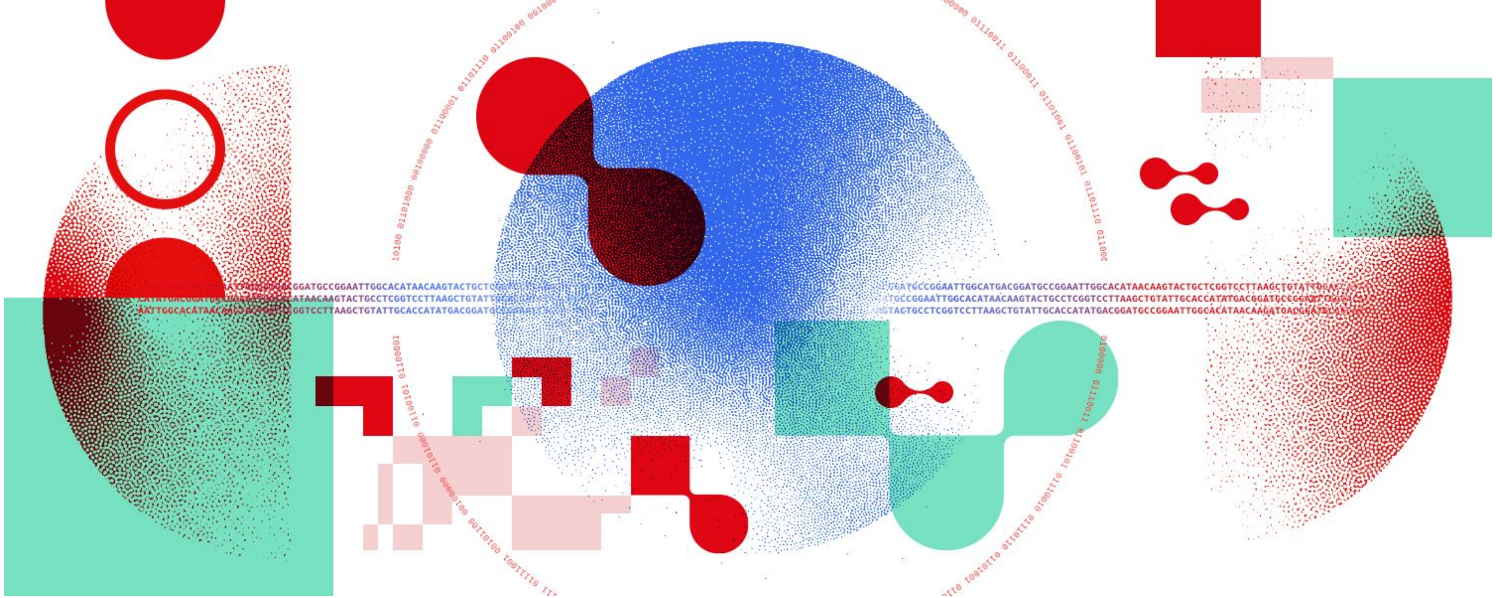


Snakemake for reproducible research

Making a more general-purpose Snakemake workflow

Centre hospitalier
universitaire vaudois

Empa
Materials Science and Technology

Antonin Thiébaut & Rafael Riudavets Puig
antonin.thiebaut@chuv.ch
Rafael.RiudavetsPuig@empa.ch

SIB
Swiss Institute of
Bioinformatics

What could we improve?

```
rule hello_world:
    output:
        'results/hello.txt'
    shell:
        'echo "Hello world!" > results/hello.txt'

rule copy_file:
    input:
        rules.hello_world.output
    output:
        'results/copied_file.txt'
    shell:
        'cp results/hello.txt results/copied_file.txt'
```

What could we improve?

```
rule hello_world:
    output:
        'results/hello.txt'
    shell:
        'echo "Hello world!" > results/hello.txt'

rule copy_file:
    input:
        rules.hello_world.output
    output:
        'results/copied_file.txt'
    shell:
        'cp results/hello.txt results/copied_file.txt'
```

- Using hard-coded file paths
- Having multiple inputs/outputs per rule
- (Checking Snakemake behaviour)

What could we improve?

```
rule hello_world:
    output:
        'results/hello.txt'
    shell:
        'echo "Hello world!" > results/hello.txt'

rule copy_file:
    input:
        rules.hello_world.output
    output:
        'results/copied_file.txt'
    shell:
        'cp results/hello.txt results/copied_file.txt'
```

- Using hard-coded file paths → Placeholders and wildcards
- Having multiple inputs/outputs per rule → Numbered/named inputs/outputs
- (Checking Snakemake behaviour) → (Log files)

