Module 4 - day 2

Reproducible data analysis and workflows

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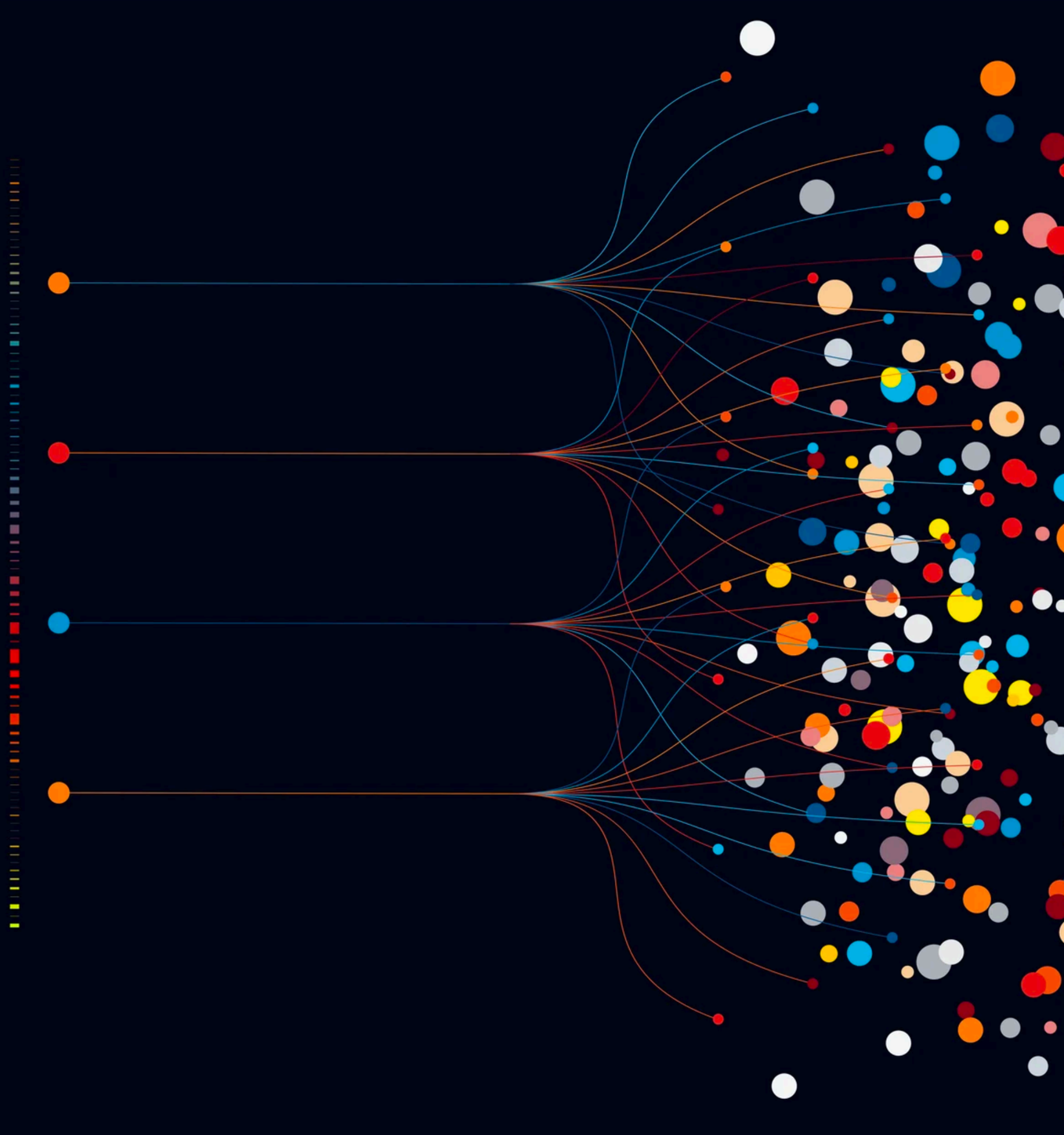
Fundamentals Data Analysis | May 28 2023 - Copenhagen



1. **Understanding Workflow Management Systems (WfMS)**
   What they are and why they matter

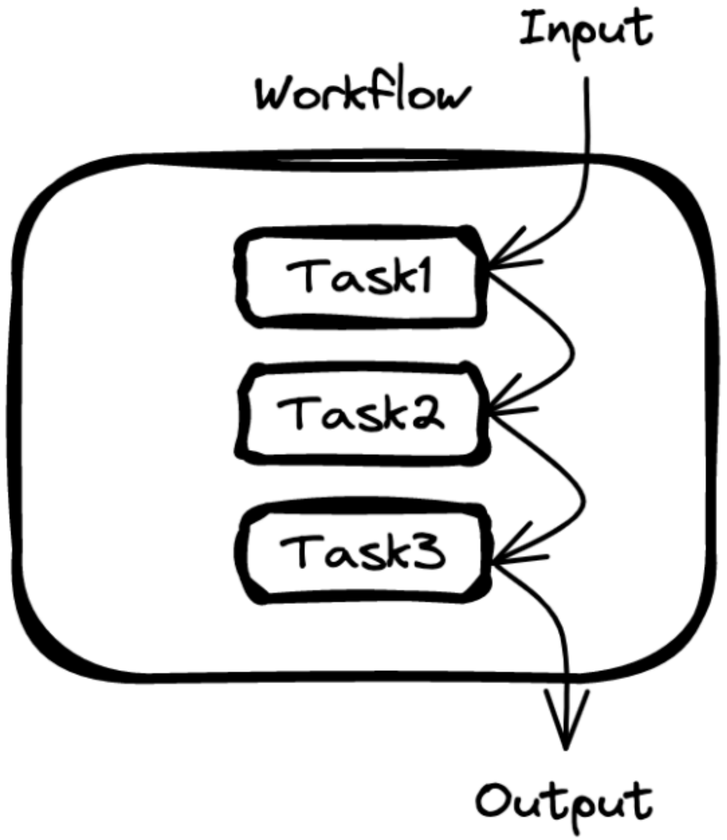
2. **Workflow Management Systems in Bioinformatics**
   A gentle introduction

4. **Environments and containers**
   Creating and managing reproducible computational environments

5. **An Introduction to Snakemake**
   A Python-based WfMS for reproducible research

