

# Snakemake for reproducible research

Making a more general-purpose Snakemake workflow

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

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- Using hard-coded file paths → Placeholders and wildcards
- Having multiple **inputs/outputs** per rule → Numbered/named inputs/outputs
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- Using hard-coded file paths —————→ **Placeholders and wildcards**
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# 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'
```

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    output:
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        'mv data/test.txt results/renamed_test.txt'
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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}`...

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    input:
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    shell:
        'mv {input} {output}'
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```

} 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'
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} 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
```



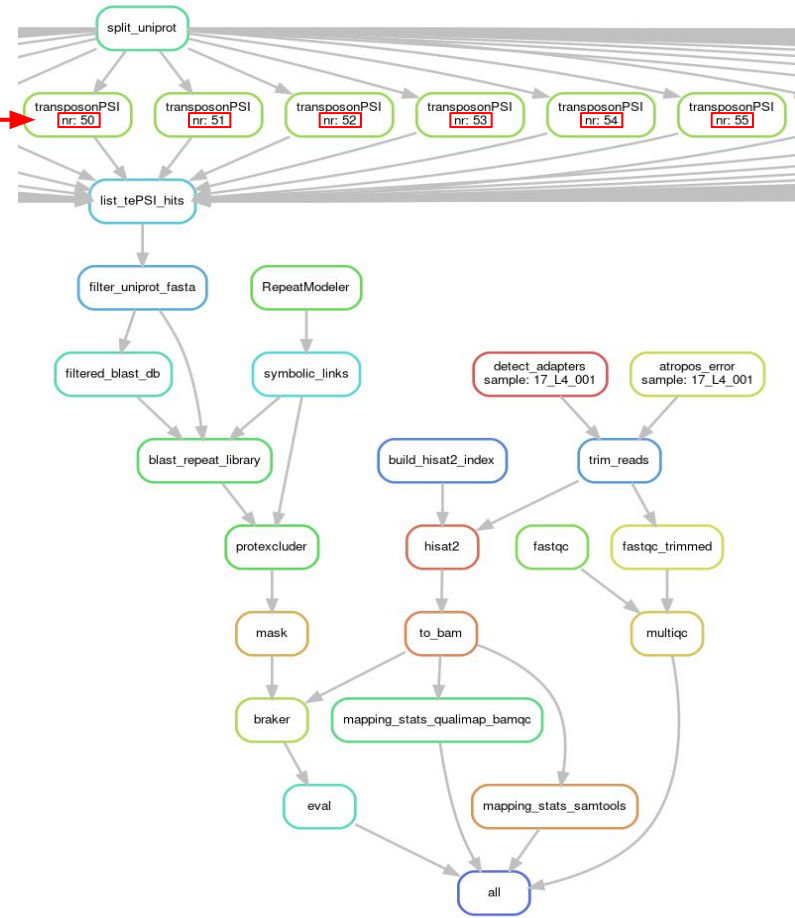
```
{file} = "test"; {nb} = "1"
```



```
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?

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rule hello_world:
    output:
        'results/hello.txt'
    shell:
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rule copy_file:
    input:
        rules.hello_world.output
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        'cp {input} {output}'
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# Creating rules with multiple inputs/outputs

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  - 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

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

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  - 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}
        '''
```



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  - 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'
```

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    output:
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    shell:
        'echo "Hello world!" >{output}'

rule copy_file:
    input:
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# 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}'
```

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- You need to **manually redirect messages to logs**, but Snakemake automatically creates the folder path

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- Log files must have the **same wildcards as the output!**
- Best practice: put all logs in same folder

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```

# 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)