What could we improve?

```
rule hello_world:
    output:
        'results/hello.txt'
    shell:
        'echo "Hello world!" > results/hello.txt'

rule copy_file:
    input:
        rules.hello_world.output
    output:
        'results/copied_file.txt'
    shell:
        'cp results/hello.txt results/copied_file.txt'
```

- Using hard-coded file paths → Placeholders and wildcards
- Having multiple inputs/outputs per rule → Numbered/named inputs/outputs
- (Checking Snakemake behaviour) → (Log files)

Avoiding hard-coded filepaths: placeholders

- Placeholder:
  - A person or thing that occupies the position or place of another person or thing
  - A symbol in a mathematical or logical expression that may be replaced by the name of any element of a set

(From the Merriam-Webster dictionary)

Avoiding hard-coded filepaths: placeholders

```
rule rename_file:
    input:
        'data/test.txt'
    output:
        'results/renamed_test.txt'
    shell:
        'mv data/test.txt results/renamed_test.txt'
```

Avoiding hard-coded filepaths: placeholders

```
rule rename_file:
    input:
        'data/test.txt'
    output:
        'results/renamed_test.txt'
    shell:
        'mv data/test.txt results/renamed_test.txt'
```

```
rule rename_file:
    input:
        'data/test.txt'
    output:
        'results/renamed_test.txt'
    shell:
        'mv {input} {output} '
```

Avoiding hard-coded filepaths: placeholders

- {input} and {output} are placeholders
- Used in shell directive
- Similar to python f-string
- Snakemake will replace them with appropriate values before running the command
- Many directives can use placeholders: {log}, {benchmark}, {params}…

```
rule rename_file:
    input:
        'data/test.txt'
    output:
       'results/renamed_test.txt'
    shell:
        'mv {input} {output} '
```

What could we improve?

```
rule hello_world:
    output:
        'results/hello.txt'
    shell:
        'echo "Hello world!" >{output}'

rule copy_file:
    input:
        rules.hello_world.output
    output:
        'results/copied_file.txt'
    shell:
        'cp {input} {output}'
```

- Using hard-coded file paths → Placeholders and wildcards
- Having multiple inputs/outputs per rule → Numbered/named inputs/outputs
- (Checking Snakemake behaviour) → (Log files)

Making more general-purpose rules: wildcards

- Wildcards ≈ "variables" automatically inferred by Snakemake

Making more general-purpose rules: wildcards

```
rule rename_file:
    input:
        'data/test.txt'
    output:
       'results/renamed_test.txt'
    shell:
        'mv {input} {output}'
```

Defined paths

- Wildcards ≈ "variables" automatically inferred by Snakemake

Making more general-purpose rules: wildcards

- Wildcards ≈ "variables" automatically inferred by Snakemake

```
rule rename_file:
    input:
        'data/test.txt'
    output:
       'results/renamed_test.txt'
    shell:
        'mv {input} {output}'
```

Defined paths

```
rule rename_file:
    input:
        'data/{file}.txt'
    output:
        'results/renamed_{file}.txt'
    shell:
        'mv {input} {output}'
```

Adaptable paths with wildcards

Making more general-purpose rules: wildcards

- Wildcards ≈ "variables" automatically inferred by Snakemake

- Enclose wildcard name with curly brackets `{ }`

```
rule rename_file:
    input:
        'data/test.txt'
    output:
       'results/renamed_test.txt'
    shell:
        'mv {input} {output}'
```

Defined paths

```
rule rename_file:
    input:
        'data/{file}.txt'
    output:
        'results/renamed_{file}.txt'
    shell:
        'mv {input} {output}'
```

Adaptable paths with wildcards

Making more general-purpose rules: wildcards

- Wildcards are "resolved" from the target and propagated to other directives
  - Regular expression matching: `.+`
    - "1 or more occurrences of any character except newline"
  - Can be constrained

- Using **wildcards forces to ask for output(s)**: Snakemake doesn't guess!
  - Target rules cannot contain wildcards

```
rule rename_file:
     input:
          'data/{file}.txt'
     output:
          'results/renamed_{file}.txt'
     shell:
          'mv {input} {output}'
```

```
snakemake --cores 1 results/renamed_test.txt
```

⇩

`{file} = "test"`

⇩

```
input: 'data/test.txt'
```

Making more general-purpose rules: wildcards

- Wildcards are "resolved" from the target and propagated to other directives
    - Regular expression matching: `.+`

- Both a workflow and a rule can use multiple wildcards

```
rule rename_file:
    input:
        'data/{file}_{nb}.txt'
    output:
        'results/renamed_{file}_{nb}.txt'
    shell:
        'mv {input} {output}'
```

```
snakemake --cores 1 results/renamed_test_1.txt
```

```
{file} = "test"; {nb} = "1"
```

```
input: 'data/test_1.txt'
```

