FAIR Bioinfo 2023

Introduction to workflow language with Snakemake

P. Marin, M. Hiriart, P. Ruiz, Nadia Goué
aubi@uca.fr

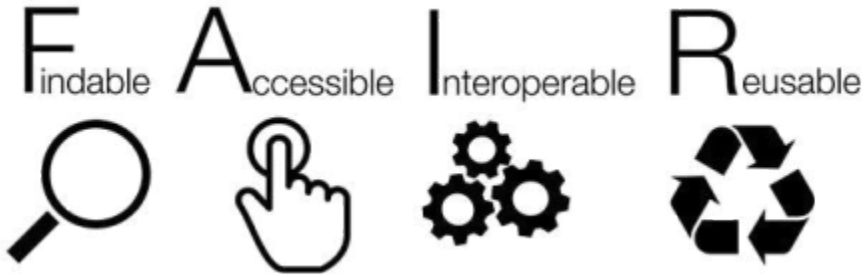
Université Clermont Auvergne, AuBi, Mésocentre

Du 10 au 13 & 14 juillet 2023

Contents

- Workflow introduction
- Snakemake introduction
- A little more on snakefile and configuration files

Interest in workflow management



- The standardization, portability, and reproducibility of analysis pipelines is a renowned problem within the bioinformatics community.
- It had struggled with issues of reproducibility and data provenance.
- Being able to reproduce scientific results is the central tenet of the scientific method.

Moving towards FAIR research methods in data-driven science is complex

What is a workflow ?

A pool of commands, progressively linked by the treatments,
from the input data towards the results

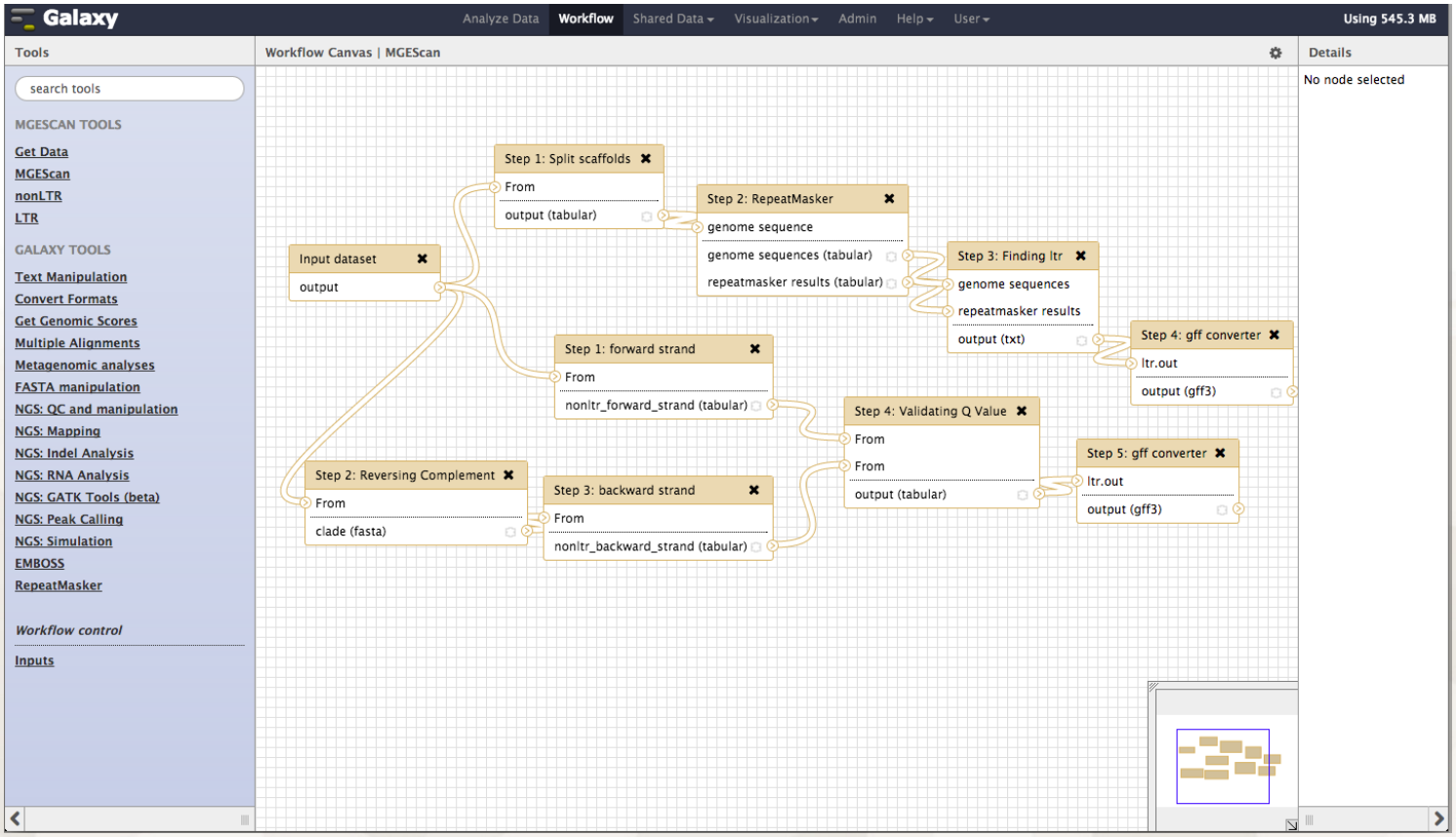
In case of data parallelization, several data flows can be processed in parallel:

