Making reproducible workflows with

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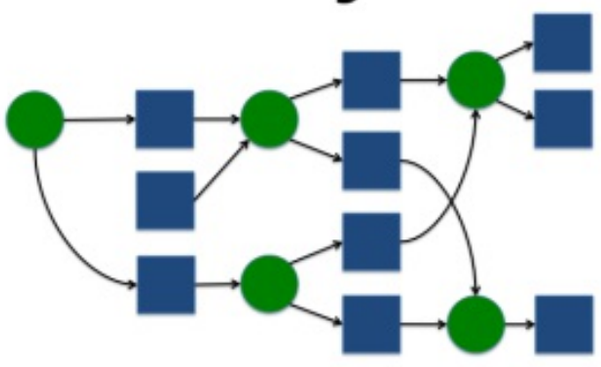
Why do we need workflow managers?

As projects grow or age, it becomes increasingly difficult to keep track of all the parts and how they fit together.

Workflow managers

Makeflow



GNU Make

nextflow

snakemake

A framework for reproducible data analysis

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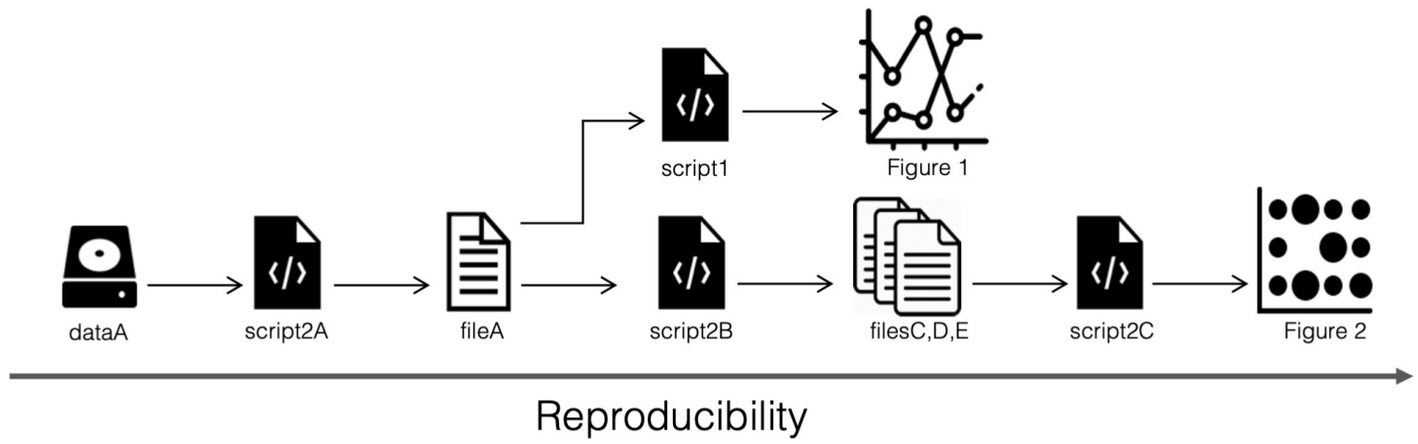
Snakemake workflows

- 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...



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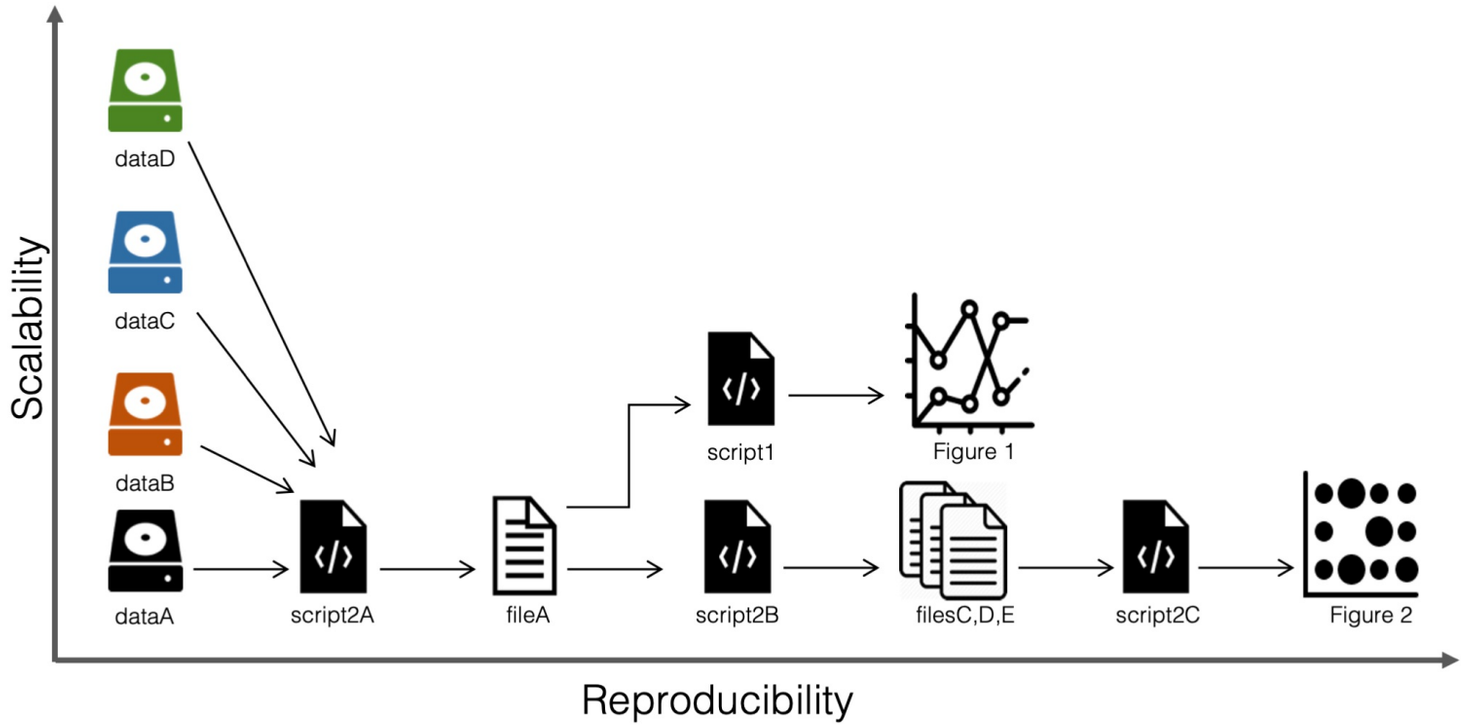
...and scalable workflows