Understanding Workflow Management Systems

What They Are and Why They Matter

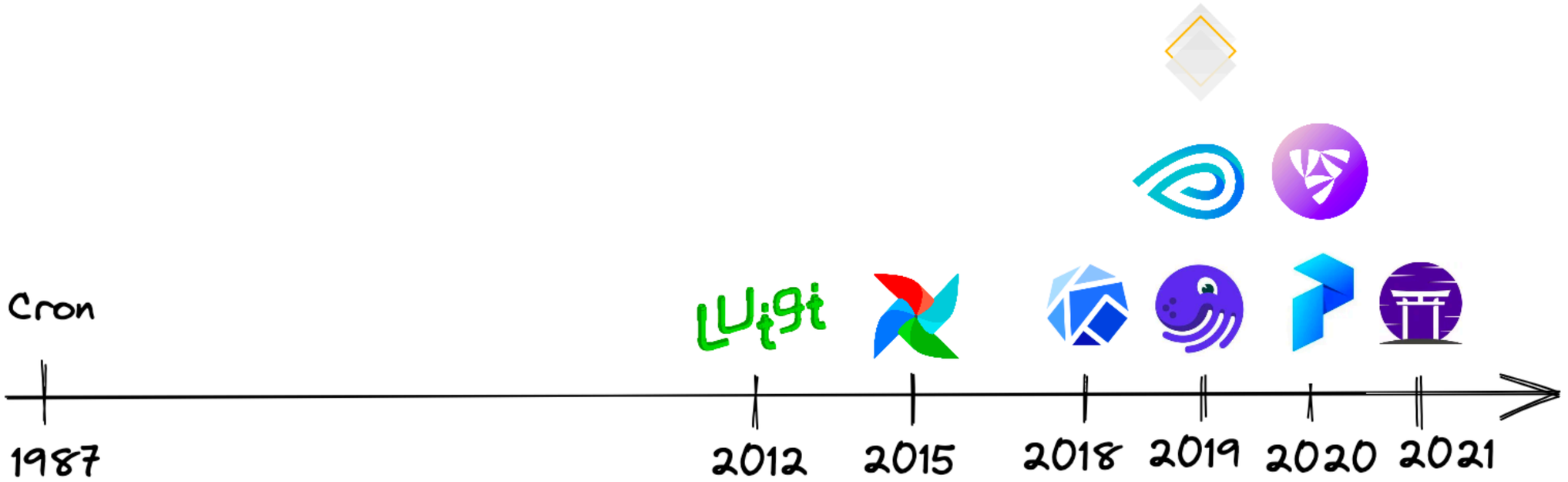

Input
Workflow
Task1
Task2
Task3
Output

- Workflow management systems (WfMS) are software tools that help researchers and data scientists **automate** and **streamline complex data analysis workflows**

- WfMS enable users to **define, execute, and monitor tasks and dependencies** in a modular and scalable manner, making it **easier to manage and reproduce analyses**

- By using WfMS, researchers can **reduce the risk of errors** and inconsistencies in their analyses, while increasing the **efficiency and reproducibility** of their research.

Orchestration

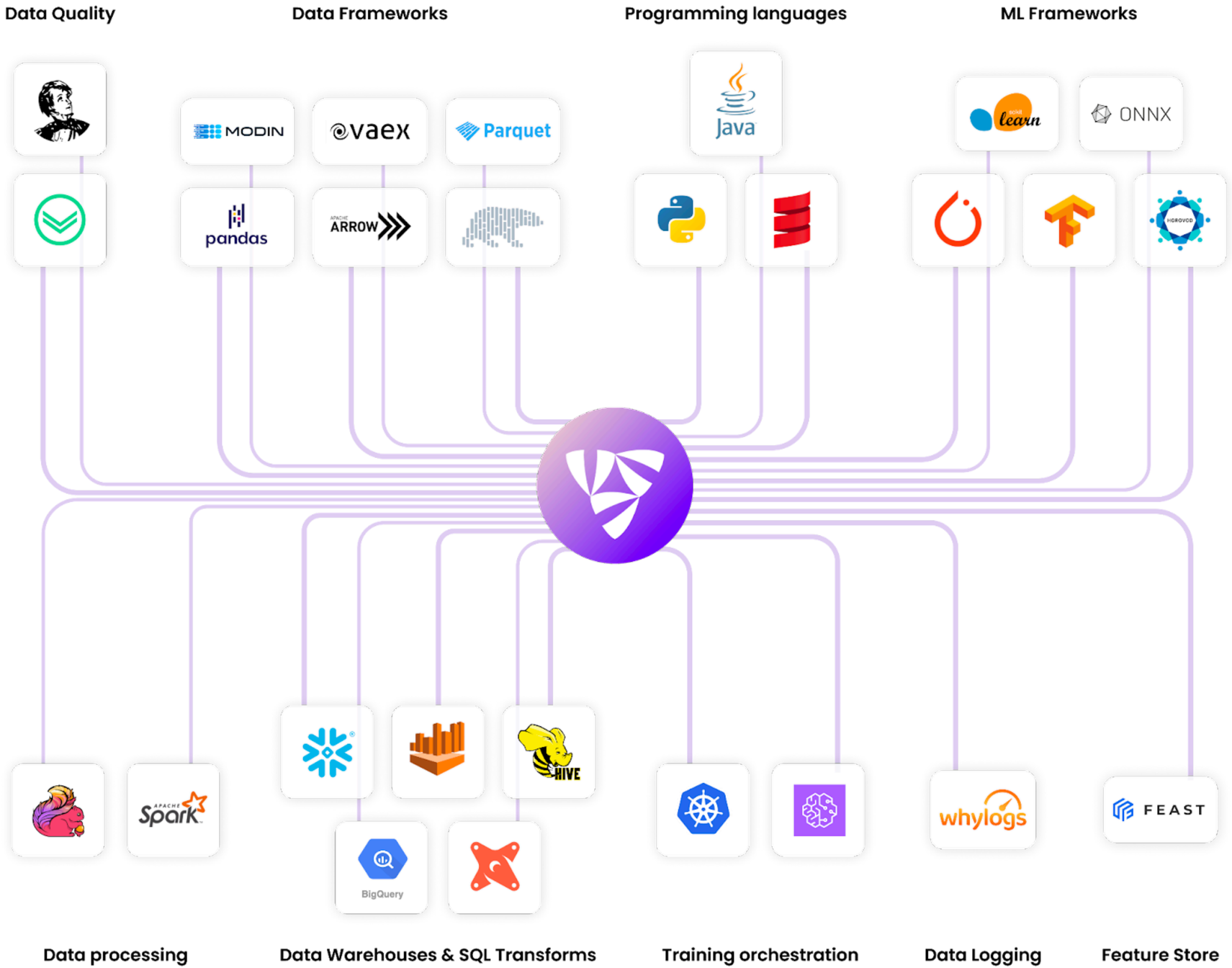


keep software processes, workflows, systems and services running at the right time and in the right order

