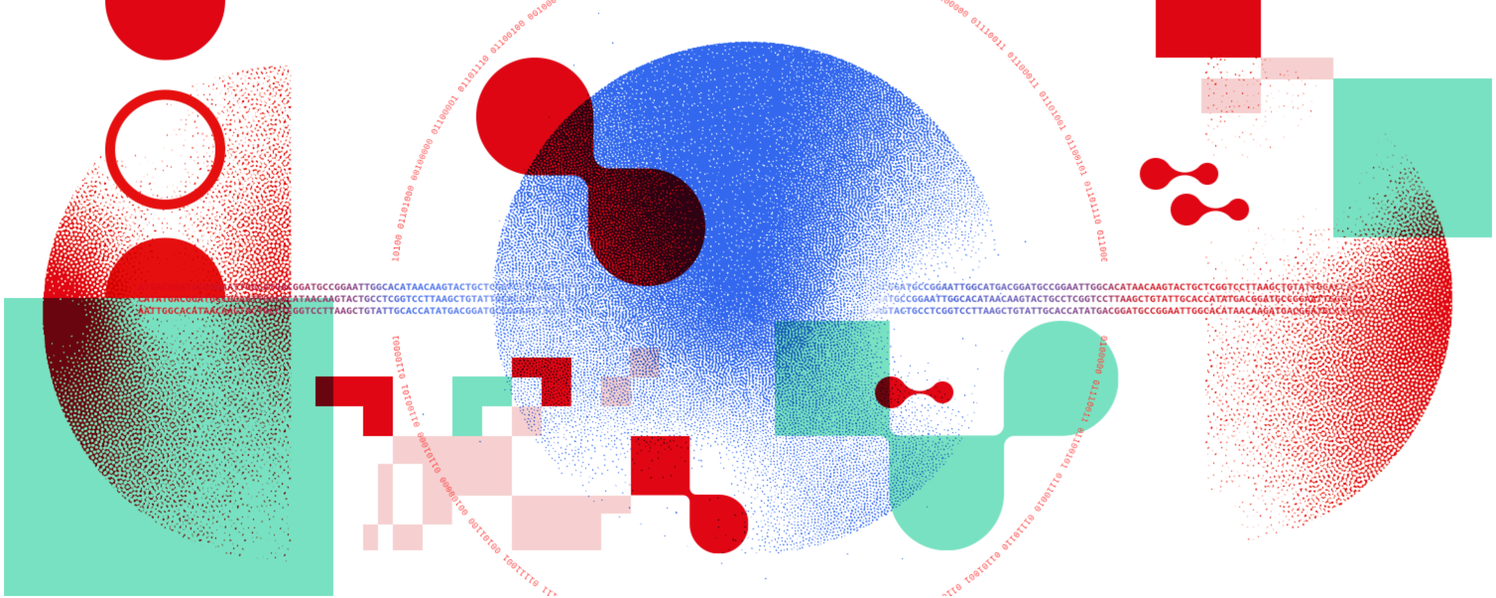


Snakemake for reproducible research

Introduction to Snakemake

Antonin Thiébaut

antonin.thiebaut@chuv.ch

Centre hospitalier
universitaire vaudois

SIB
Swiss Institute of
Bioinformatics

Reproducibility

- Question 1

What is reproducibility?

