Introduction to Snakemake

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class: inverse, center, middle name: lesson3

Lesson 3

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Lesson 3

1. Assignment 2 Answer
2. Fixing when things go wrong
3. Priorities
4. Script files (Python, R, and Julia)
5. Modularizing workflows
6. Visualizing Workflows
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Assignment 2

When Things Go Wrong

Locked Working Directories

- Snakemake locks its working directory when running
  - Prevents other snakemake instances from running in the same place
- Snakemake removes the lock when it completes (success *or* failure)
- Lockfile may not be removed when if snakemake crashes or is killed by slurm
  - `scancel --user your_username`

```
Unable to lock working directory.
```

Unlocking a Stale Lock

The Correct Way: `--unlock`

```
sbatch -c 1 --mem 2G --wrap "snakemake --unlock -s path/to/your/workflow.smk -j 1"
```

☠☠☠ Nuclear Option ☠☠☠

```
rm -r ./.snakemake
```

When Things Go Wrong

It Should Have Worked But It Didn't!

- Sometimes a job finishes successfully but snakemake doesn't detect the outputs
- Filesystem latency *especially* on a cluster like Waffles can be a factor
    - It takes some non-zero amount of time to write results to disk
- Consider setting `--latency-wait` with larger number (default: `5` seconds)

Priorities

- Rule priorities may be set
- These **are not** the same as slurm partitions
- Only determine the priority of execution *within* the workflow
- Rules default to priority `0`
- Bigger numbers are higher priority

```
rule my_example:
    input: ...
    output: ...
    priority: 50
    shell: ...
```

Script Files

- Not to be confuse with an external command
- Like a `run` block, but stored in another file
  - Path is specified relative to the workflow
- Available languages:
  - Python
  - R
  - Julia
- Snakemake will use special variables in the script
  - These scripts won't be general purpose!
  - Tied to snakemake

Script Files

```
# workflow.smk
rule scriptfile_example:
    input:
        "path/to/inputfile",
        "path/to/other/inputfile"
    output:
        "path/to/outputfile",
        "path/to/another/outputfile"
    script:
        "scripts/script.py"
```

```
# scripts/script.py
def do_something(data_path, out_path, threads, myparam):
    # python code here

do_something(snakemake.input[0], snakemake.output[0],
             snakemake.threads, snakemake.config["myparam"])
```

Including Workflows

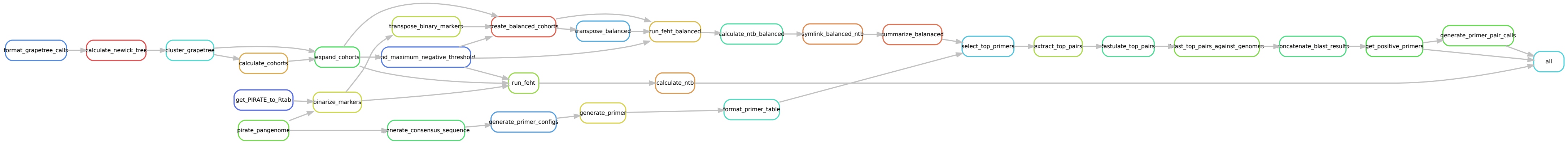
- Existing workflows can be included with `include`
- Allows more modular design of workflows
- Like copy/pasting another workflow in

```
rule all:
    input: "summary_report.txt"

include: "summary_report.smk"
include: "determine_amr.smk"
include: "assemble_genomes.smk"
```

Visualizing Workflows

```
# Shows just the abstract graph of rules
snakemake -s your/workflow.smk --rulegraph | dot -Tpng > workflow.png
# OR
# Show every sample's journey through the workflow
snakemake -s your/workflow.smk --dag | dot -Tpng > workflow.png
```



Clinic

Please feel free to ask any questions!