- with a multi-cores PC or a computational cluster (ex. ~ 3 100 cores)
- one (or more) core can be attributed to one workflow

What is a workflow ?

- From informatics point of view : Group of programs executed in series
  so that the output of 1 program is used as input for the next one.

- From a bioinformatics point of view : a workflow is a set of pipelines



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What are workflow management systems ?

- Many workflow management systems, many forms

https://github.com/common-workflow-language/common-workflow-language/wiki/Existing-Workflow-systems

- command line: shell (needs competences into scripting)
- rule: snakemake, c-make, nextflow, ...
- graphic interface: Galaxy, Taverna, Keppler, ...

Reproducibility

Manage parallelization

Learning effort

What is Snakemake ?

Workflow manager

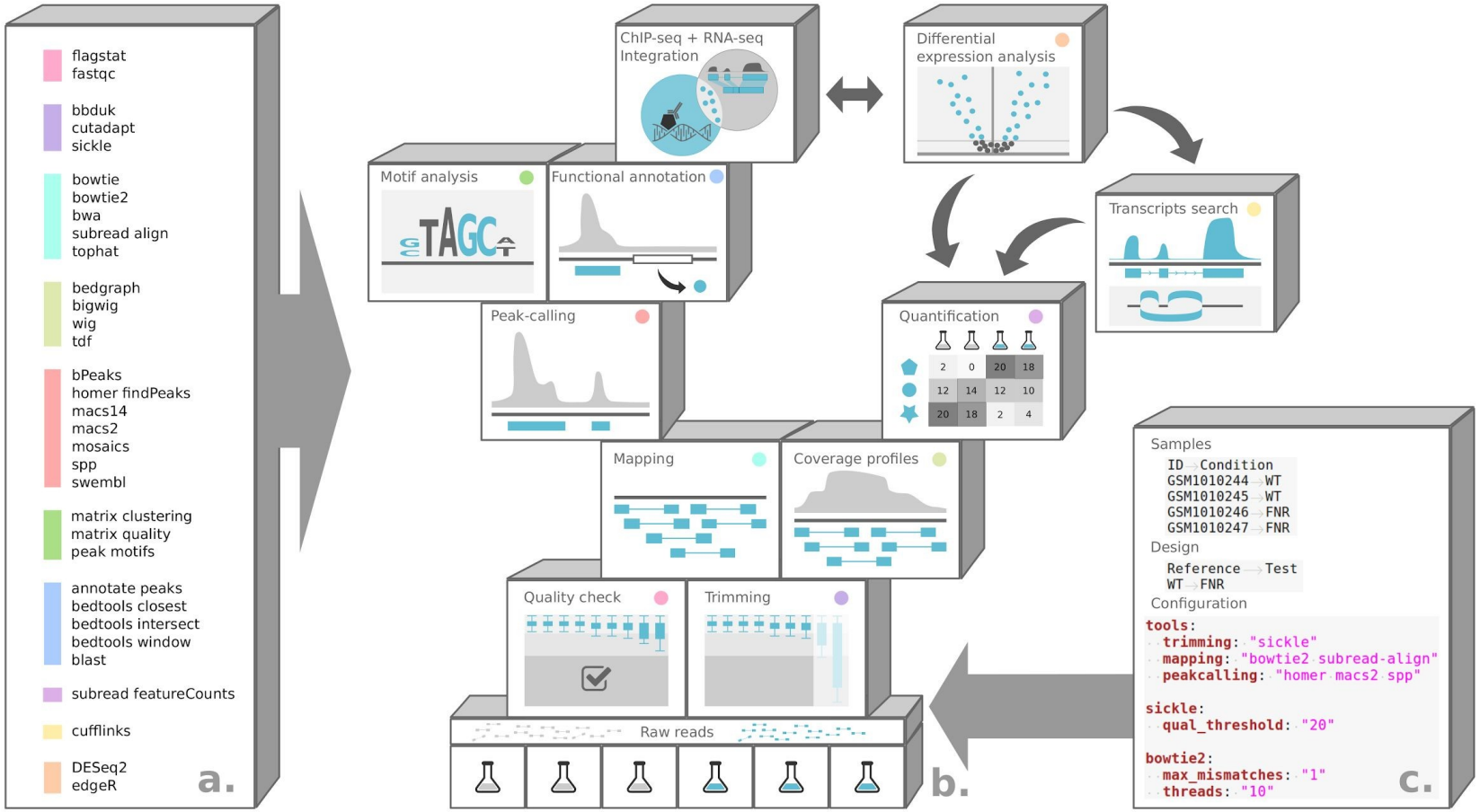
- Supports for dependencies
  - ✔ Refers to upstream files (or tasks) that downstream transformation steps require as input.
  - ✔ When a dependency is updated, associated downstream files should be updated as well.

- Support for reentrancy
  - ✔ Reentrancy is the ability of a program to continue where it left off if interrupted.
  - ✔ It's obviating the need to restart from the beginning of a process.

Köster and Rahmann, 2012. https://doi.org/10.1093/bioinformatics/bts480
Köster and Rahmann, 2018. https://doi.org/10.1093/bioinformatics/bty350

What is Snakemake ?

Reproducible and scalable analysis



Rioualen *et al.* 2017, https://doi.org/10.1101/165191, Rioualen *et al.* 2019 https://doi.org/10.1002/cpbi.72