- Replicability vs repeatability vs reproducibility

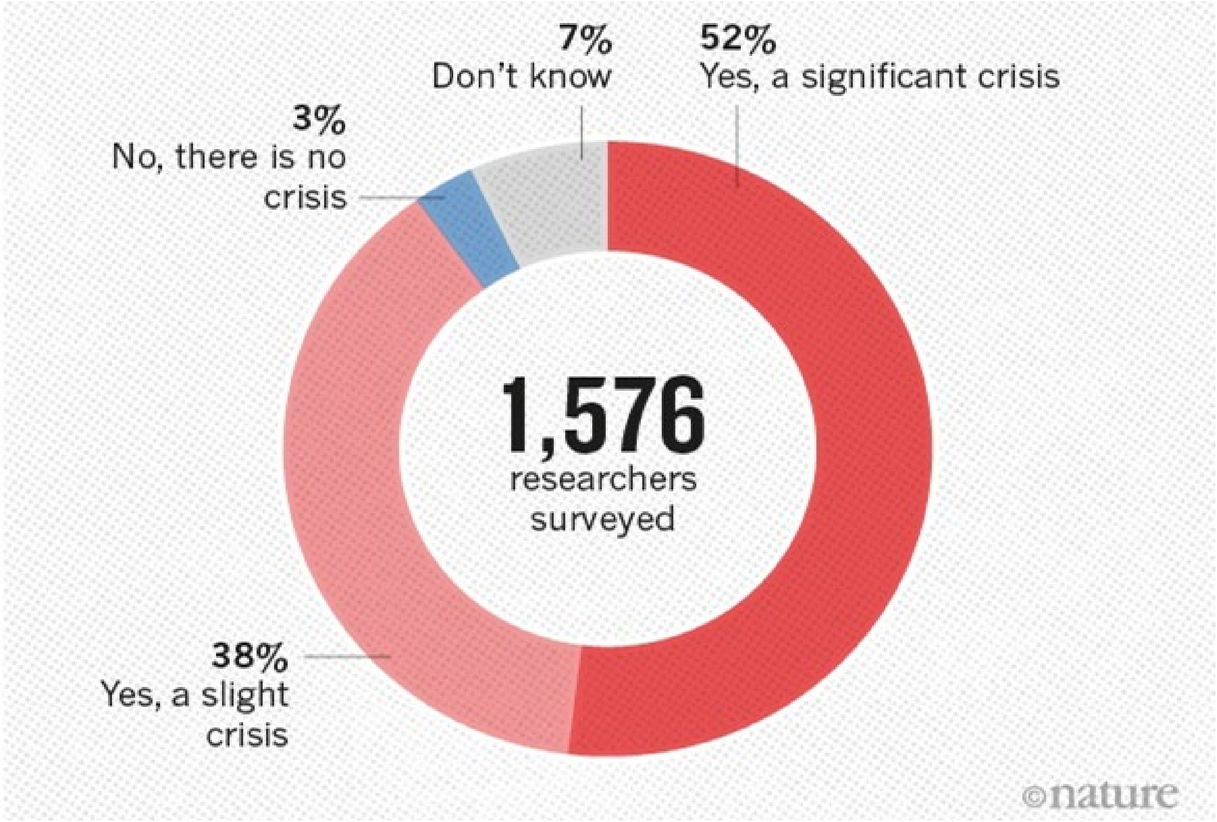
- “Reproducibility is more or less the ability to draw similar conclusions from replicates studies”
  - Diaba-Nuhoho, P., Amponsah-Offeh, M., *BMC Research Notes* (2021), https://doi.org/10.1186/s13104-021-05875-3

- Key component of the scientific method, “cornerstone of science”

Reproducibility crisis

- Question 2

Is there a reproducibility crisis?



