

Snakemake for reproducible research

Introduction to Snakemake



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Reproducibility

- Question 1

What is reproducibility?

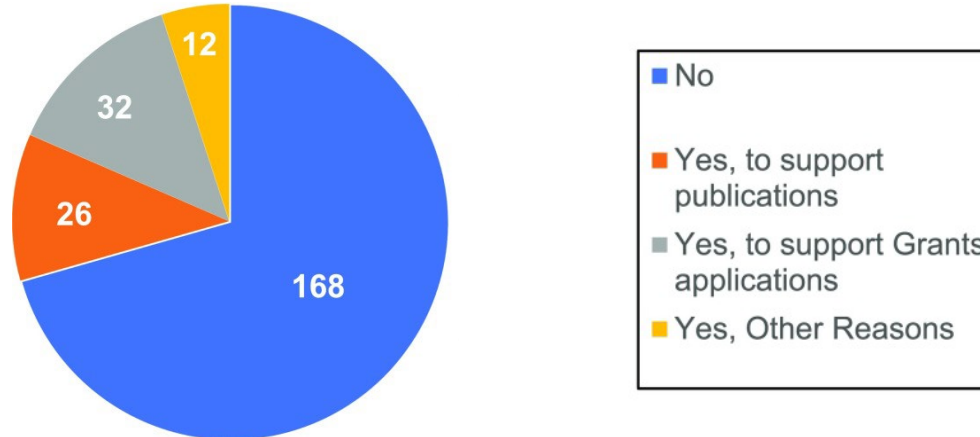
- Replicability vs repeatability vs reproducibility
- "Reproducibility is more or less the ability to draw similar conclusions from replicates studies"
 - Diaba-Nuhoho, P., Amponsah-Offeh, M., *BMC Research Notes* (2021), <https://doi.org/10.1186/s13104-021-05875-3>
- Key component of the scientific method, "cornerstone of science"

Reproducibility crisis

- Question 2

Is there a reproducibility crisis?

- Baker, M., *Nature* (2016), <https://doi.org/10.1038/533452a>:
 - ~1600 researchers: 52% significant crisis, 38% slight crisis (90% in total)
- Alfredo Sánchez-Tójar, Universität Bielefeld:
 - Publication bias in ecology: <https://www.youtube.com/watch?v=wdhzLrPUJJY>
 - 83 articles of 3 fields: ~30% of partial replication, **0% of true replication**
- Knudtson, K. L., *J Biomol Tech.* (2019), <https://doi.org/10.7171%2Fjbt.19-3003-001>
 - Has your core's rigor and reproducibility practice statement ever been requested?



Why is that?

Why is that?

- 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

COMPLETED

50 experiments

INITIATED

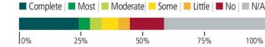
87 experiments

DESIGNED

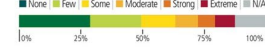
193 experiments

BARRIERS

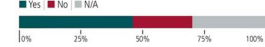
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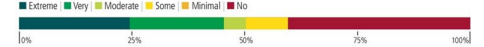
Modifications needed



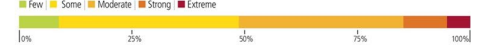
Reagents shared



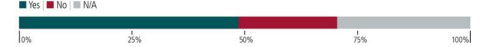
Authors helped



Protocol clarifications needed



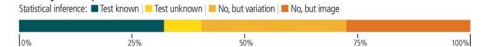
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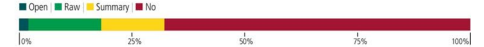
Code shared



Analysis reported



Data shared



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

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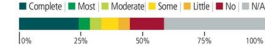
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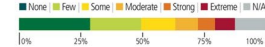
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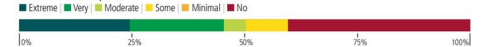
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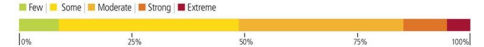
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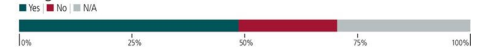
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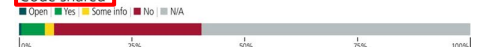
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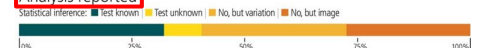
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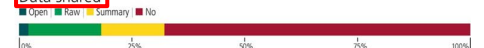
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Workflow Management Systems (WMS)

- Question 3

What do WMS bring?

- WMS can solve several hidden reproducibility issues:
 - Entirely:
 - OS
 - Version
 - Language
 - Readability
 - Availability
 - Partially (at least):
 - File format
 - Metadata
 - Parameters/options

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- Provide reproducible and scalable infrastructures to set-up, perform, and monitor a defined sequence of tasks

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Python, you said?

