



# Snakemake for reproducible research

Making Snakemake even more reproducible

Antonin Thiébaut & Rafael Riudavets Puig

[antonin.thiebaut@chuv.ch](mailto:antonin.thiebaut@chuv.ch)

[Rafael.RiudavetsPuig@empa.ch](mailto:Rafael.RiudavetsPuig@empa.ch)

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  - **Conda/mamba**: open-source, cross-platform, language-agnostic package manager and environment management system
  - **Channels**: field-specific repositories of software
    - [Conda-forge](#): general computation
    - [Bioconda](#): bioinformatics

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  - **Channels**: field-specific repositories of software
    - [Conda-forge](#): general computation
    - [Bioconda](#): bioinformatics
  - Environments defined in YAML files

```
name: python_env
channels:
  - conda-forge
  - bioconda
dependencies:
  - python >= 3.12
  - pandas == 2.2.3
```

py.yaml

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    - Value: path to the environment file relative to the rule's snakefile

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rule rename_file:
    input:
        'data/test.txt'
    output:
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    conda:
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    shell:
        'mv {input} {output}'
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- Snakemake provides integrated package management via Conda to define isolated software environments per rule
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  - Value: path to the environment file relative to the rule's snakefile
- Execution parameter:

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```

- v7 and before: `--use-conda`

```
snakemake --cores 1 --use-conda results/rename_file.txt
```

- v8+: `--software-deployment-method` or `--sdm` (shorthand version)

```
snakemake --cores 1 --sdm conda
results/rename_file.txt
```

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    - Handles Docker and Apptainer images
    - **Global** OR **rule-specific**

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container:
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snakemake -c 1 --use-singularity
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snakemake -c 1 --sdm apptainer
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  - Execution parameter
    - v7 and before: `--use-singularity`
    - V8+: `--sdm apptainer`
  - Can be combined with conda `--sdm conda apptainer`
    - Pull the image
    - Create the conda env from **within the container**
  - Containerisation of Conda-based workflows

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```
snakemake -c 1 --sdm conda apptainer
results/renamed_file.txt
```

```
snakemake -c 1 --containerize > Dockerfile
```

# Snakemake environments

- Question 6

# What is the best setting for Snakemake environments?

- Use package and container managers!
- Same as Snakefile and config files: split things reasonably
  - 1 .smk file  $\approx$  1 'thematic' module  $\approx$  1 environment
- Always check for version conflicts



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    params:
        lines = 5
    run:
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- Replaces **shell/run**
- Access to directive values and variables, like in **shell**
- Value = path to the script relative to the rule's snakefile
- Advantages:
  - Great for long code
  - Can use **conda/singularity** directive!!!



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```
# Retrieve information from Snakemake
input_file = open(snakemake.input[0])
output_file = open(snakemake.output[0], 'w')
n_lines = snakemake.params.lines

# Process file
for i in range(n_lines):
    output_file.write(input_file.readline())
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first\_step.py

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```
library(readr)

# Retrieve information from Snakemake
input_path <- snakemake@input[[1]]
output_path <- snakemake@output[[1]]
n_lines <- snakemake@params$lines[1]

# Process file
data <- read_delim(input_path, '\t',
```

first\_step.R

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    - No parentheses, no argument

```
def seq_input(wildcards):  
    type = wildcards.type  
    if type == 'SE':  
        return 'data/file1.fq'  
    else:  
        return ['data/file1.fq', 'data/file2.fq']  
  
rule merge_files:  
    input:  
        seq_input  
    output:  
        'results/{type}.txt'  
    shell:  
        'cat {input} > {output}'
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- Input functions = Python functions
  - Single argument: **wildcards**
  - Return a file or list of files
  - Can also return a dictionary with **input** names as keys
    - Use `input: unpack(<function_name>)` to obtain named inputs

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  - Can also return a dictionary with **input** names as keys
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- Functions are evaluated before workflow execution  $\Rightarrow$  can't list **output** files
  - **No output functions!**

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```

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



```
{type} = "NotSE"
```



```
input:  
    ['data/file1.fq', 'data/file2.fq']
```

# Working after an unknown number of inputs/outputs

- *aka* 'Data-dependent conditional execution' *aka* **checkpoint** (instead of **rule**)
- When:
  - An unknown number of files is generated by a rule
  - **Output** files are unknown before execution
- Conditional reevaluation of the DAG of jobs based on the outputs content
  - Since DAG is re-evaluated midway □ you can't see the whole workflow at the start
- **Very complicated!**



# Exercises

- Through the day:
  - Develop a simple RNAseq analysis workflow, from reads (fastq files) to Differentially Expressed Genes (DEG)
- For this session:
  - Use an input function
  - Use R and Python scripts
  - Run a rule inside a conda environment
  - Run a rule inside a Docker/Singularity container