Baker, M., *Nature* (2016), https://doi.org/10.1038/533452a

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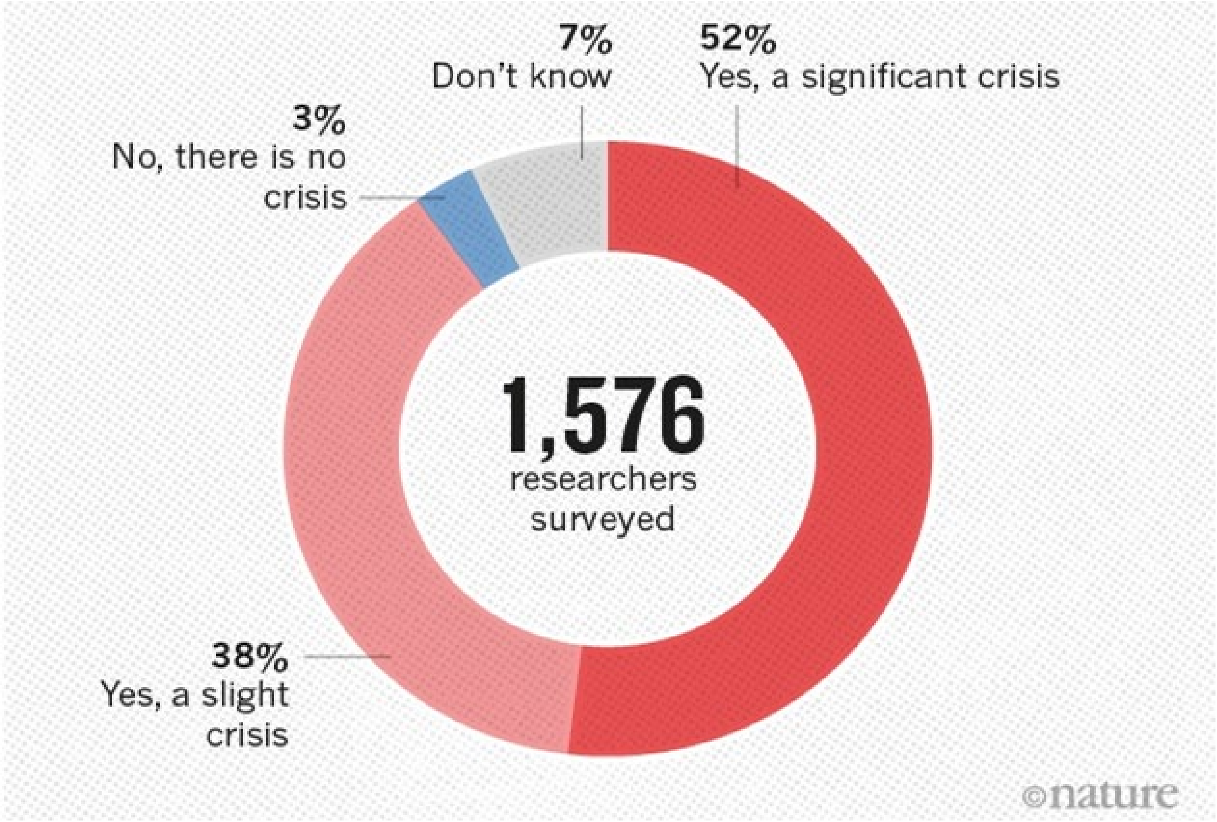

- Alfredo Sánchez-Tójar, Universität Bielefeld
- Publication bias in ecology and evolutionary biology:
  - https://www.youtube.com/watch?v=wdhzLrPUJJY
- 83 articles of 3 fields:
  - ~30% of partial replication
  - **0% of true replication**

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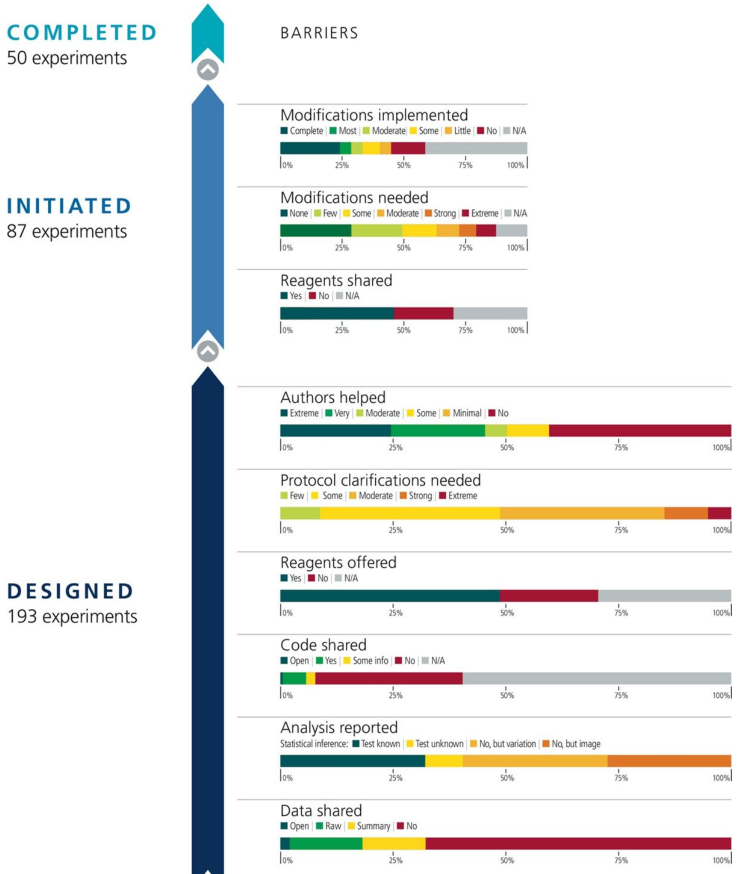
- Absence of knowledge/infrastructure
- Questionable research practices and fraud
- Statistical issues
  - Low statistical power
  - Statistical heterogeneity
- Publication system in science
  - Publication bias (non-significant results/unoriginal replications not published)
  - "Publish or perish"
  - Standards of reporting, open-access