- Question 4

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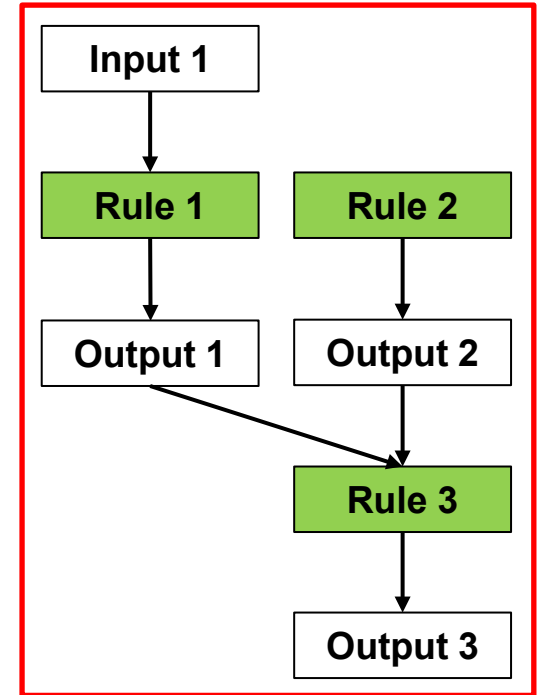
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- Easily deployable/executable **locally** or **remotely** (computation clusters and clouds)
- Integrated package management via **conda/mamba** (package manager) and **apptainer** (container manager)
- Once you have downloaded a workflow, it is easy to:
 - Run Snakemake in a **strictly controlled environment** (OS, software, versions, parameters...)
 - Efficiently and automatically reproduce analyses, results and figures

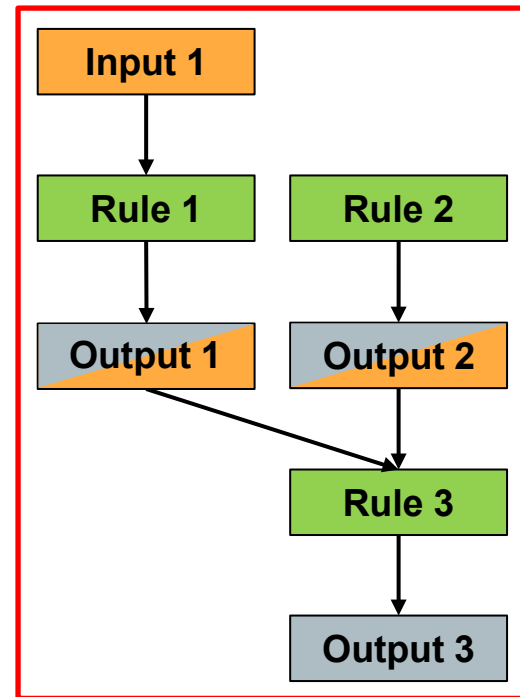
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- **Workflow:**
 - Network of dependent **rules**



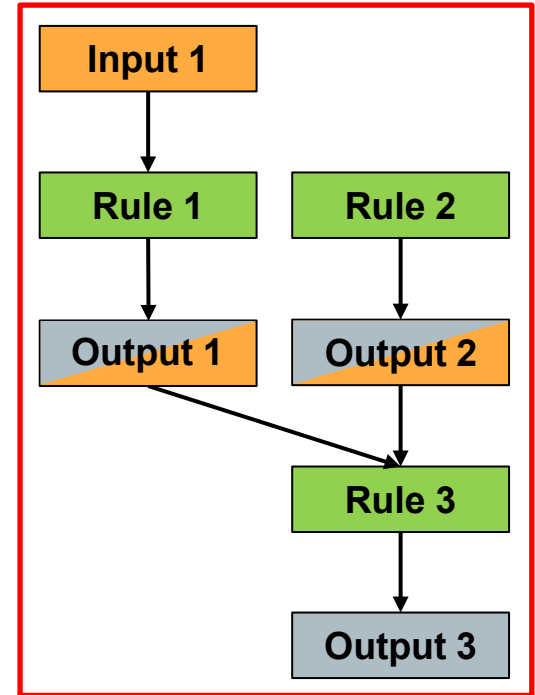
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- **Workflow:**
 - Network of dependent **rules**
- **Rule:**
 - Smallest part of a workflow
 - **Set of instructions** to create one or more **output(s)** from zero or more **input(s)**
- **Job:**
 - **Execution** of a **rule** with **specific input(s)/output(s)**
 - Success conditions:
 - **No error**
 - **All expected outputs present**



What does Snakemake really look like?

```
rule rename_file:
    input:
        'data/file.txt'
    output:
        'results/renamed_file.txt'
    shell:
        'mv data/file.txt results/file_renamed.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

