Making reproducible workflows with

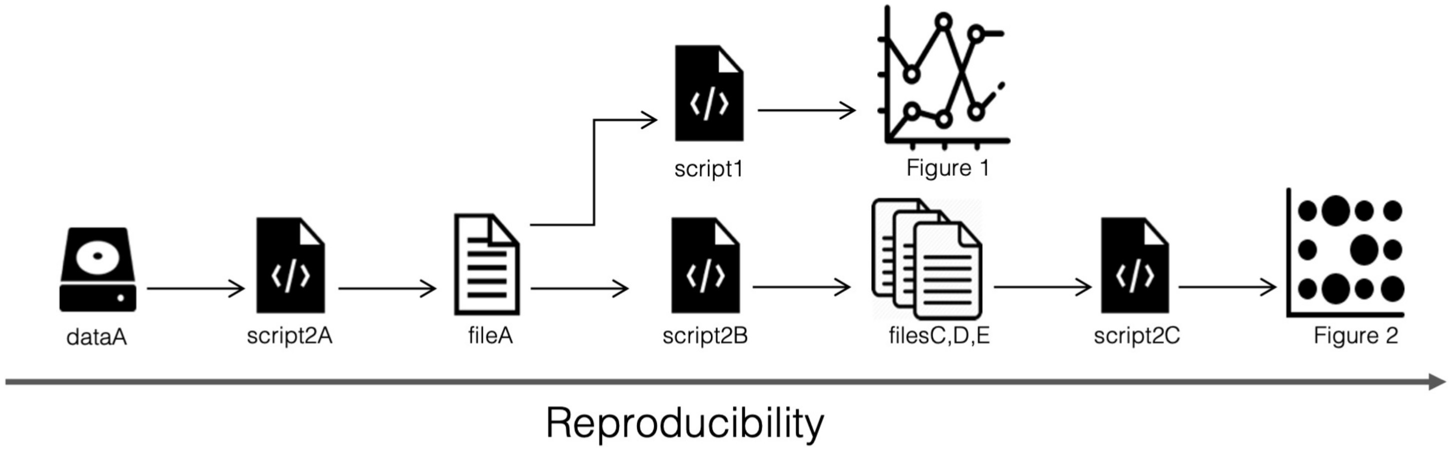
snakemake

A framework for reproducible data analysis

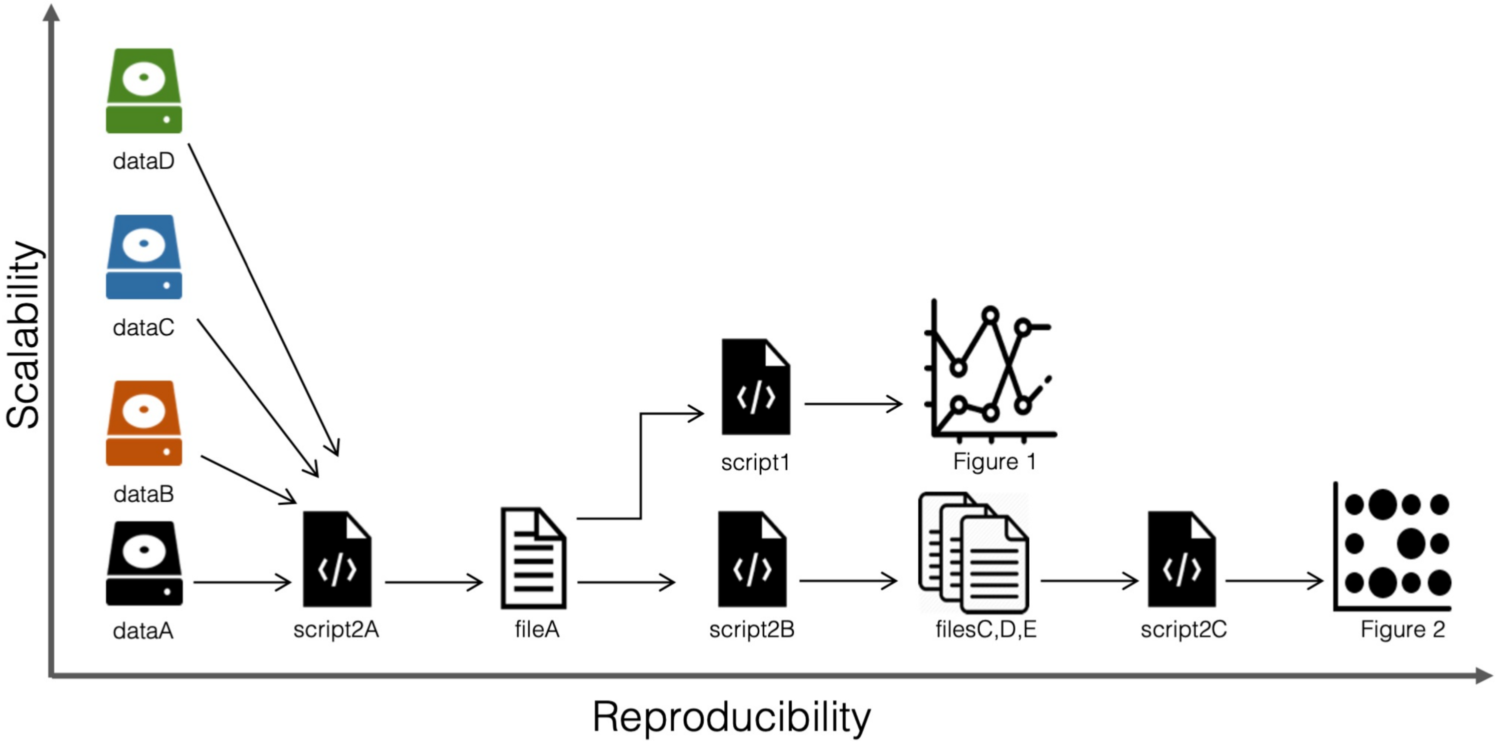
Snakemake workflows

- automatically track input/output file dependencies
- are built from rules
- are generalized with wildcards
- use a Python-based definition language
- easily scale from laptops to HPC clusters

Reproducible…



…and scalable workflows



Example: sequence trimming

Using a bash-script:

```
for sample in *.fastq
do
  id=$(echo ${sample} | sed 's/.fastq//')

  # 1. Trim fastq file
  seqtk trimfq -b 5 -e 10 $sample > ${id}.trimmed.fastq

  # 2. Compress fastq file
  gzip -c ${id}.trimmed.fastq > ${id}.trimmed.fastq.gz

  # 3. Remove intermediate files
  rm ${id}.trimmed.fastq
done
```

Example: sequence trimming

Using snakemake rules:

```
rule trim_fastq:
    output: temp("{prefix}.trimmed.fastq")
    input: "{prefix}.fastq"
    shell:
        "seqtk trimfq -b 5 -e 10 {input} > {output}"

rule gzip:
    output: "{prefix}.trimmed.fastq.gz"
    input: "{prefix}.trimmed.fastq"
    shell:
        "gzip -c {input} > {output}"
```

Example: sequence trimming

Using snakemake rules:

```
$ snakemake -c 1 {a,b}.trimmed.fastq.gz
```

Example: sequence trimming

Using snakemake rules:

```
$ snakemake -c 1 {a,b}.trimmed.fastq.gz
Provided cores: 1
Rules claiming more threads will be scaled down.
Job counts:
count   jobs
2       gzip
2       trim_fastq
4

rule trim_fastq:
    input: a.fastq
    output: a.trimmed.fastq
    wildcards: prefix=a
    1 of 4 steps (25%) done

rule gzip:
    input: a.trimmed.fastq
    output: a.trimmed.fastq.gz
    wildcards: prefix=a
Removing temporary output file a.trimmed.fastq.
2 of 4 steps (50%) done
```

Example: sequence trimming

Using snakemake rules:

```
$ snakemake -c 1 {a,b}.trimmed.fastq.gz
```

...

