Snakemake for reproducible research

Decorating and optimising a 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? (again)

- Avoiding hard-coded parameters
- Processing list of files
- Optimising resource usage

What could we improve? (again)

- Avoiding hard-coded parameters → config file
- Processing list of files → expand() syntax
- Optimising resource usage → Threads directive

What could we improve? (again)

- Avoiding hard-coded parameters → config file
- Processing list of files → expand() syntax
- Optimising resource usage → Threads directive

Avoiding hard-coded parameters: config file

- Snakemake can use configuration files to render workflows more flexible
  - Change config instead of code!

Avoiding hard-coded parameters: config file

- Snakemake can use configuration files to render workflows more flexible
  - Change config instead of code!
- Imported file with configfile keyword in Snakefile
  - configfile: 'path/to/config.yaml' (relative to working directory)
- 2 possible formats: JSON and YAML
  - Personal opinion: YAML is easier to write, understand and can be commented

```json
{
  "retries": 5,
  "samples": [
    "file1",
    "file2"
  ],
  "resources": {
    "threads": 8,
    "memory": "500M"
  }
}
```

JSON

```yaml
retries: 5  # Single value
samples:  # Multiple values
    - file1
    - file2
resources:  # Nested parameters
    threads: 8
    memory: 500M
```

YAML

Avoiding hard-coded parameters: config file

- Snakemake can use configuration files to render workflows more flexible
  - Change config instead of code!
- Imported file with configfile keyword in Snakefile
  - configfile: 'path/to/config.yaml' (relative to working directory)
- 2 possible formats: JSON and YAML
  - Personal opinion: YAML is easier to write, understand and can be commented
- Accessed via global variable config
  - Imported as a Python dictionary (use keys to access values): config['samples']

```
{
  "retries": 5,
  "samples": [
    "file1",
    "file2"
  ],
  "resources": {
    "threads": 8,
    "memory": "500M"
  }
}
```

JSON

```
retries: 5  # Single value
samples:  # Multiple values
    - file1
    - file2
resources:  # Nested parameters
    threads: 8
    memory: 500M
```

YAML

Config file?

- Question 5

What should appear in a config file?

- Ideally, everything that should not be hard-coded:
  - File locations
  - Sample names and associated information
  - Rule computing resources
  - Etc…

What should appear in a config file?

- Ideally, everything that should not be hard-coded:
  - File locations
  - Sample names and associated information
  - Rule computing resources
  - Etc…

- But it is preferable to use paths to other smaller config files
  - Same as Snakefile and snakefiles
  - Example:
    - Table containing the sample names and information: `config/samples_info.tsv`
      - Tab-separated format is easy to write, read and parse
    - In the config file: `samples: 'config/samples_info.tsv'`
    - Add a function in a Snakefile to parse the table

What should **NOT** appear in a config file?

- Credentials: access tokens, passwords…

➔ Use environment variables (envvars)

What could we improve? (again)

- Avoiding hard-coded parameters → config file
- Processing list of files → expand() syntax
- Optimising resource usage → Threads directive

Processing list of files: the expand syntax

- expand(): Snakemake function to expand a wildcard expression to several values
  - Useful to define multiple inputs or outputs with a common pattern

Processing list of files: the expand syntax

- expand(): Snakemake function to expand a wildcard expression to several values
  - Useful to define multiple inputs or outputs with a common pattern
  - Syntax: expand('{wildcard_name}', wildcard_name=<values>)
    - <values>: iterable (*i.e.* list, tuple, set) containing the wildcard values

```
rule merge_files:
    input:
        'data/test_1.txt',
        'data/test_2.txt',
        'data/test_3.txt'
    output:
        'results/total.tsv'
    shell:
        'cat {input} > {output}'
```

```
rule merge_files:
    input:
        expand('data/test_{file}.txt', file=[1, 2, 3])
    output:
        'results/total.tsv'
    shell:
        'cat {input} > {output}'
```

➢ The rule merge_files uses all three input files to generate a single output file
  ➢ **expand() does not apply the rule three times, once per input!**

Processing list of files: the expand syntax

- When there are several wildcards, expand() creates **all possible combinations**

Processing list of files: the expand syntax

- When there are several wildcards, expand() creates **all possible combinations**

```
files=['test_A','test_B']
nbs = [1, 2]

rule merge_files:
    input:
        expand('data/{file}_{nb}.tsv', file=files, nb=nbs)
    output:
        'results/total.tsv'
    shell:
        'cat {input} > {output}'
```

```
input:
    ['data/test_A_1.tsv', 'data/test_A_2.tsv',
     'data/test_B_1.tsv', 'data/test_B_2.tsv']
```

Processing list of files: the expand syntax

- The wildcards in expand() are **independent** from wildcards in the rule

Processing list of files: the expand syntax

- The wildcards in expand() are **independent** from wildcards in the rule

```
files=['test_A','test_B']
nbs = [1, 2]

rule merge_files:
    input:
        expand('data/{file}_{nb}.tsv', file=files, nb=nbs)
    output:
        'results/{file}.tsv'
    shell:
        'cat {input} > {output}'
```

➢ Here, {file} value will NOT be propagated to the input

What could we improve? (again)

- Avoiding hard-coded parameters → config file
- Processing list of files → expand() syntax
- Optimising resource usage → Threads directive

Optimising resource usage: threads

- 'threads' is a directive; its value is the number of threads to allocate to each job spawned by a rule
  - New type of value: numeric (integer)
  - When executed locally, '--cores' controls the total number of threads allocated to Snakemake; threads is automatically decreased if it's lower than '--cores'
  - **Check whether software can actually multithread!**

```
rule example:
    input:
        'data/test.txt'
    output:
        'results/modified_test.txt'
    threads: 4
    shell:
        'command --threads {threads} {input} > {output}'
```

Exercises

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

- For this session:
  - Use a config file
  - Process list of inputs
  - Modularise a workflow
  - Aggregate outputs
  - (Optimise resource usage)
  - (Manage non-conventional outputs)