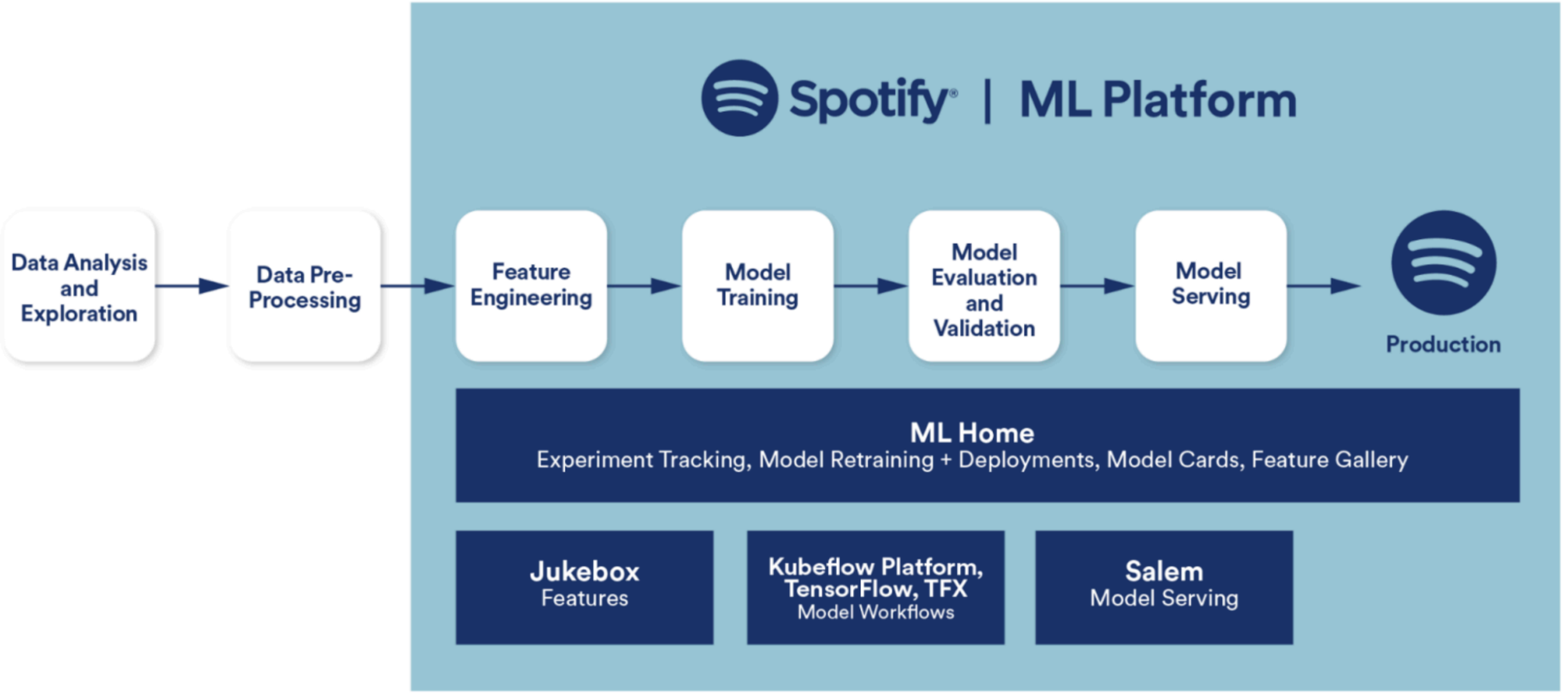
https://www.union.ai/blog-post/orchestration-for-data-machine-learning-and-infrastructure

Data Orchestration
the process of gathering, cleansing, organizing and analyzing data to make informed decisions

Machine Learning Orchestration
effective implementation, management and deployment of production-grade ML pipelines to simplify the creation of building ML-powered products

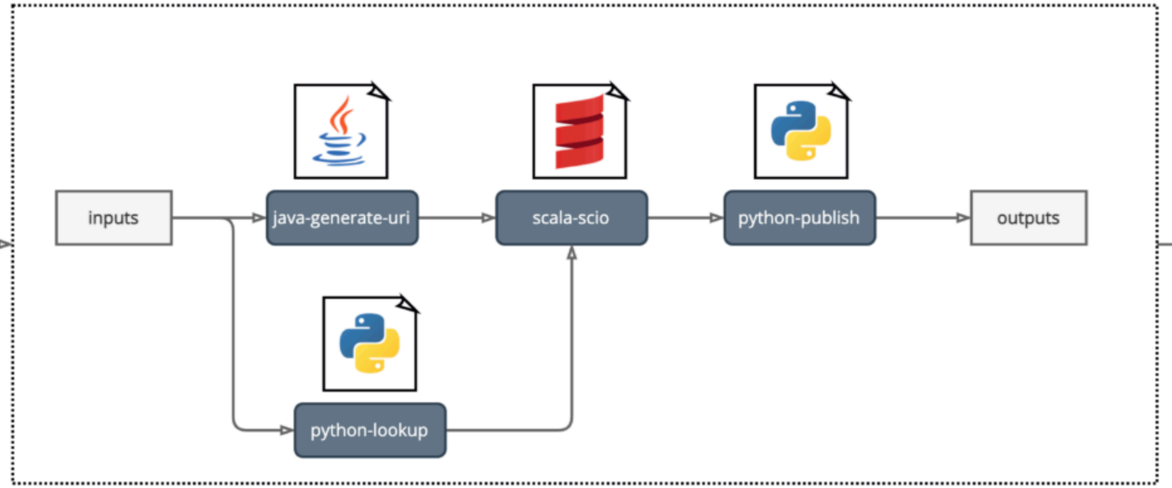

Data Quality
Data Frameworks
Programming languages
ML Frameworks
MODIN
vaex
Parquet
pandas
ARROW
Java
ONNX
HOROVOD
Spark
HIVE
BigQuery
whylogs
FEAST
Data processing
Data Warehouses & SQL Transforms
Training orchestration
Data Logging
Feature Store


Spotify R&D
Spotify® + Flyte


Spotify | ML Platform
Data Analysis and Exploration
Data Pre-Processing
Feature Engineering
Model Training
Model Evaluation and Validation
Model Serving
Production
ML Home
Experiment Tracking, Model Retraining + Deployments, Model Cards, Feature Gallery
Jukebox
Features
Kubeflow Platform, TensorFlow, TFX
Model Workflows
Salem
Model Serving

Flyte

```
@workflow_class
class WorkflowDemo:
    endpoint = Input(Types.String, '
    partition = Input(Types.Datetime

    python_lookup = python_LookupDa

    java_generate_uri = java_Generat

    scala_scio = scala_ScioTask(ins=

    python_publish = python_Publish(

    Output(python_publish.outputs.ou
```



Flyte

Styx

WfMS in Bioinformatics

A gentle introduction

- Bioinformatics researchers often deal with **large and complex datasets** that require **advanced computational methods** and tools

- WfMS enable researchers to **automate and streamline** analyses, making it easier to manage and reproduce results

- We should design workflows that are **modular, scalable, and reproducible**, and using tools like **containerization** and **version control** to ensure **consistency and transparency** in the analysis pipeline

	Bioinformatics	Data Engineering
Size of data files	Large	Small
Data type	Compressed text, proprietary formats	Common formats (text, images, etc)
Number of data files	Small	Large
Compute Intensity per step	Medium to large	Small to medium
Store results in databases?	No	Yes

https://www.bsiranosian.com/bioinformatics/why-are-bioinformatics-workflows-different/

