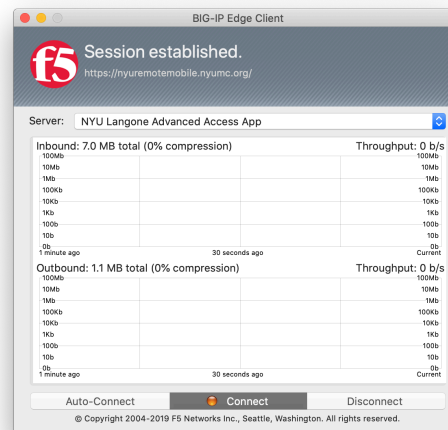
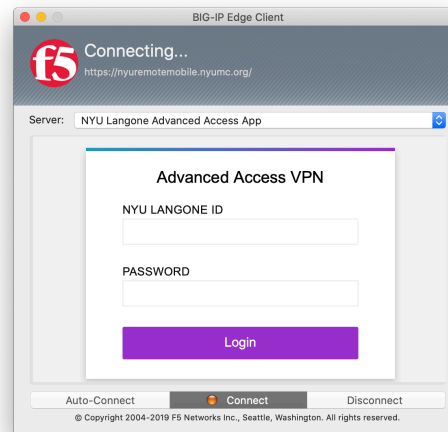


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Connecting to the VPN

- Open the F5 App
- Enter your Kerberos ID and Password
- Complete the 2 – Factor authentication
- You are now logged in



Log into Big Purple

- Open your terminal/powershell
- Enter:
 - `ssh <kid>@bigpurple.nyumc.org`
- You should now be in your home directory

```

[red] [green] [blue] [yellow] markgrivainis — grivam01@bigpurple-ln3: ~ -- ssh grivam01@bigpurple.n...
+ ssh grivam01@bigpurple.nyumc.org
Last login: Wed Oct 7 13:33:30 2020 from 10.128.222.103

BigPurple
NYU Langone Health HPC

Use the following commands to adjust your environment:

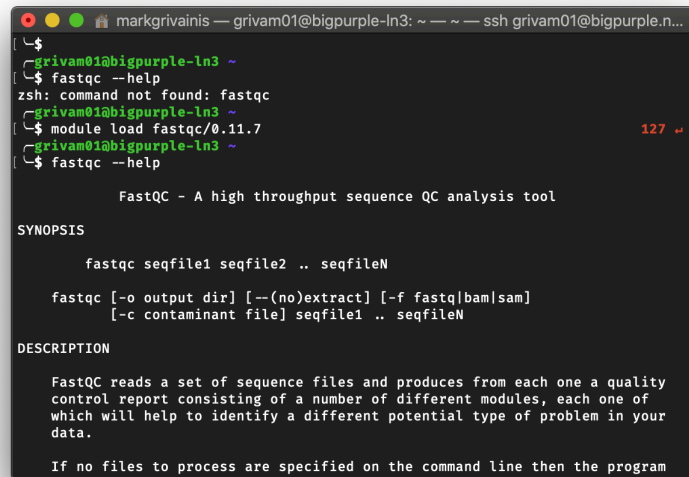
'module avail'           - show available modules
'module add <module>'    - adds a module to your environment for this session
'module initadd <module>' - configure module to be loaded at every login


2020-07-16 The HPC virtual Town Halls are held on Thursdays, 12:00-1:00.
            You may join via https://nyumc.webex.com/meet/siavoa01
            You may also contact us through email. We can use phone or Webex
x to help you.

BigPurple User Guide available at: http://bigpurple-ws.nyumc.org/wiki
New HPC Portal: https://hpcmed.org/
You may email <hpc_admins@nyumc.org> for any further assistance.
```