Errington, T.M. *et al.*, *eLife* (2021), https://doi.org/10.7554/eLife.67995

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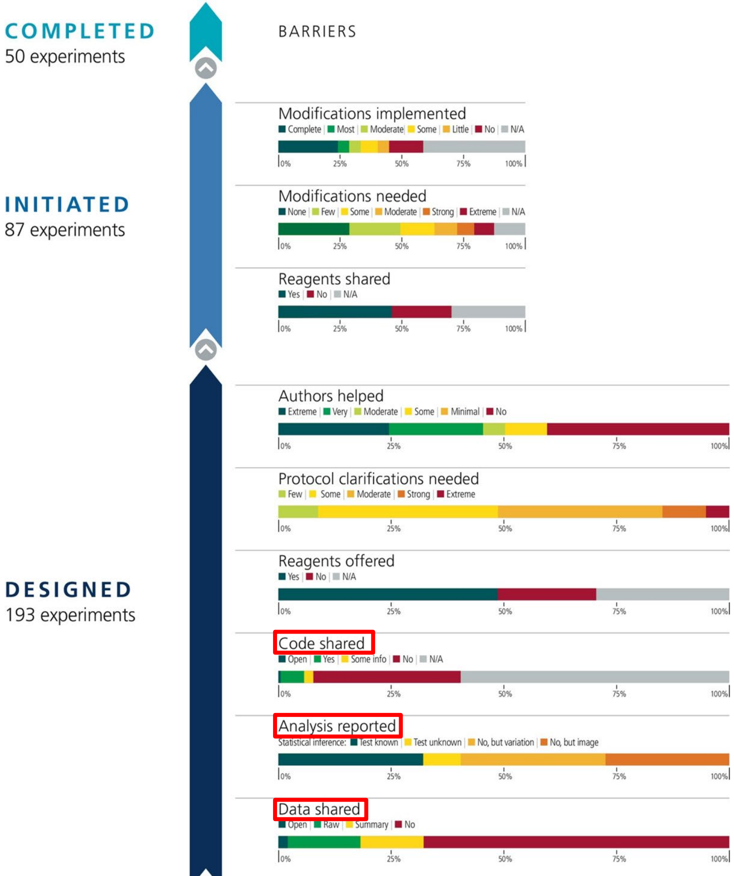