Tool	Class	Ease of use[a]	Expressiveness[b]	Portability[c]	Scalability[d]	Learning resources[e]	Pipeline initiatives[f]
Galaxy	Graphical	●●●	●○○	●●●	●●●	●●●	●●○
KNIME	Graphical	●●●	●○○	○○○	●●◐	●●●	●●○
Nextflow	DSL	●●○	●●●	●●●	●●●	●●●	●●●
Snakemake	DSL	●●○	●●●	●●◐	●●●	●●○	●●●
GenPipes	DSL	●●○	●●●	●●○	●●○	●●○	●●○
bPipe	DSL	●●○	●●●	●●○	●●◐	●●○	●○○
Pachyderm	DSL	●●○	●●●	●○○	●●○	●●●	○○○
SciPipe	Library	●●○	●●●	○○○	○○○	●●○	○○○
Luigi	Library	●●○	●●●	●○○	●●◐	●●○	○○○
Cromwell + WDL	Execution + workflow specification	●○○	●●○	●●●	●●◐	●●○	●●○
cwltool + CWL	Execution + workflow specification	●○○	●●○	●●◐	○○○	●●●	●●○
Toil + CWL/WDL/Python	Execution + workflow specification	●○○	●●●	●◐○	●●●	●●○	●●○

Tool	Class	Ease of use[a]	Expressiveness[b]	Portability[c]	Scalability[d]	Learning resources[e]	Pipeline initiatives[f]
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KNIME	Graphical	●●●	●○○	○○○	●●◐	●●●	●●○
Nextflow ★	DSL	●●○	●●●	●●●	●●●	●●●	●●●
Snakemake ★	DSL	●●○	●●●	●●◐	●●●	●●○	●●●
GenPipes	DSL	●●○	●●●	●●○	●●○	●●○	●●○
bPipe	DSL	●●○	●●●	●●○	●●◐	●●○	●○○
Pachyderm	DSL	●●○	●●●	●○○	●●○	●●●	○○○
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Luigi	Library	●●○	●●●	●○○	●●◐	●●○	○○○
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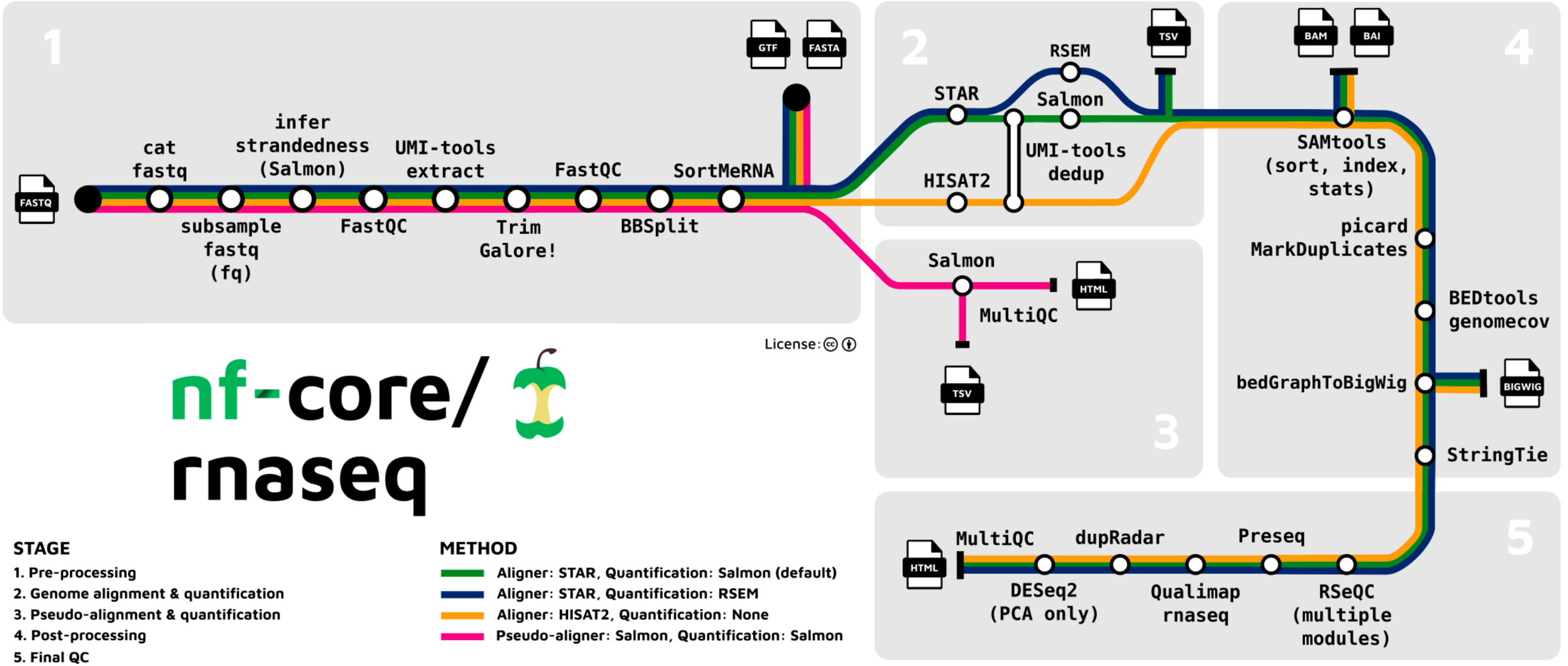

1
FASTQ
cat fastq
infer strandedness (Salmon)
UMI-tools extract
FastQC
SortMeRNA
subsample fastq (fq)
FastQC
Trim Galore!
BBSplit
GTF
FASTA
2
STAR
RSEM
Salmon
HISAT2
UMI-tools dedup
TSV
3
Salmon
HTML
MultiQC
TSV
4
BAM
BAI
SAMtools (sort, index, stats)
picard MarkDuplicates
BEDtools genomecov
bedGraphToBigWig
BIGWIG
StringTie
5
HTML
MultiQC
dupRadar
Preseq
DESeq2 (PCA only)
Qualimap rnaseq
RSeQC (multiple modules)
License:
nf-core/
rnaseq
STAGE
1. Pre-processing
2. Genome alignment & quantification
3. Pseudo-alignment & quantification
4. Post-processing
5. Final QC
METHOD
Aligner: STAR, Quantification: Salmon (default)
Aligner: STAR, Quantification: RSEM
Aligner: HISAT2, Quantification: None
Pseudo-aligner: Salmon, Quantification: Salmon

