Computational Reproducibility With Scientific Workflows: Analysing viral genomes with Nextflow

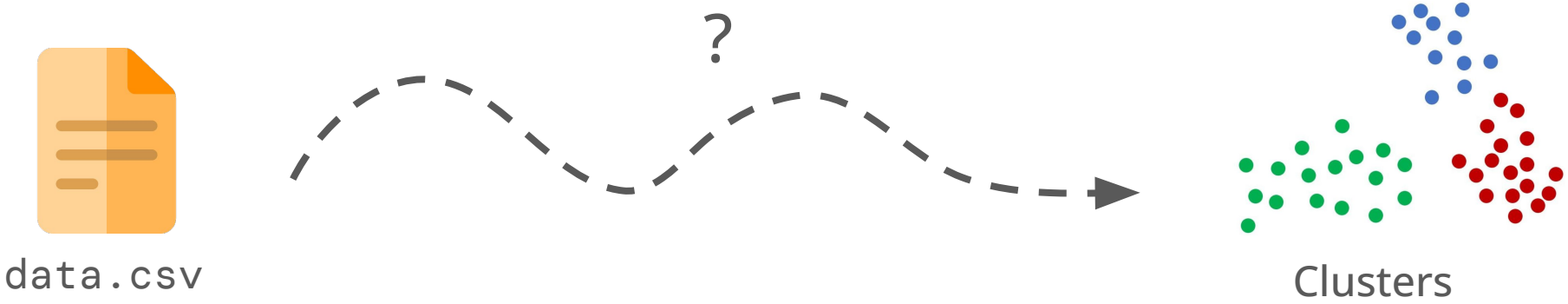
George Marchment, Sarah Cohen-Boulakia and Frédéric Lemoine

29/07/2025

ACM REP '25

Motivational Example

Motivational Example



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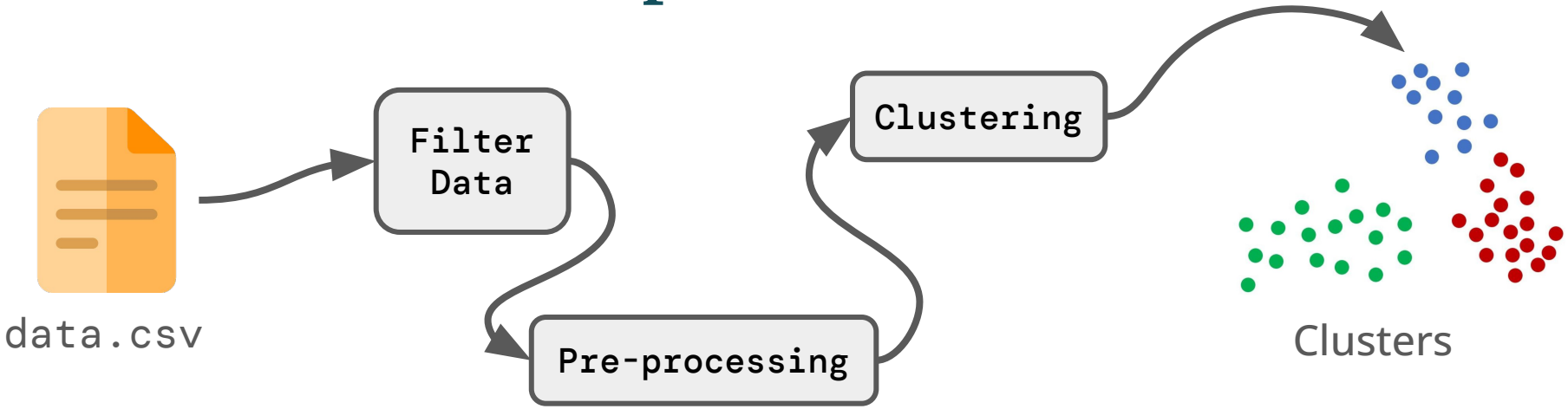