Making more general-purpose rules: wildcards

- Wildcards are "resolved" from the target and propagated to other directives
    - Regular expression matching: `.+`
- Both a workflow and a rule can use multiple wildcards
- Input and output files do not need to share the same wildcards
- **All outputs, logs… created by a rule must have the same wildcards!**

```
rule rename_file:
    input:
        'data/{file}.txt'
    output:
        'results/renamed_{file}_{nb}.txt'
    shell:
        'mv {input} {output}'
```

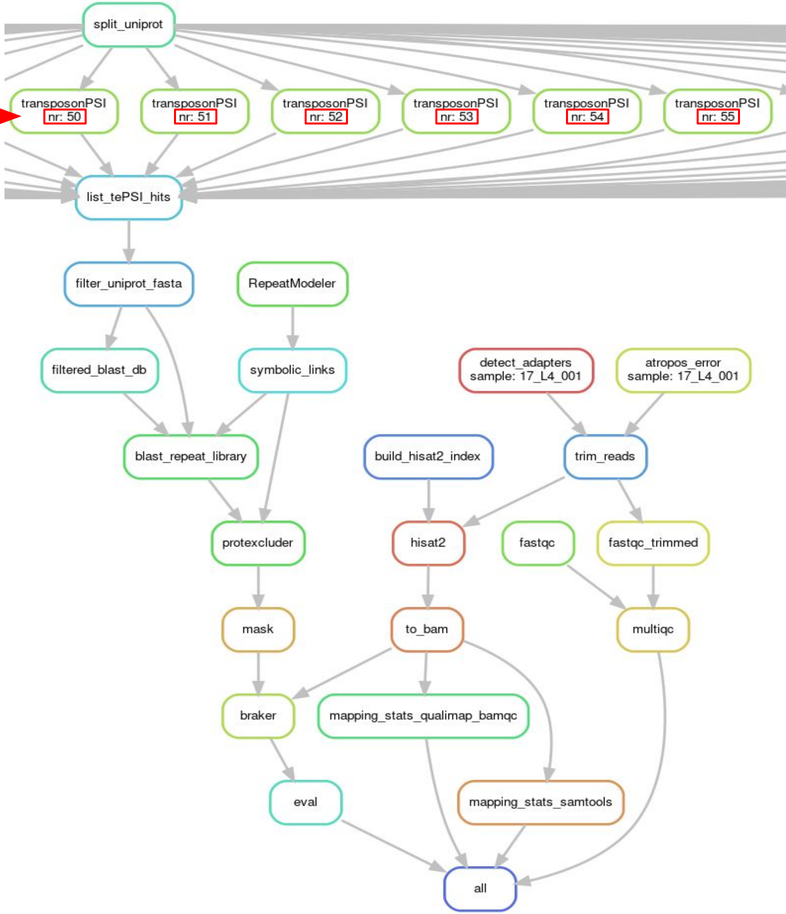
```
snakemake --cores 1 results/renamed_test_1.txt
```

```
{file} = "test"; {nb} = "1"
```

```
input: 'data/test.txt'
```

Building a Directed Acyclic Graph (DAG)

- Rule can appear more than once, with different wildcards
  - 1 rule + 1 wildcard values = 1 job



What could we improve?

```
rule hello_world:
    output:
        'results/hello.txt'
    shell:
        'echo "Hello world!" >{output}'

rule copy_file:
    input:
        rules.hello_world.output
    output:
        'results/copied_file.txt'
    shell:
        'cp {input} {output}'
```

- Using hard-coded file paths → Placeholders and wildcards
- Having multiple inputs/outputs per rule → Numbered/named inputs/outputs
- (Checking Snakemake behaviour) → (Log files)

Creating rules with multiple inputs/outputs

- Rules can use multiple inputs/outputs

Creating rules with multiple inputs/outputs

- Rules can use multiple inputs/outputs
    - Separated by a comma
    - Input values are **unpacked** (replaced by a space-separated list)

```
rule gather_files:
    input:
        'data/test1.txt',
        'data/test2.txt'
    output:
        'results/merged_test.txt'
    shell:
        'cat {input} > {output}'
```

⇩

```
shell:
    'cat data/test1.txt data/test2.txt > results/merged_test.txt'
```

Creating rules with multiple inputs/outputs

- Rules can use multiple inputs/outputs
    - Separated by a comma
    - Input values are **unpacked** (replaced by a space-separated list)
- Shell can have multiple commands
    - Separated by a semicolon
    - Commands are concatenated

```
rule gather_files:
    input:
        'data/test1.txt',
        'data/test2.txt'
    output:
        'results/merged_test.txt'
    shell:
        'cat {input} > {output}';
        'cat {input} >> {output}'
```

