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Introduction to workflow language with Snakemake

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- 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

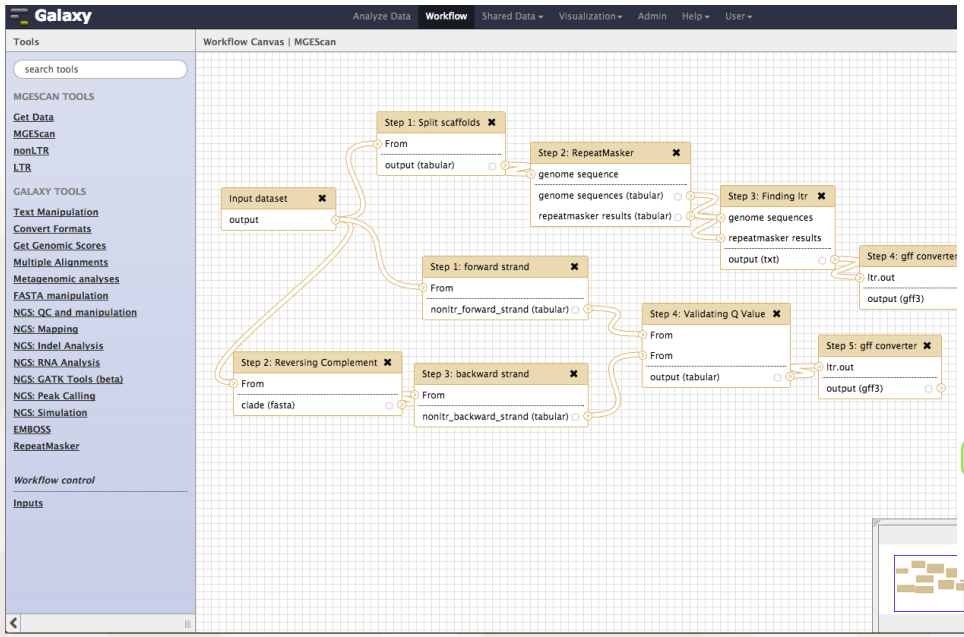
What is a workflow ?

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



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

Support for dependencies

Refer 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.

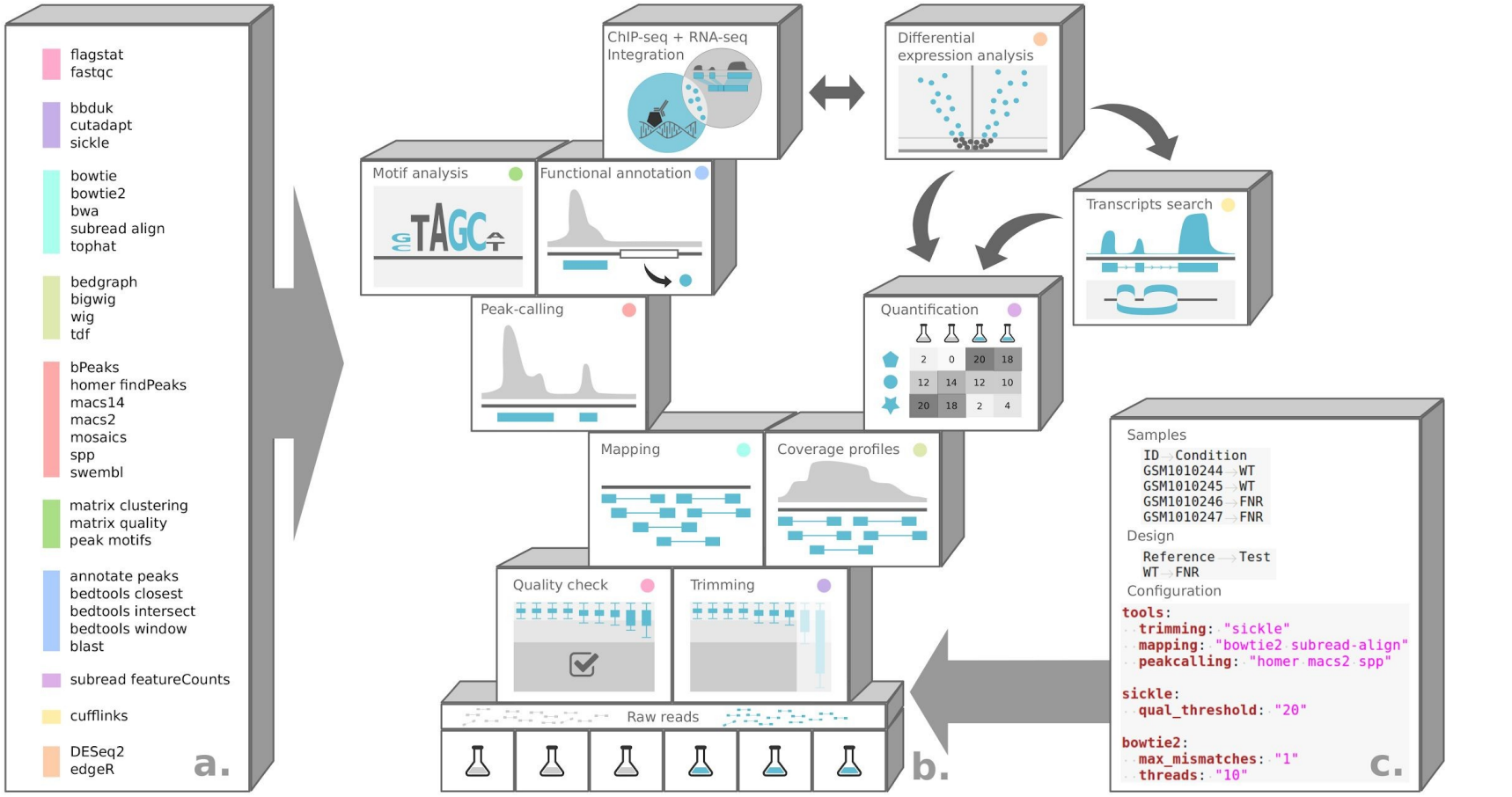
Support for reentrancy

Reentrancy is the ability of a program to continue where it left off if interrupted, 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
  - the programing language Python (Snake)
  - GNU Make, a rule-based automation tool
- Understanding the Rule concept. It has:
  - an understandable name
  - an input, list one or more filenames
  - an output, list one or more filenames
  - a 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}"
```

GNU Make Reference Manual. Stallman and McGrath, 1991

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

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

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

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Workflow PRACTICE

Snakemake for a 2-steps workflow on Biosphere BioPipes VM