Environments and containers

Creating and managing reproducible computational environments

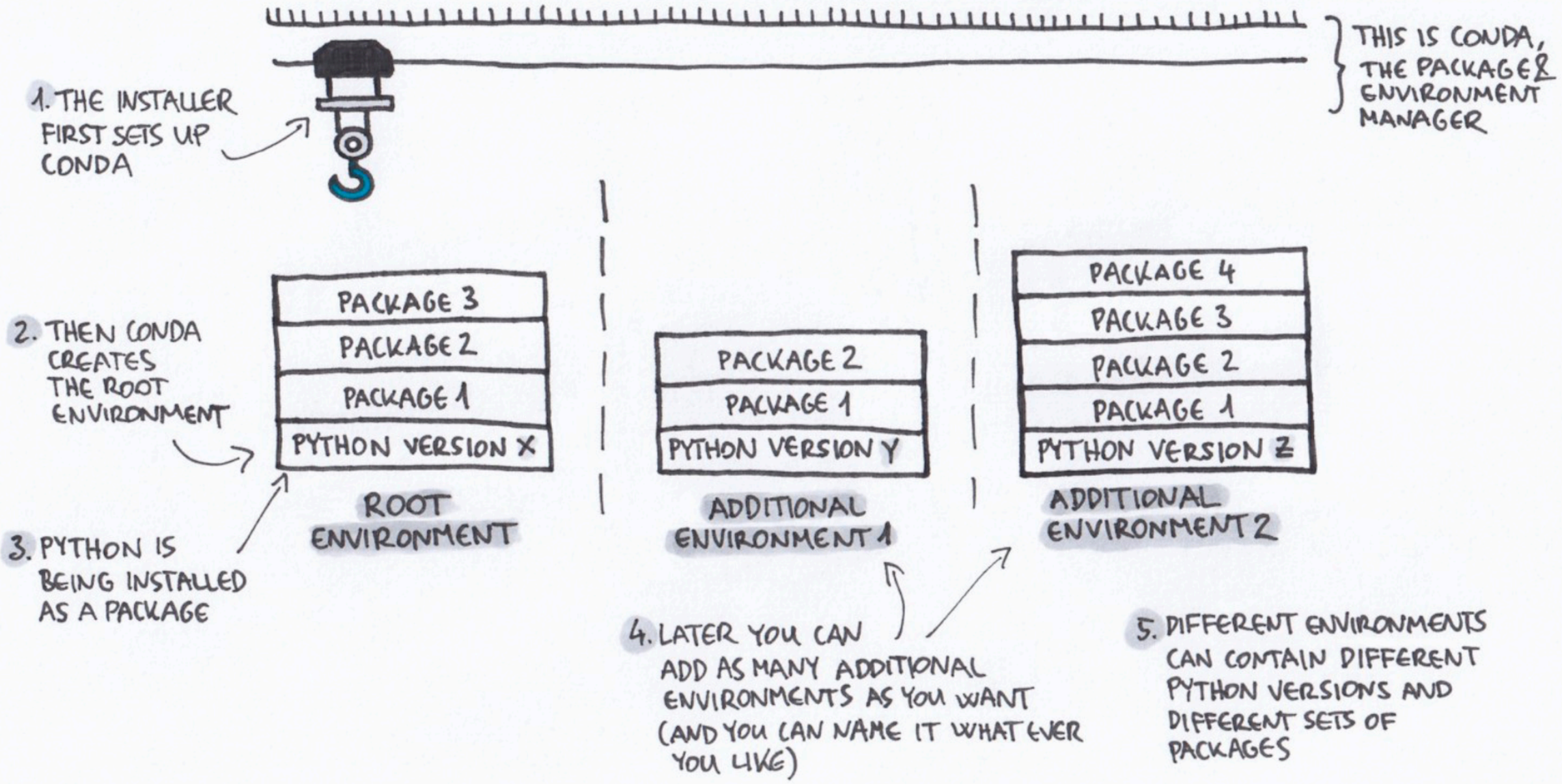

ANACONDA®


docker

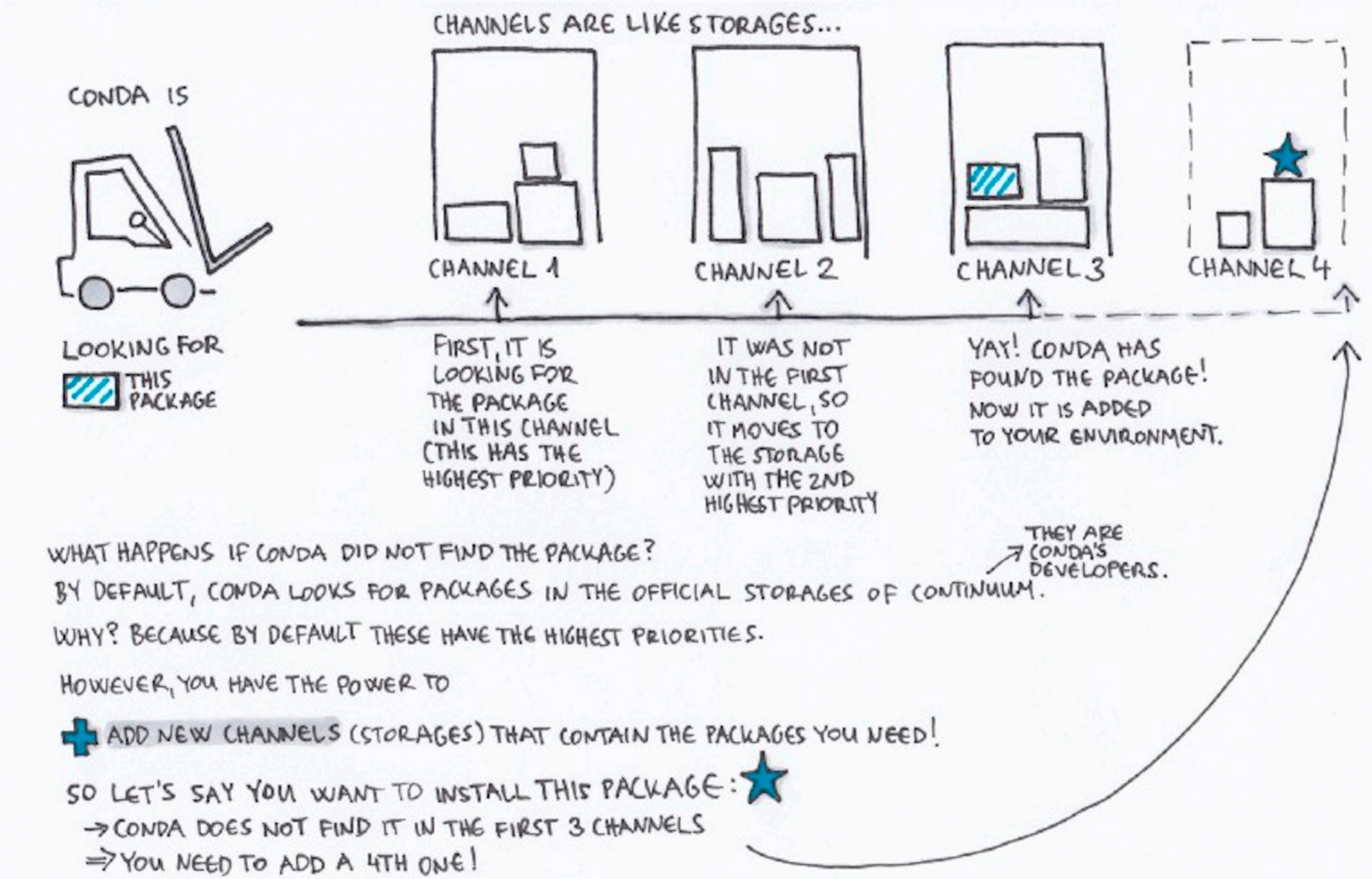
- Conda is an open-source package manager that allows users to **easily create, manage, and share reproducible software environments** for data analysis and scientific computing