Creating rules with multiple inputs/outputs

- Rules can use multiple inputs/outputs
  - Separated by a comma
  - Input values are **unpacked** (replaced by a space-separated list)
- Shell can have multiple commands
  - ~~Separated by a semicolon~~
  - Commands are concatenated

```
rule gather_files:
    input:
        'data/test1.txt',
        'data/test2.txt'
    output:
        'results/merged_test.txt'
    shell:
        '''
        cat {input} > {output}
        cat {input} >> {output}
        '''
```

Creating rules with multiple inputs/outputs

- Rules can use multiple inputs/outputs
  - Separated by a comma
  - Input values are **unpacked** (replaced by a space-separated list)
- Shell can have multiple commands
  - ~~Separated by a semicolon~~
  - Commands are concatenated
- Inputs can be accessed by their positional index: input[n]
  - **Numbering starts at 0**

```
rule gather_files:
    input:
        'data/test1.txt',
        'data/test2.txt'
    output:
        'results/merged_test.txt'
    shell:
        '''
        cat {input[0]} > {output}
        cat {input[1]} >> {output}
        '''
```

Creating rules with multiple inputs/outputs

- Rules can use multiple inputs/outputs
    - Separated by a comma
    - Input values are **unpacked** (replaced by a space-separated list)
- Shell can have multiple commands
    - ~~Separated by a semicolon~~
    - Commands are concatenated
- Inputs can be accessed by their positional index: `input[n]`
    - **Numbering starts at 0**
- Named inputs can be accessed by their names: `input.input_name`

```
rule gather_files:
    input:
        file_1='data/test1.txt',
        file_2='data/test2.txt'
    output:
        'results/merged_test.txt'
    shell:
        '''
        cat {input.file_1} > {output}
        cat {input.file_2} >>
{output}
        '''
```

Creating rules with multiple inputs/outputs

- Outputs work like inputs
    - Separated by ','
    - Can be named
    - Can be accessed by positional index or by name
- All outputs need to be created or the job will fail

```
rule gather_files:
    input:
        file_1='data/test1.txt',
        file_2='data/test2.txt'
    output:
        copy_1='results/copied_test1.txt',
        copy_2='results/copied_test2.txt'
    shell:
        '''
        cat {input.file_1} > {output.copy_1}
        cat {input.file_2} > {output.copy_2}
        '''
```

```
snakemake --cores 1 results/copied_test1.txt
```

```
'results/copied_test1.txt', 'results/copied_test1.txt'
```

What could we improve?

```
rule hello_world:
    output:
        'results/hello.txt'
    shell:
        'echo "Hello world!" >{output}'

rule copy_file:
    input:
        rules.hello_world.output
    output:
        'results/copied_file.txt'
    shell:
        'cp {input} {output}'
```

- Using hard-coded file paths → Placeholders and wildcards
- Having multiple inputs/outputs per rule → Numbered/named inputs/outputs
- (Checking Snakemake behaviour) → (Log files)

Checking Snakemake behaviour: log files

- 'log' is a directive; its value is a path to a log file for one rule
    - Can be accessed with a placeholder in shell: {log}

```
rule rename_file:
    input:
        'data/test.txt'
    output:
        'results/renamed_file.txt'
    log:
        'logs/renaming.log'
    shell:
        'mv {input} {output} 2> {log}'
```

Checking Snakemake behaviour: log files

- 'log' is a directive; its value is a path to a log file for one rule
  - Can be accessed with a placeholder in shell: {log}
- You need to manually redirect messages to logs, but Snakemake automatically creates the folder path

```
rule rename_file:
    input:
        'data/test.txt'
    output:
        'results/renamed_file.txt'
    log:
        'logs/renaming.log'
    shell:
        'mv {input} {output} 2> {log}'
```

Checking Snakemake behaviour: log files

- 'log' is a directive; its value is a path to a log file for one rule
    - Can be accessed with a placeholder in shell: {log}
- You need to manually redirect messages to logs, but Snakemake automatically creates the folder path
- Log files must have the **same wildcards as the output**!
- Best practice: put all logs in same folder

```
rule rename_file:
    input:
        'data/test.txt'
    output:
        'results/renamed_file.txt'
    log:
        'logs/renaming.log'
    shell:
        'mv {input} {output} 2> {log}'
```

Exercises

- Through the day:
  - Develop a simple RNAseq analysis workflow, from reads (fastq files) to Differentially Expressed Genes (DEG)

- For this session:
  - Use multiple inputs and outputs
  - Use placeholders and wildcards
  - Visualise a workflow DAG
  - (Check a workflow's behaviour)