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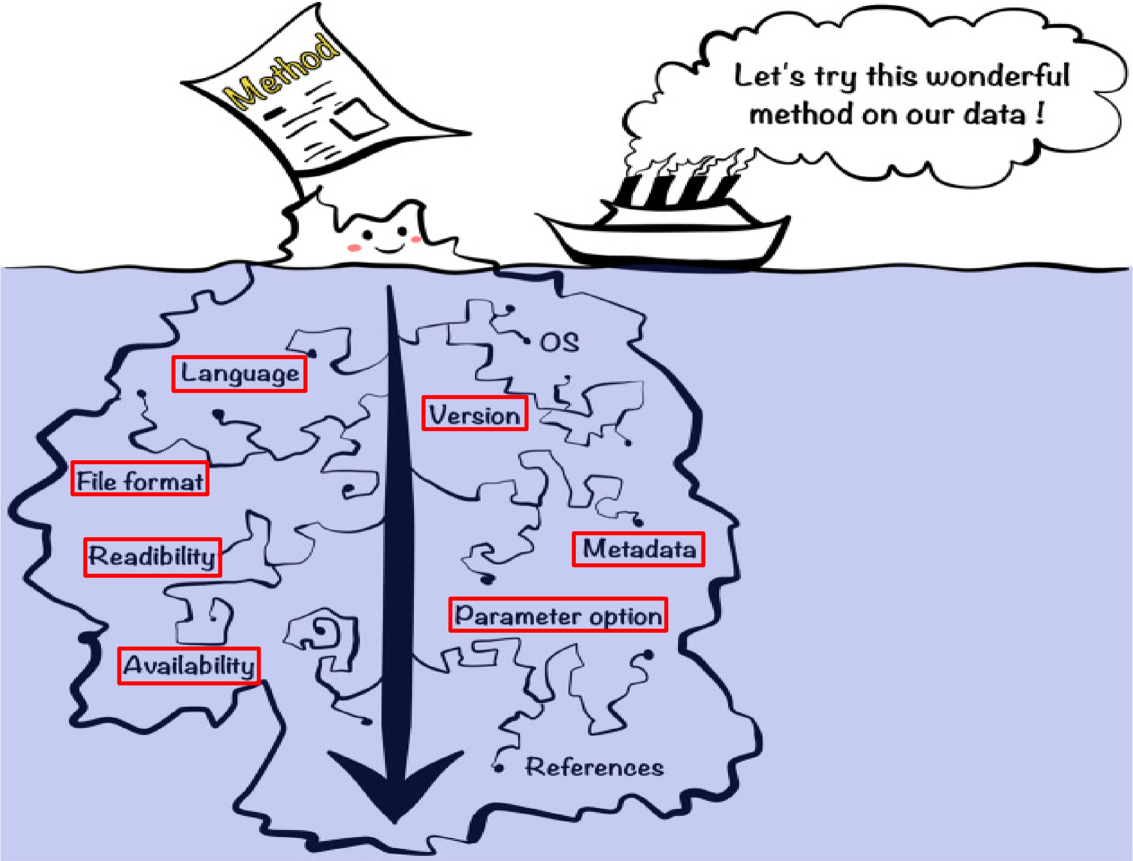
Workflow Management Systems (WMS)

- Question 3

What do WMS bring?



Kim Y.M. *et al.*, *Gigascience* (2018) https://doi.org/10.1093/gigascience/giy077

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- Multiple systems exist. Most popular ones are:
  - **Nextflow**: “top-down” approach, implemented in Groovy (~ Java)
  - **Snakemake**: “bottom-up” approach resolving dependencies, implemented in Python
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Python, you said?

- Question 4

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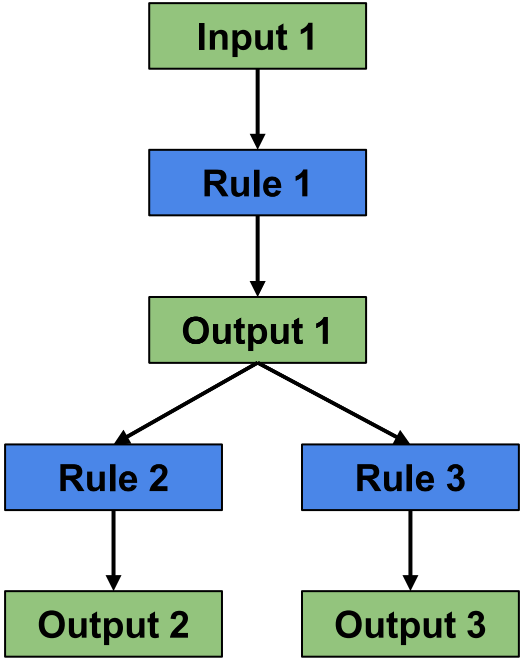
- Can be easily executed on local machines, HPCs, and clouds
- Handles dependencies with **conda/mamba** (package manager) and **docker/singularity** (containers)
- With Snakemake, conda, and docker installed, you can:
    - Download a workflow (*e.g.* from a Github or Gitlab repository)
    - Run Snakemake in a controlled environments (software, versions, parameters, OS…)
    - Automatically and efficiently reproduce all the analyses and results

How does Snakemake work?