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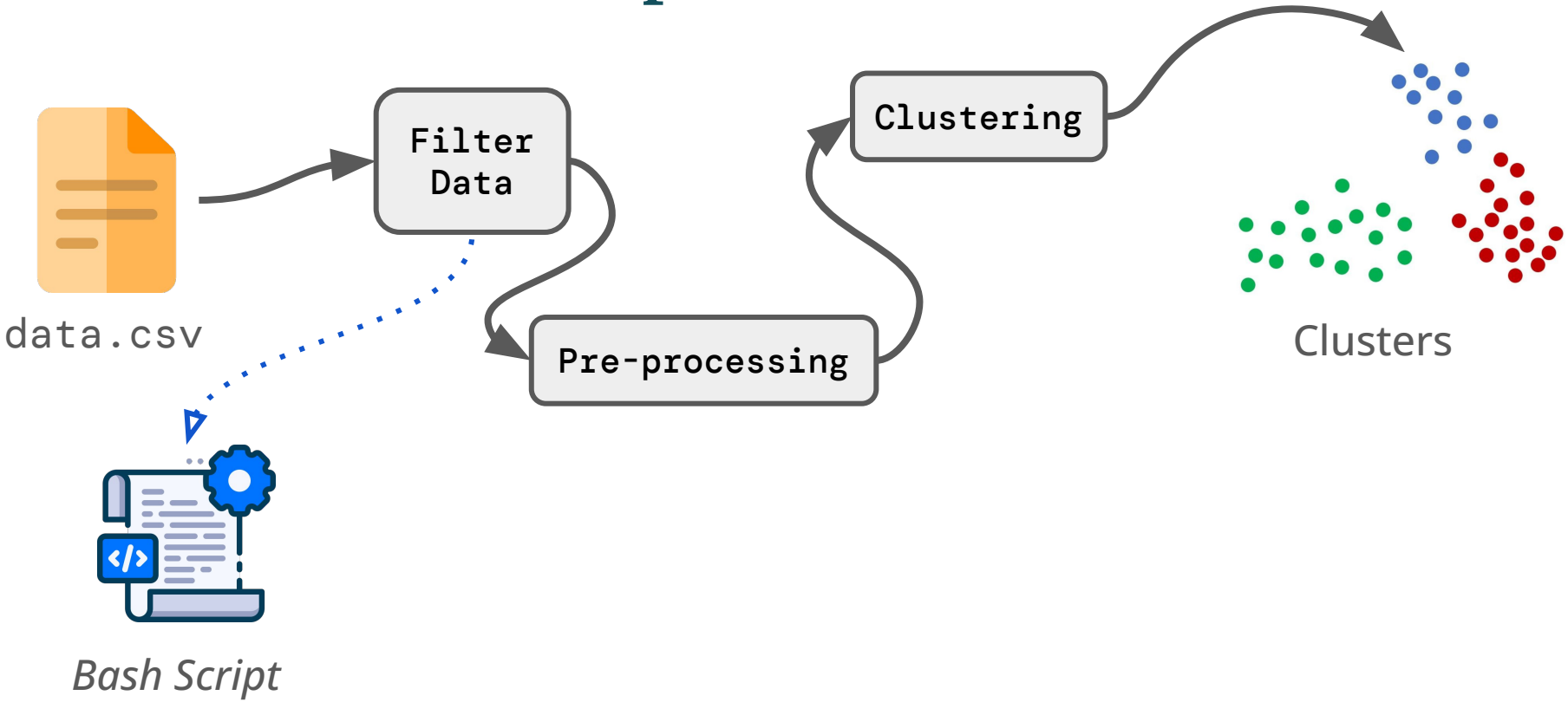

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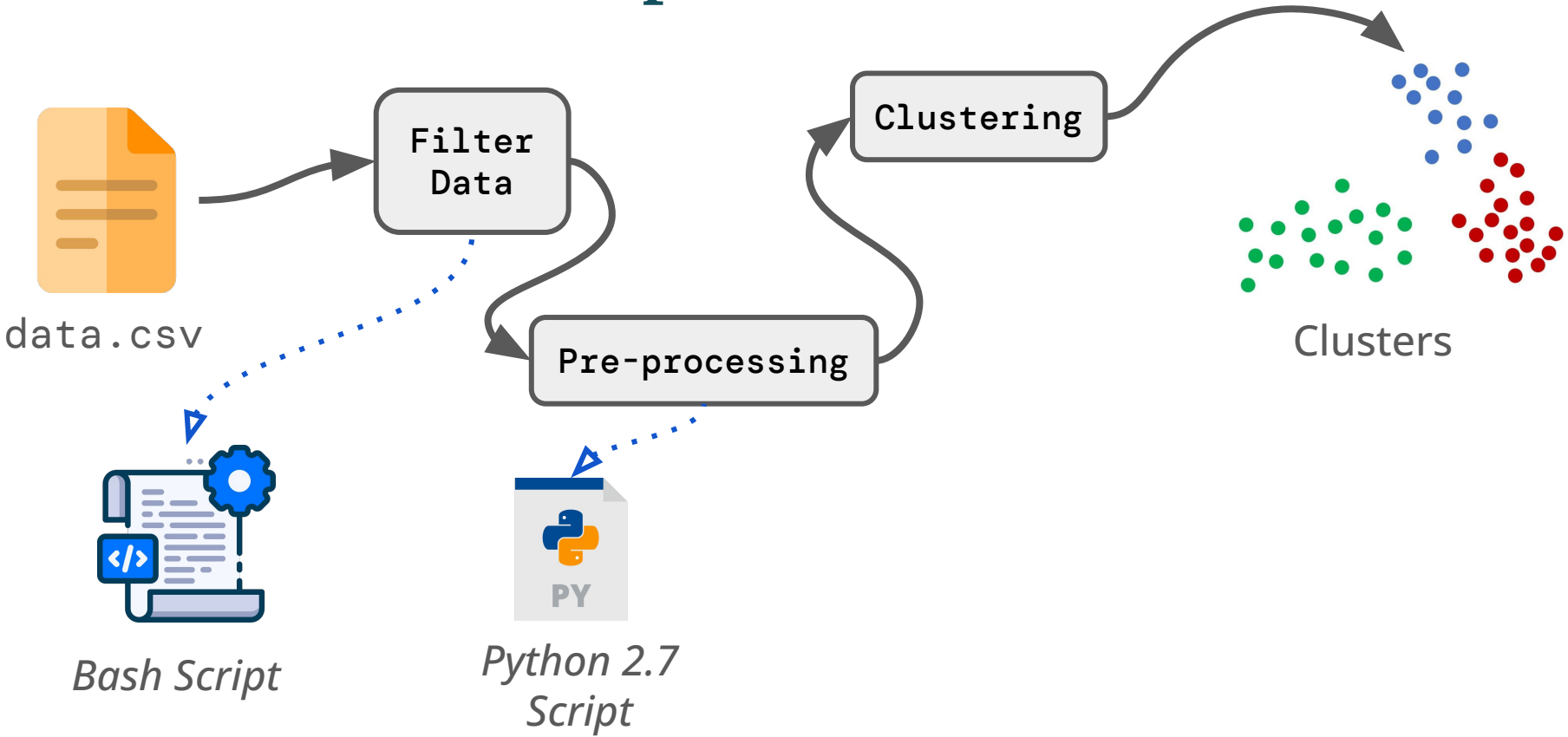