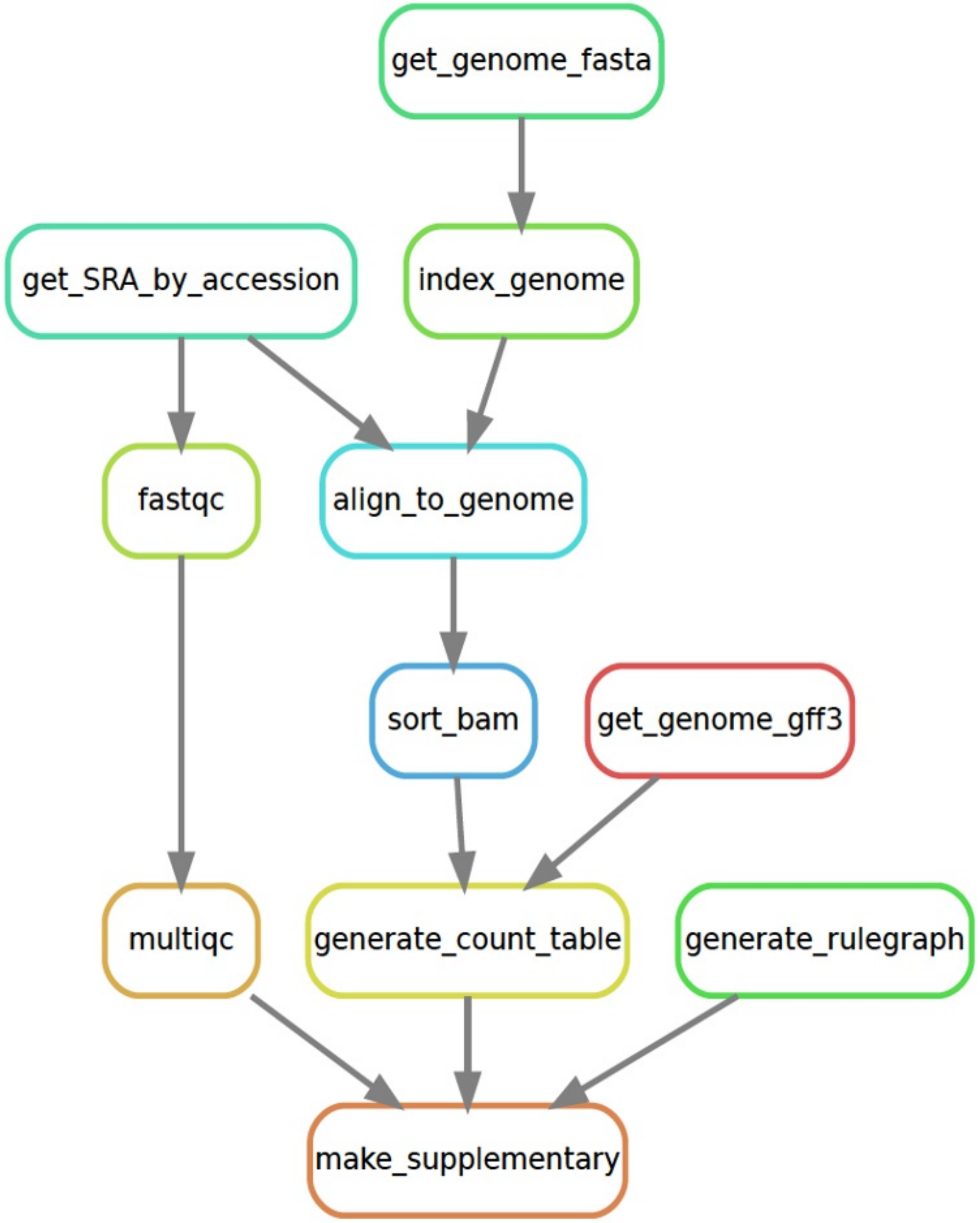
```
rule trim_fastq:
    input: b.fastq
    output: b.trimmed.fastq
    wildcards: prefix=b
3 of 4 steps (75%) done

rule gzip:
    input: b.trimmed.fastq
    output: b.trimmed.fastq.gz
    wildcards: prefix=b
Removing temporary output file b.trimmed.fastq.
4 of 4 steps (100%) done
```