- Workflow:
  - Collection of **interdependent** **rules** to generate specific **outputs**



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    - Basic workflow unit
    - **Template (recipe)** to produce an **output** (1 or more files)
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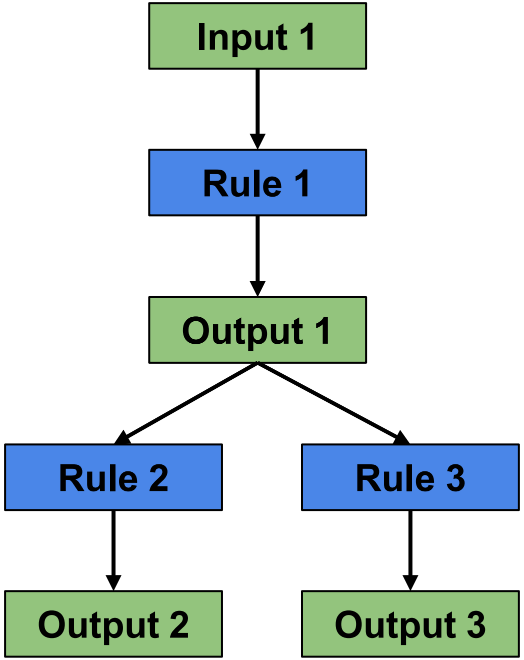
    - Generates **jobs** when executed



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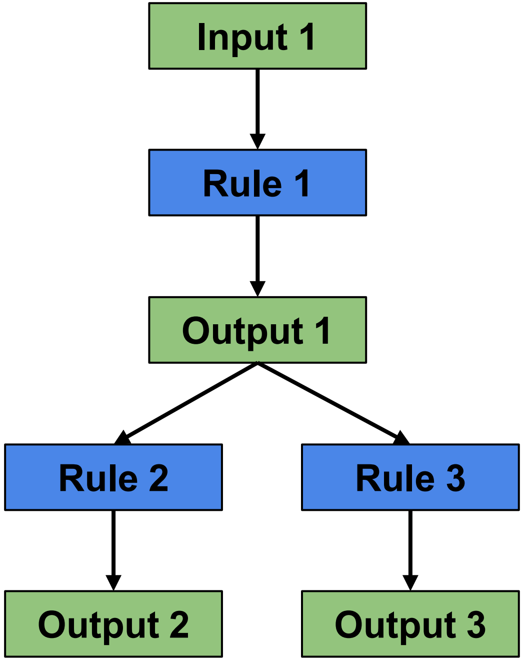
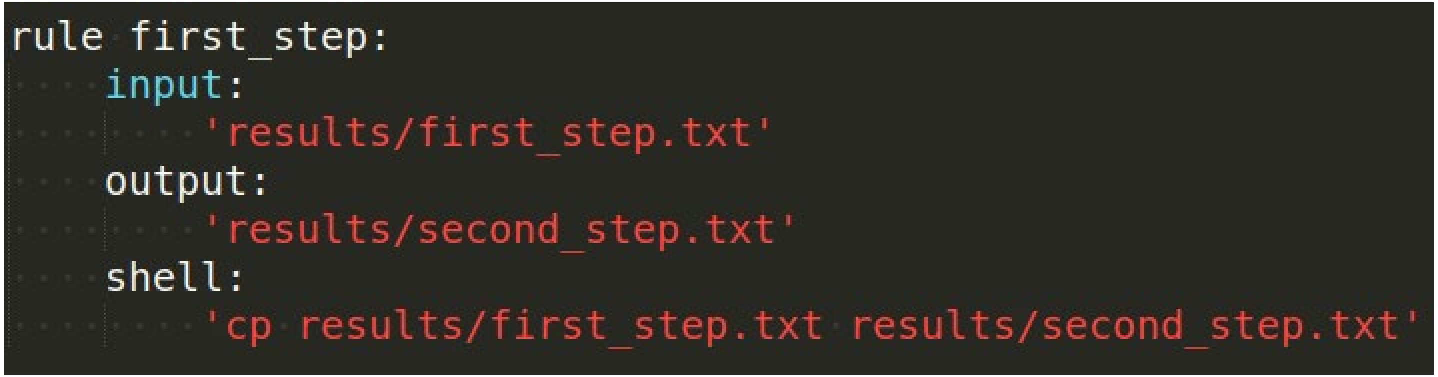
- Job:
  - Single **execution** of a rule (apply the recipe to specific data)
  - Successful if **all outputs are present and no error**



What does Snakemake really look like?



```
rule first_step:
    input:
        'results/first_step.txt'
    output:
        'results/second_step.txt'
    shell:
        'cp results/first_step.txt results/second_step.txt'
```

Exercises

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

- For this session:
  - Understand the structure of a Snakemake workflow
  - Create your first rules and Snakefile
  - Chain rules together
  - Run your first workflow