Loading Modules

- If you do not know exactly what module you need use:
 - module avail
- If a module is not loaded you will get an error:
 - Command not found: <module_name>
- Load a module using:
 - module load <module_name>/version/...



```
markgrivainis — grivam01@bigpurple-ln3: ~ — ssh grivam01@bigpurple.n...
$
grivam01@bigpurple-ln3 ~
$ fastqc --help
zsh: command not found: fastqc
grivam01@bigpurple-ln3 ~
$ module load fastqc/0.11.7
grivam01@bigpurple-ln3 ~
$ fastqc --help

FastQC - A high throughput sequence QC analysis tool

SYNOPSIS

fastqc seqfile1 seqfile2 .. seqfileN

fastqc [-o output dir] [--(no)extract] [-f fastq|bam|sam]
        [-c contaminant file] seqfile1 .. seqfileN

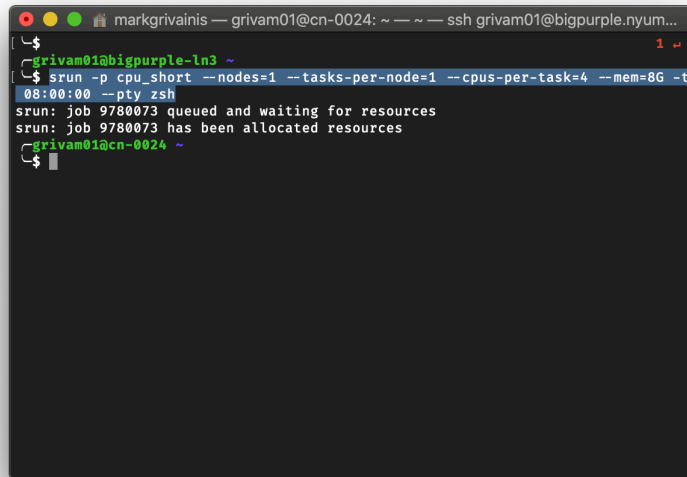
DESCRIPTION

FastQC reads a set of sequence files and produces from each one a quality
control report consisting of a number of different modules, each one of
which will help to identify a different potential type of problem in your
data.

If no files to process are specified on the command line then the program
```

Running an interactive job

- Use the 'srun' slurm command
 - `srun -p cpu_short --nodes=1 --tasks-per-node=1 --cpus-per-task=4 --mem=8G -t 08:00:00 --pty bash`
- -p: the type of node
- --nodes: How many nodes (use 1)
- --tasks-per-node: How many tasks (use 1)
- --cpus-per-task: How many CPUs to assign
 - This varies depending on what you are doing
 - For alignment use 8 or 16
 - For trimming / fastqc use 4 or 8 (remember to set the flag when calling the program)



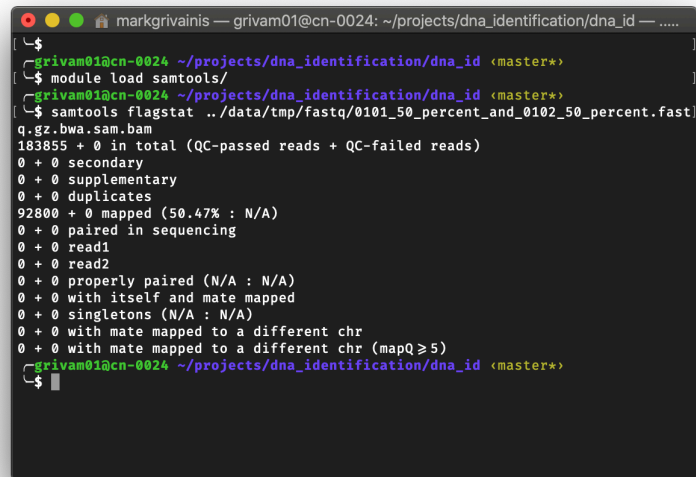
```
markgrivainis — grivam01@cn-0024: ~ — ssh grivam01@bigpurple.nyum...  
grivam01@bigpurple-ln3 ~  
$ srun -p cpu_short --nodes=1 --tasks-per-node=1 --cpus-per-task=4 --mem=8G -t  
08:00:00 --pty zsh  
srun: job 9780073 queued and waiting for resources  
srun: job 9780073 has been allocated resources  
grivam01@cn-0024 ~  
$
```

BBMap CPU/Ntask comparisons

- 1 node; 1 task; 8 CPUs per task
 - 21978.373 seconds
- 1 node; 1 task; 16 CPUs per task
 - 10641.761 seconds.
- 1 node; 1 task; 1 CPUs per task
 - > 12 hours
- 1 node; 8 tasks; 1 CPUs per task
 - 24770.645 seconds.