Piecing the rules together

Snakemake figures out how rules can be pieced together to generate some requested output.

Here we ask for supplementary.pdf, which is an R Markdown report generated by the rule `make_supplementary`.



```
$ snakemake supplementary.pdf
```

Re-running the workflow

Here Snakemake detects that a file used in `align_to_genome` is newer than downstream files, so it reruns the necessary rules.

```
$ touch intermediate/NCTC8325.1.bt2
$ snakemake supplementary.pdf
```

Anatomy of a Snakemake rule

```
rule trim_fastq:
    output: temp("{prefix}.trimmed.fastq")
    input: "{prefix}.fastq"
    log: "logs/{prefix}.trim_fastq.log"
```

Anatomy of a Snakemake rule

```
rule trim_fastq:
    output: temp("{prefix}.trimmed.fastq")
    input: "{prefix}.fastq"
    log: "logs/{prefix}.trim_fastq.log"

    shell:
        """
        seqtk trimfq -t 8 –b 5 -e 10 {input} > {output} \
                    2> {log}
        """
```

Anatomy of a Snakemake rule

```
rule trim_fastq:
    output: temp("{prefix}.trimmed.fastq")
    input: "{prefix}.fastq"
    log: "logs/{prefix}.trim_fastq.log"

    # rule settings
    params:
        leftTrim=5,
        rightTrim=10

    shell:
      """
      seqtk trimfq -t 8 –b {params.leftTrim} \
                   -e {params.rightTrim} {input} > {output} \
                   2> {log}
      """
```

Anatomy of a Snakemake rule

```
rule trim_fastq:
    output: temp("{prefix}.trimmed.fastq")
    input: "{prefix}.fastq"
    log: "logs/{prefix}.trim_fastq.log"

    # rule settings
    params:
        leftTrim=5,
        rightTrim=10

    # resources
    threads: 8
    resources: mem=64

    shell:
      """
      seqtk trimfq -t {threads} –b {params.leftTrim} \
                    -e {params.rightTrim} {input} > {output} \
                    2> {log}
      """
```

Anatomy of a Snakemake rule

```
rule trim_fastq:
    output: temp("{prefix}.trimmed.fastq")
    input: "{prefix}.fastq"
    log: "logs/{prefix}.trim_fastq.log"

    # rule settings
    params:
        leftTrim=5,
        rightTrim=10

    # resources
    threads: 8
    resources: mem=64

    # software management
    conda: "envs/seqtk.yaml"
    container: "docker://quay.io/biocontainers/seqtk"

    shell:
      """
      seqtk trimfq -t {threads} –b {params.leftTrim} \
                   -e {params.rightTrim} {input} > {output} \
                   2> {log}
      """
```

Snakemake commandline

```
# Generate the output of the first rule in Snakefile
$ snakemake -s Snakefile
```

```
# Run the workflow in dry mode and print shell commands
$ snakemake -n -p
```

```
# Execute the workflow with 8 cores
$ snakemake --cores 8
```

```
# Specify a configuration file
$ snakemake --configfile config.yaml
```

```
# Run rules with specific conda environments
$ snakemake --use-conda
```

```
# Run rules with specific Singularity or Docker containers
$ snakemake --use-singularity
```

Questions?