- Conda can **create isolated environments for different projects**, allowing users to install different versions of software and packages without conflicts

- Conda **environments can be easily shared and reproduced across different systems and platforms**, making it a useful tool for **collaboration and reproducibility**



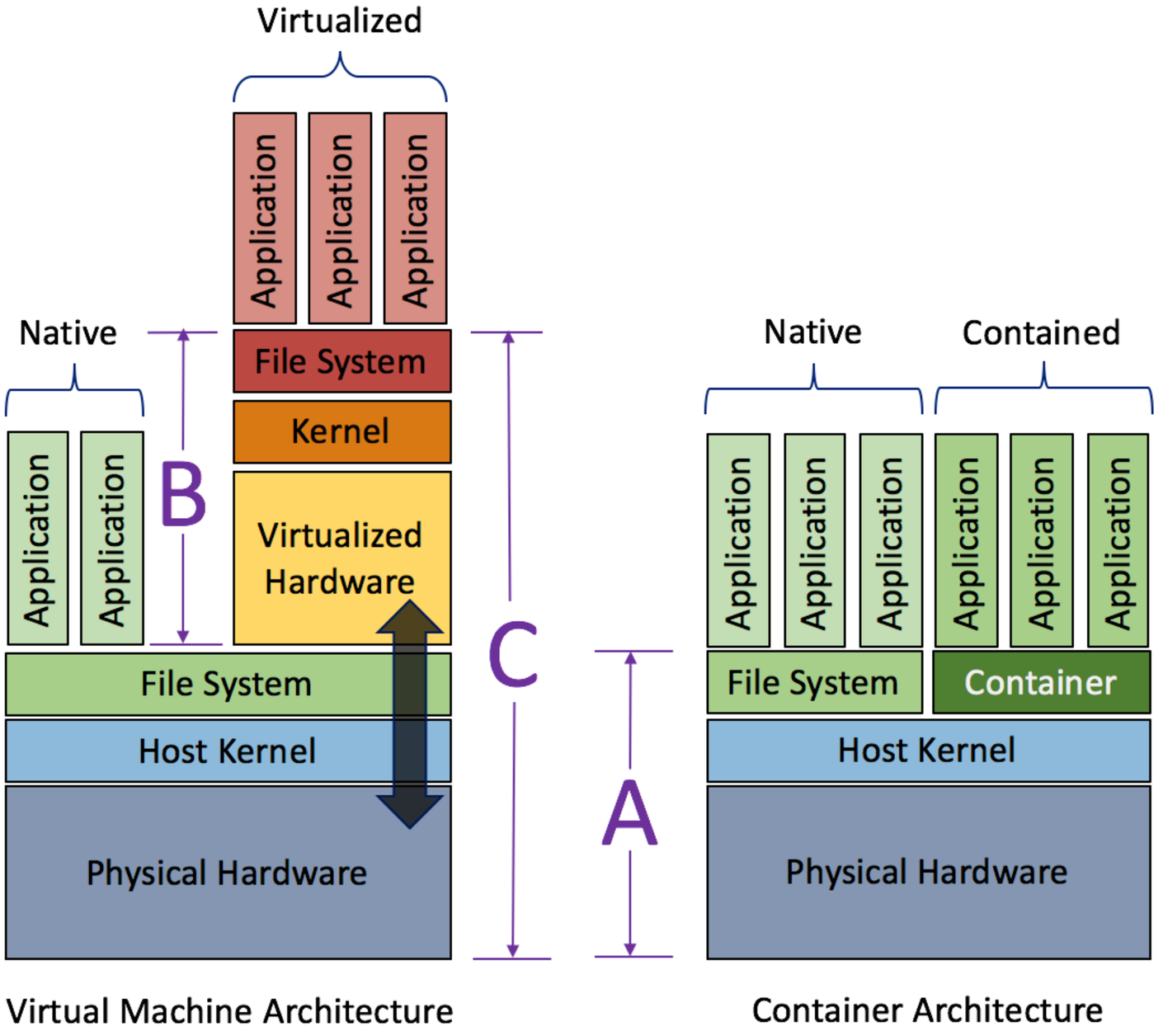
https://angus.readthedocs.io/en/2019/conda_tutorial.html



https://angus.readthedocs.io/en/2019/conda_tutorial.html

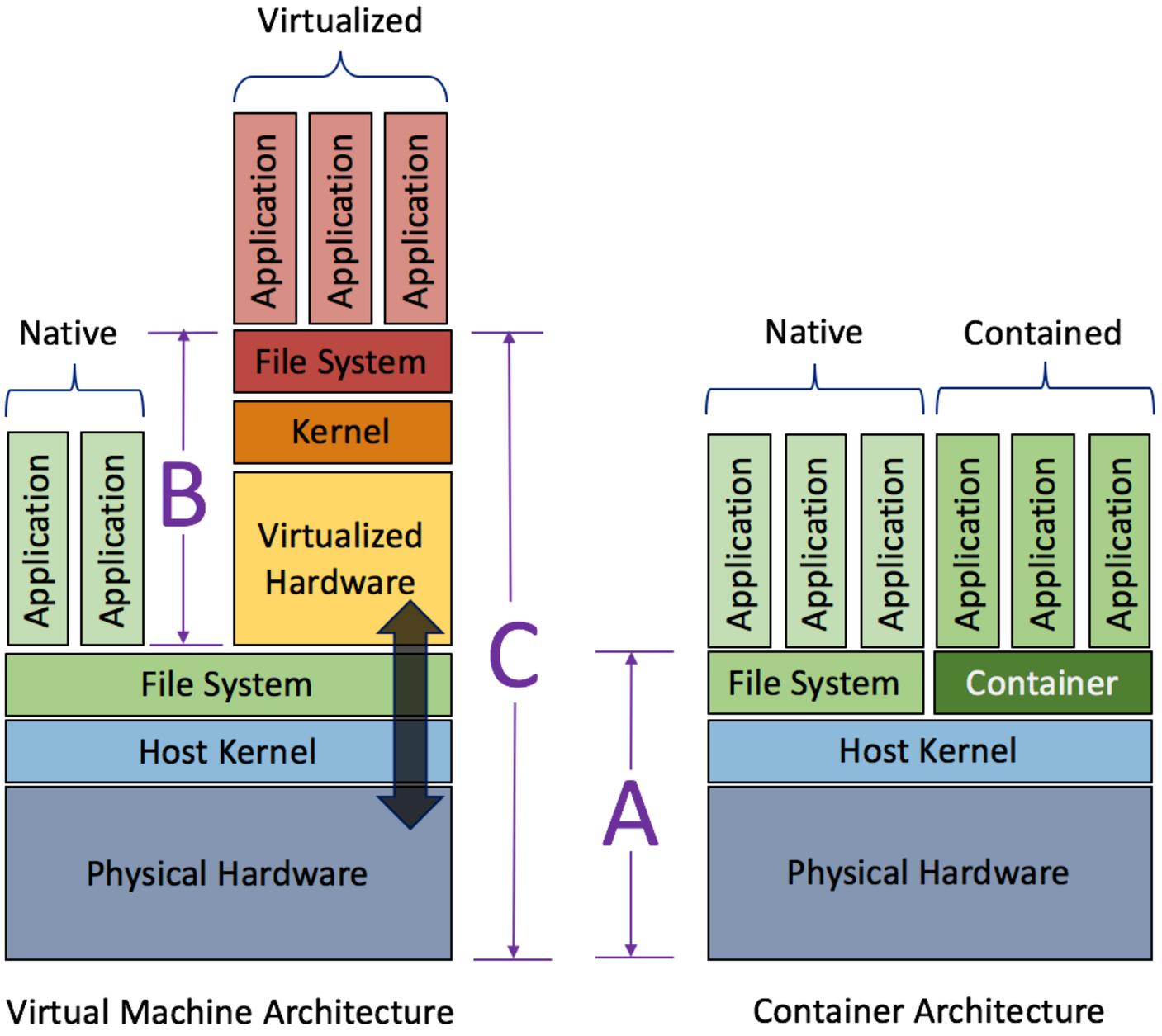
- Docker is a **containerization platform** that allows users to **package an entire software environment**, including dependencies and configuration settings, into a **portable container** that can be run on any system with Docker installed.

