Snakemake

https://github.com/nichollskc/IMPC analysis

https://snakemake.readthedocs.io/en/stable/index.html

Idea of snakemake – defines dependencies

- Python version of Make
- Rules define inputs, outputs and commands to go from inputs to outputs
- Re-runs a rule if the inputs are older than the outputs

```
1 configfile: "config.yml"
2
3 rule fetch_fastq:
4
      params:
          url=lambda wildcards: config['FASTQ_URLS'][wildcards.ID]
5
6
      output:
          temp("data/fastq/{ID}.fastq.gz")
8
      shell:
          "wget -0 {output} --no-verbose {params.url} 2>&1"
9
10
11 rule run kallisto:
12
      input:
13
          "data/fastq/{ID}.fastq.gz"
14
      output:
15
          "data/kallisto/{ID}/abundance.tsv"
16
      shell:
          "kallisto quant --index={confiq[INDEX FILE]} --output-dir=$(dir
17
  name {output}) --single -l 50 -s 2 {input} 2>&1"
18
19
  rule generate_count_matrix:
20
      input:
21
          expand("data/kallisto/{ID}/abundance.tsv",
                 ID=list(config['FASTQ URLS'].keys()))
22
23
      output:
24
          df="data/tpm.tsv"
25
      run:
                                  fetch fastq
                                                         fetch fastq
                                                                               fetch fastq
                                                                                                      fetch fastq
26
          import worker
          df = worker generat | ID: ERS1370449
27
                                                      ID: ERS1370450
                                                                             ID: ERS1370451
                                                                                                   ID: ERS1370452
          df.to_csv(output.df
28
                                      run_kallisto |
                                                          run kallisto I
                                                                              run kallisto I
                                                                                                   run kallisto I
                                                               generate_count_matrix
                         snakemake data/tpm.tsv
```

snakemake --cluster "<COMMAND>" --jobs 100
--cluster-config cluster/slurm_config.json

Nice features

- Temporary/protected outputs
- Special status for log files
- Job groups run jobs in one SLURM job
- R/python scripts can access snakemake variables e.g. list of inputs
- Different cluster settings for different jobs

Excellent documentation

https://snakemake.readthedocs.io/en/stable/index.html