The Snakemake rule

- Hybrid between
  - Python (Snake)
  - GNU Make, a rule-based automation tool
- Understanding the Rule concept. It has:
  - understandable name
  - input, list one or more filenames
  - output, list one or more filenames
  - command (run: for python ; shell: for shell, R, ...)
  - optional directives: params: , message: , log: , threads: , ...

```
rule NAME:
        input:
                "path/to/inputfile",
                "path/to/other/inputfile"
        output:
                "path/to/outputfile",
                "path/to/another/outputfile"
        shell: "some_command {input} {output}"
```

The data flow linkage and rules order

- Snakemake workflow links rules thanks to input and output filenames
  - ✔ Until v6.15.0: the first rule (all, target, ...) need to specify the result files and the next rules describe how to achieve them
  - ✔ From v6.15.0: any rule can be the default target rule

```
rule all:
        input: "P10415.fasta"

rule get_prot:
        output: "P10415.fasta"
        shell: "wget https://www.uniprot.org/uniprot/P10415.fasta"
```

The data flow linkage and rules order

- Snakemake automatically checks that everything is up-to-date:
  - ✔ Create a directed acyclic graph (DAG), linking rules with inputs and outputs
  - ✔ Starts with the last output result files of the DAG
  - ✔ Since output files do not exits or have to be re-created, snakemake goes back through the worlflow
  - ✔ Output files have to be re-created when the input file timestamp is newer than the output file one
  - ✔ And from this point, Snakemake goes on through the workflow and apply rules