- Docker containers can be used **to ensure that a software environment is exactly the same across different machines**, making it easier to reproduce computational analyses and experiments.



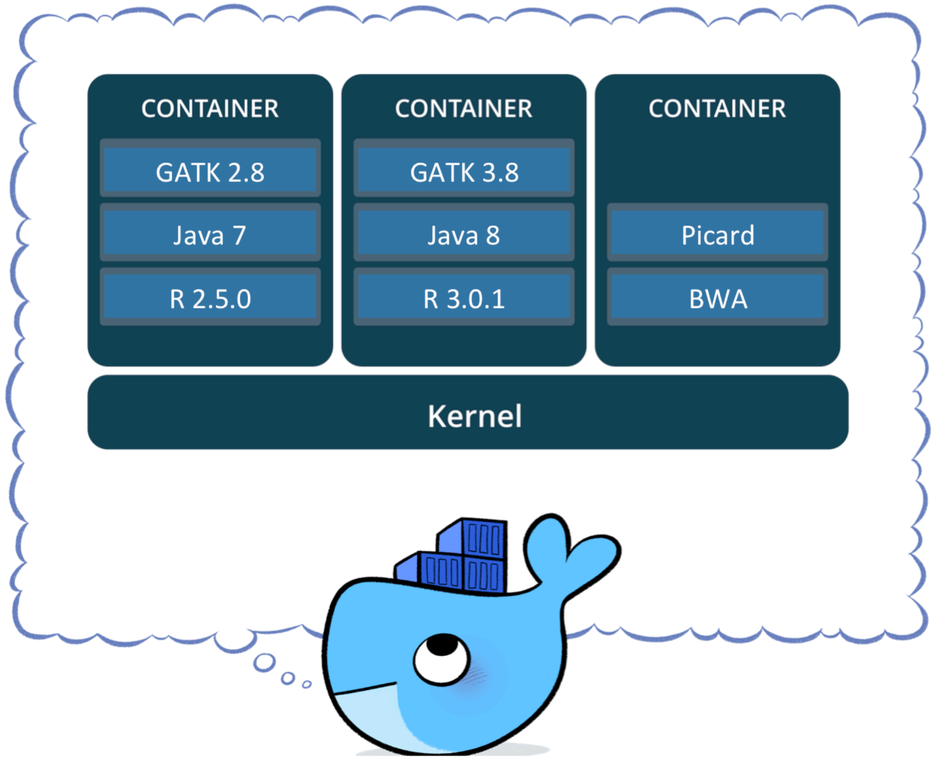
Virtual Machine Architecture

Container Architecture



Virtual Machine Architecture

Container Architecture



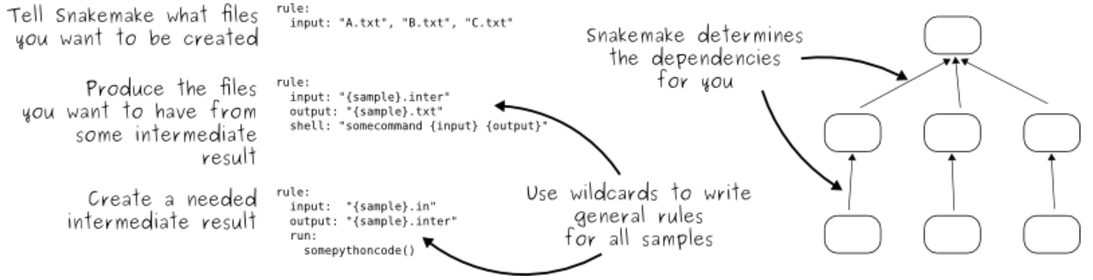
An introduction to Snakemake

A Python-based WfMS for reproducible research

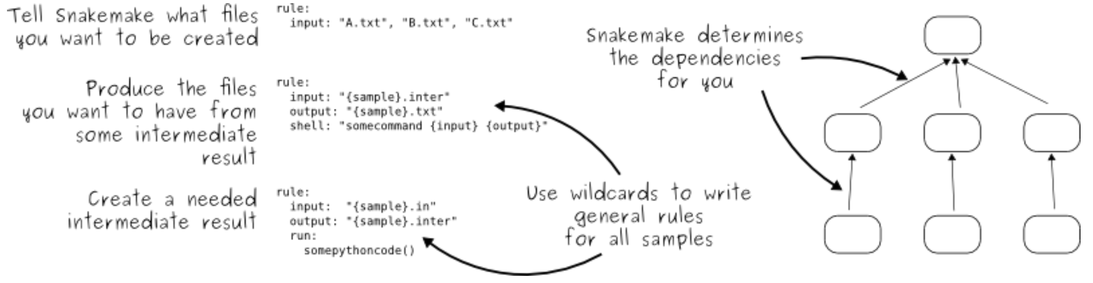
- Snakemake is a WfMS that uses a **Python-based DSL** to define and execute workflows. It is particularly well-suited for data analysis pipelines that require **complex dependencies and parallelization**

- Snakemake enables researchers to **build and manage workflows in a modular and scalable manner**, and provides a range of features and tools for reproducible research, including **version control, containerization, and automated testing**

- Snakemake is widely used in bioinformatics for data processing and analysis, and has **a large and active user community**.