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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
```

...

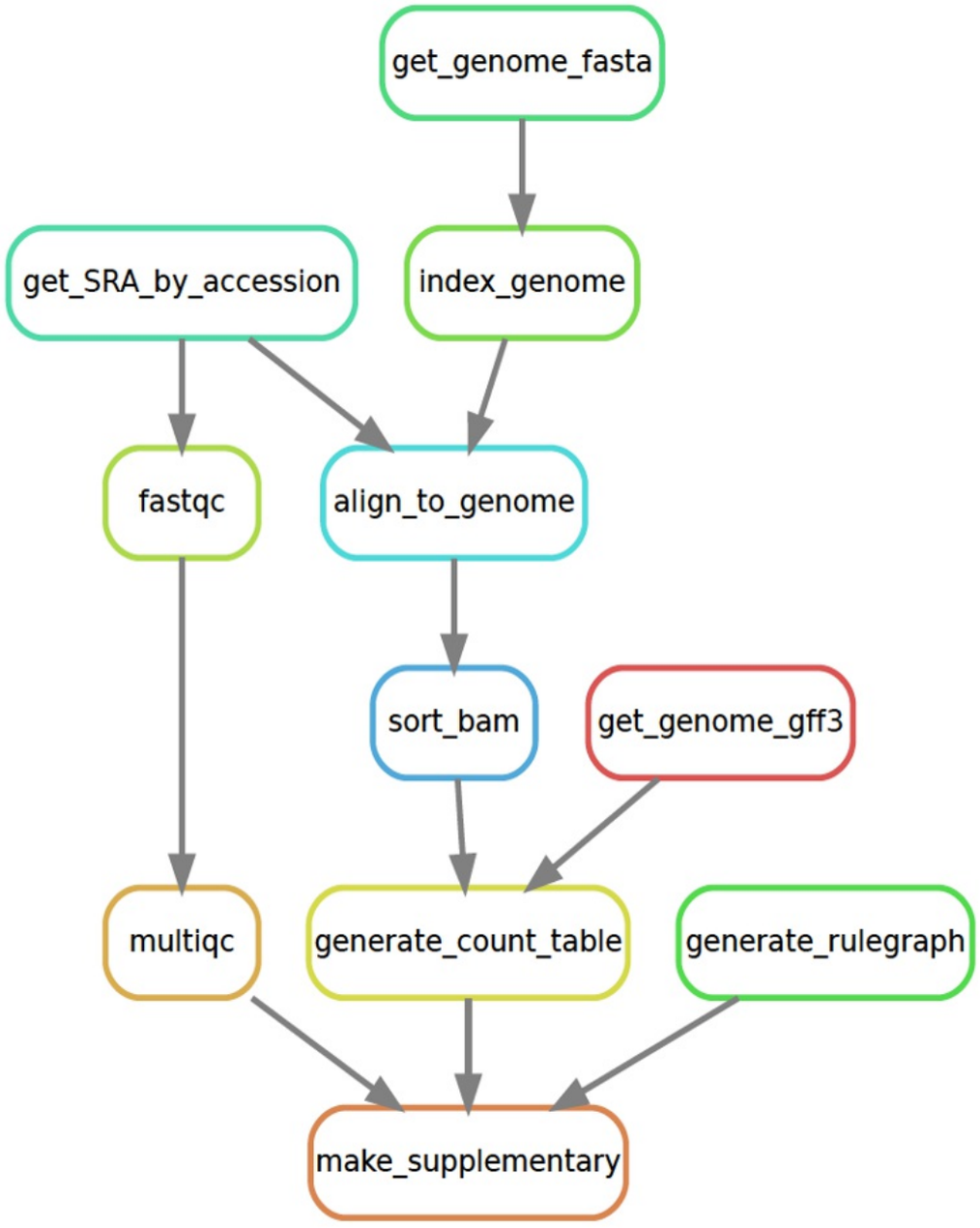
```
rule trim_fastq:
    input: b.fastq
    output: b.trimmed.fastq
    wildcards: prefix=b
3 of 4 steps (75%) done

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}
    """
```

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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?

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