Generalization with wildcards

- Snakemake use wildards to replace parts of filename:
  - ✔ Reduce hardcoding: more flexible, work with new data without modification
  - ✔ Are automatically resolved
  - ✔ Are written into {}
  - ✔ Are specific to a rule

- Examples

```
Rule read_firstlines:
        input:
                "101/file.A.txt"
        output:
                "{set}1/{file}.{grp}.txt"
          shell:
                "head -n 10 {input} > {output}"

=> set = 10, grp = A
```

```
Rule read_firstlines:
        input:
                "101/file.A.txt"
        output:
                "{set}/{file}.A.{ext}"
          shell:
                "head -n 10 {input} > {output}"

=> set = 101, ext = txt
```

Input / output specifications

- Enumerated

```
rule all:
    input:
        "P10415.fasta","P01308.fasta"
```

- Python list & wildcard

```
DATASETS=["P10415","P01308"]

rule all:
    input:
        ["{dataset}.fasta" for dataset in DATASETS]
```

- expand() & wildcards

```
DATASETS=["P10415","P01308"]
rule all:
  input: expand("{dataset}.fasta",dataset=DATASETS)
```

Snakemake Options

- Using a conda environment

Snakemake supports using explicit conda environments on a per-rule basis:

- ✔ directive in the rule definition:

```
rule NAME:
    input:
    output:
    conda: my_rule_env.yml
    shell:
```

- ✔ Run Snakemake with the --use-conda option
- ✔ The specified environment will be created and activated on the fly by Snakemake and the rule will then be run in the conda environment.

Snakemake Options

- Configuration file
  - ✔ contains all hard-coding values of the snakefile (paths to files, core numbers, parameter values, etc)
  - ✔ Is a yml or json file and call the defined items with config["myItem"]
  - ✔ Run with the --configfile myConfig.yml Snakemake option
  - ✔ Or add the directive configfile: myConfig.yml at the beginning of the snakefile

config.yaml

```
samples:
    A: data/samples/A.fastq
    B: data/samples/A.fastq
```

snakefile

```
configfile: "config.yaml"

rule NAME:
    input:
        expand("{sample}.fastq", sample=config[samples])
    output:
    shell:
```

Snakemake Options

- Some other useful options

  - ✔ dry-run, no workflow execution, display only what would be done: -n –dryrun
  - ✔ print the shell command: -p –printshellcmds
  - ✔ print a summary and status of rule: -D –summary
  - ✔ limit the number of jobs in parallel: -j 1 (cores: -c 1)
  - ✔ automatically create HTML reports (--report report.html) containing runtime statistics, a visualization of the workflow topology, used software and data provenance information (need to add the jinja2 package as a dependency)
  - ✔ DAG visualization with `dot` tool (graphviz package), to create diagrams of the complete workflow --dag or the rules dependencies --rulegraph

References

Amstutz P., *et al.* 2022. Existing Workflow systems. Common Workflow Language wiki, GitHub. https://s.apache.org/existing-workflow-systems updated 2022-08-30, accessed 2022-08-30.

Leipzig 2017. A review of bioinformatic pipeline frameworks. doi: 10.1093/bib/bbw020

Köster and Rahmann, 2012. Snakemake—a scalable bioinformatics workflow engine. https://doi.org/10.1093/bioinformatics/bts480

Köster and Rahmann, 2018. Snakemake—a scalable bioinformatics workflow engine. https://doi.org/10.1093/bioinformatics/bty350

LeipzigStallma and McGrath 1991. The GNU Make Reference Manual. ISBN-10:168092155X

Rioualen *et al.* 2017. SnakeChunks : modular blocks to build Snakemake workflows for reproducible NGS analyses. https://doi.org/10.1101/165191

Rioualen *et al.* 2019. Integrating Bacterial ChIP-seq and RNA-seq Data With SnakeChunks. https://doi.org/10.1002/cpbi.72

Workflow PRACTICE

Snakemake for a 2-steps workflow on Biosphere BioPipes VM