https://doi.org/10.12688/f1000research.29032.2

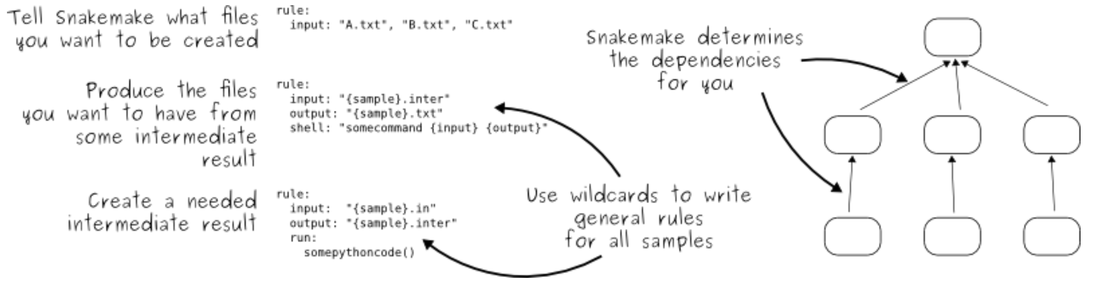


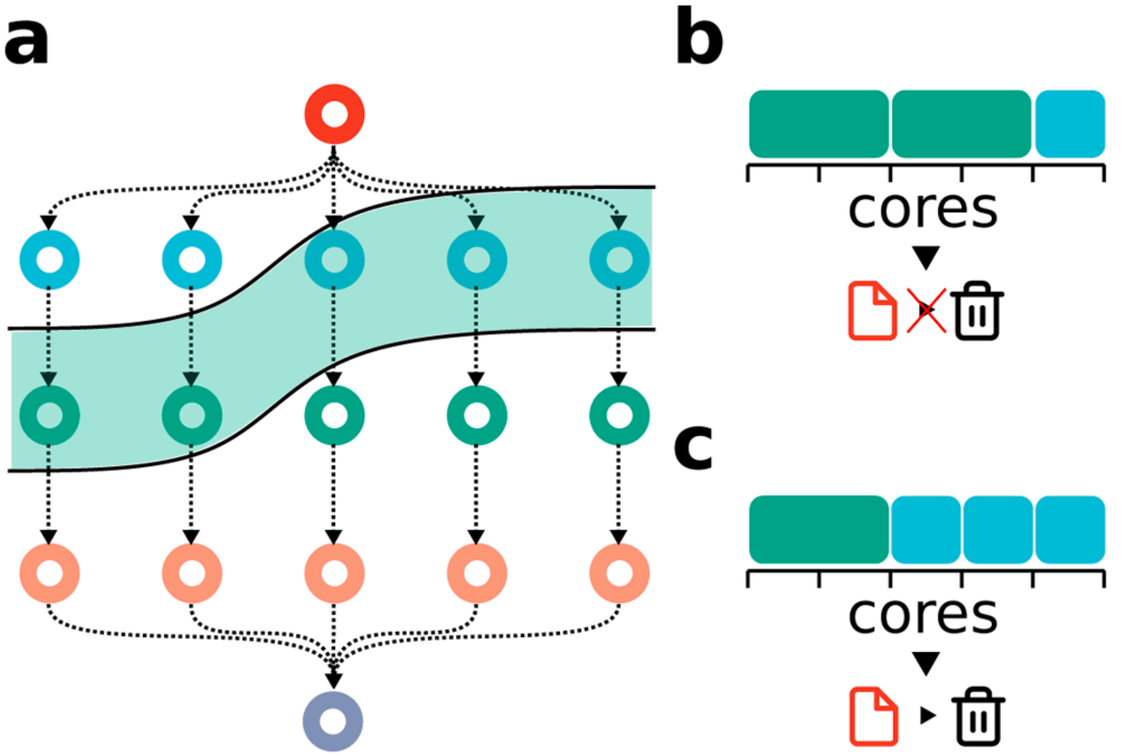

```
1  configfile: "config.yaml"
2
3  module some_workflow:
4      snakefile: "https://github.com/some/raw/v1.0.0/Snakefile"
5      config: config["some"]
6
7  use rule * from some_workflow
8
9  use rule simulate_data from some_workflow with:
10     params:
11         some_threshold=1.e-7
12
13 module other_workflow:
14     snakefile: "https://github.com/other/raw/v1.0.0/Snakefile"
15     config: config["other"]
16
17 use rule * from other_workflow as other_*
18
19 rule some_plot:
20     input:
21         "results/tables/all.csv"
22     output:
23         "results/plots/all.svg"
24     conda:
25         "envs/stats.yaml"
26     notebook:
27         "notebooks/some-plot.py.ipynb"
```

Legend

- declare module
- use rules
- modify rule
- extend workflow

https://doi.org/10.12688/f1000research.29032.2





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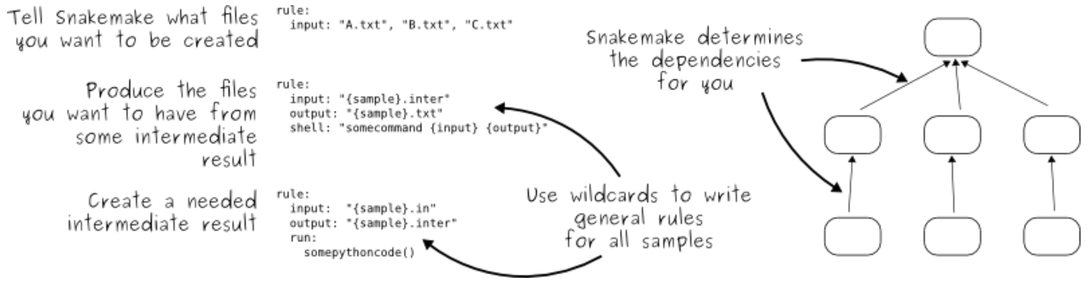

a

Legend
- domain knowledge
- technical knowledge
- Snakemake knowledge
- trivial

```
1  configfile: "config.yaml"
2
3  rule all:
4      input:
5          expand(
6              "results/plots/{country}.hist.pdf",
7              country=config["countries"]
8          )
9
10 rule download_data:
11     output:
12         "data/worldcitiespop.csv"
13     log:
14         "logs/download.log"
15     conda:
16         "envs/curl.yaml"
17     shell:
18         "curl -L https://burntsushi.net/stuff/worldcitiespop.csv > {output} 2> {log}"
19
20 rule select_by_country:
21     input:
22         "data/worldcitiespop.csv"
23     output:
24         "results/by-country/{country}.csv"
25     log:
26         "logs/select-by-country/{country}.log"
27     conda:
28         "envs/xsv.yaml"
29     shell:
30         "xsv search -s Country '{wildcards.country}' "
31         " {input} > {output} 2> {log}"
32
33 rule plot_histogram:
34     input:
35         "results/by-country/{country}.csv"
36     output:
37         "results/plots/{country}.hist.svg"
38     container:
39         "docker://faizanbashir/python-datascience:3.6"
40     log:
41         "logs/plot-hist/{country}.log"
42     script:
43         "scripts/plot-hist.py"
44
45 rule convert_to_pdf:
46     input:
47         "{prefix}.svg"
48     output:
49         "{prefix}.pdf"
50     log:
51         "logs/convert-to-pdf/{prefix}.log"
52     wrapper:
53         "0.47.0/utils/cairosvg"
```

Hands-on session

https://github.com/GeoGenetics/data-analysis-2024/reproducible-data-analysis