Running a Module in Interactive Mode

- Now that you are no longer on the head node you can run any command line applications you load
- Remember to read the documentation
 - Do this by adding the --help flag
- Once you know what the command is and what flags you need to set you can run it.
- The output that is sent to Stdout or Stderr will be printed in the terminal



```
markgrivainis — grivam01@cn-0024: ~/projects/dna_identification/dna_id — .....
```

```
$ grivam01@cn-0024 ~/projects/dna_identification/dna_id <master*>  
$ module load samtools/  
$ grivam01@cn-0024 ~/projects/dna_identification/dna_id <master*>  
$ samtools flagstat ../data/tmp/fastq/0101_50_percent_and_0102_50_percent.fast  
q.gz.bwa.sam.bam  
183855 + 0 in total (QC-passed reads + QC-failed reads)  
0 + 0 secondary  
0 + 0 supplementary  
0 + 0 duplicates  
92800 + 0 mapped (50.47% : N/A)  
0 + 0 paired in sequencing  
0 + 0 read1  
0 + 0 read2  
0 + 0 properly paired (N/A : N/A)  
0 + 0 with itself and mate mapped  
0 + 0 singletons (N/A : N/A)  
0 + 0 with mate mapped to a different chr  
0 + 0 with mate mapped to a different chr (mapQ ≥ 5)  
$ grivam01@cn-0024 ~/projects/dna_identification/dna_id <master*>
```


Installing Python Packages

- You can either use conda (anaconda / miniconda) or pip
- I prefer using pip as I have encountered less issues
- My go-to versions of python is:
 - `module load python/cpu/3.7.2`
 - `module load python/gcc/3.6.5`
- Pip should be installed with this version of Python, it is not with all the versions on BP
- If it is not installed, this command will install it after loading the python module
 - `python -m pip install --user pip`
- Pip will normally try to install packages into a folder that you do not have access to on BP
- To avoid any issues, install packages into your home directory using the `--user` flag
 - `pip install --user cutadapt`
- Remember to load the same version of python that was used to install the packages every time.

Shell Scripts

- Shell scripts can range from a few lines to thousands of lines of code
- For this course, shell scripts will act as wrapper scripts when running sbatch.
 - A wrapper script will configure the environment for the batch job run by Slurm
 - The main components in the script are:
 - Shebang
 - Setting up the Slurm parameters
 - Purging and loading the correct modules
 - Loading a virtual environment / conda environment
 - Setting up any folders for output.
 - Running the program required for the analysis

```
driver.sh
1 #!/bin/bash shebang
2 #SBATCH --job-name=optimization_driver # Job name
3 #SBATCH --ntasks=1 # Run on a single CPU
4 #SBATCH --cpus-per-task=1
5 #SBATCH --mem=4gb # Job memory request
6 #SBATCH --time=12:00:00 # Time limit hrs:min:sec
7 #SBATCH -p=cpu_short
8
9
10 # Load all the packages you need
11 module purge
12 module load anaconda3
13 #conda activate py36
14 module load slurm/current
15
16 echo "Running Driver"
17 # run the python driver script
18 python driver.py
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```

Slurm Parameters

Set up required modules

Run the script

NORMAL driver.sh sh 77% 14/18 h:25

My Workflow

1. Start with an interactive job
 1. Load the modules you require (Keep track of the modules you use for writing .sh script)
 2. Use the command line application to run your analysis
 1. If your dataset is large, try to make a small version of it for testing
 1. For example, if you are working with FASTQ files, just include the first 100 reads from both files
 2. Read the documentation, focus on what flags are available to you, and what flags you require
 3. Once the script is running build your shell script using the commands you ran in the interactive session
2. Run the shell script using sbatch and the subset of the data, does it match the ijob
3. Run the same shell script using the entire dataset

Adding Command Line Arguments to Shell

- Positional command line arguments are represented as variables in a shell script
- Variables start with a '\$' symbol
 - \$0 is the name of the script
 - Any subsequent numbers will be the argument in those positions
- Use these variables to pass on command line arguments to the wrapped script
 - In qc.sh
 - ...
 - fastqc <flags> \$1 \$2
 - sbatch qc.sh test.R1 test.R2

```
# shell script 'cmd_args.sh'
echo $1
echo $2
# ---- end of script ----
```

```
$ sh cmd_args.sh argument1 argument2
argument1
argument2
```

Some Useful Commands

- `head <file>`
 - Output the first 10 lines of the file
 - “-n 100” flag will output the first 100 lines
- Piping
 - `<cmd> | <cmd>`
 - will feed the output of one command to the next
 - `cat <filename> | head`
 - `cmd > file`
 - output the result of the command to specified file
- `cmd >> file`
 - Append the result of the command to the file
- `grep “pattern” file`
 - Search for the specified pattern in the file
- `cat <file>, less <file>, more <file>`
 - Will all output the file to the terminal, all have different features.
 - `cat` can also be used to join files together