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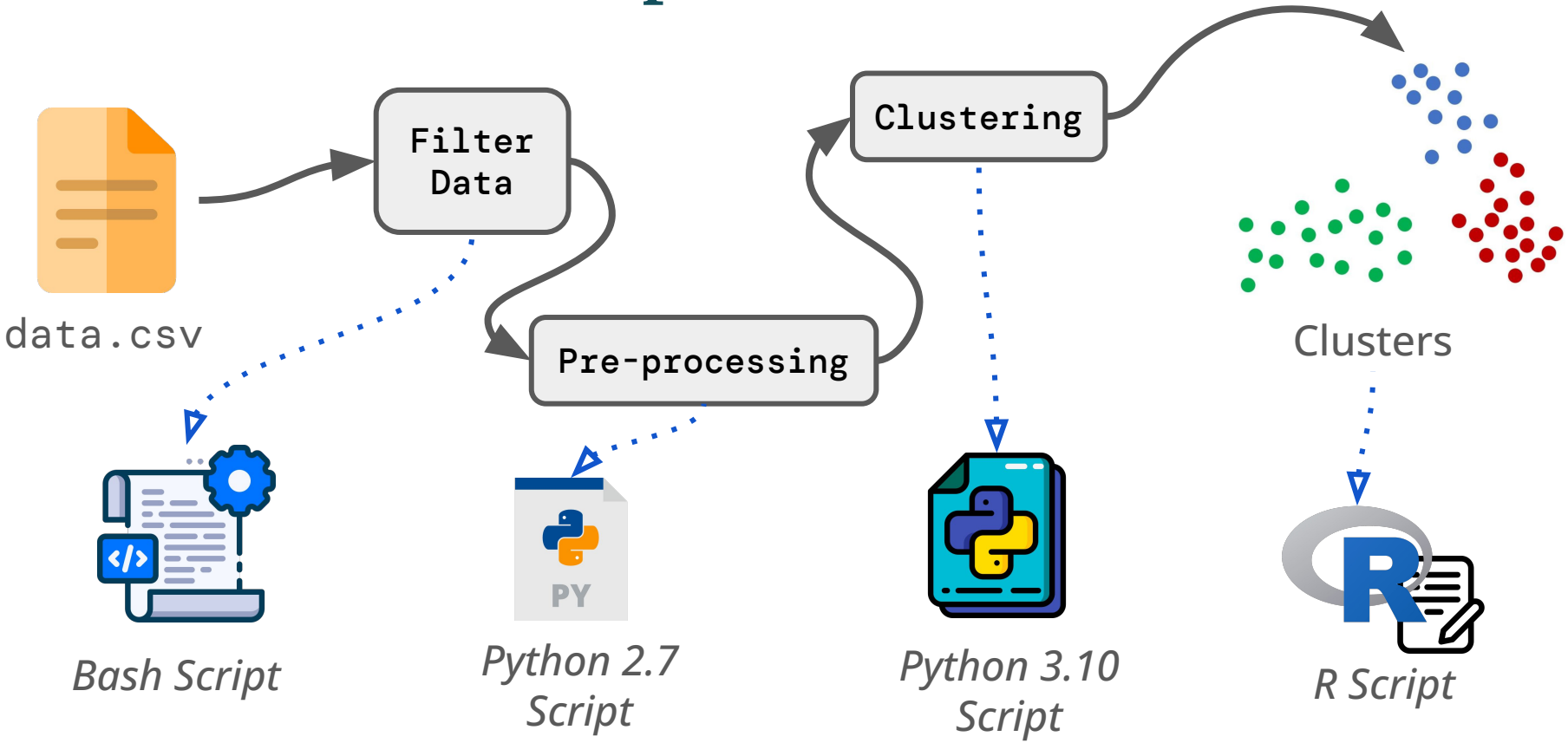

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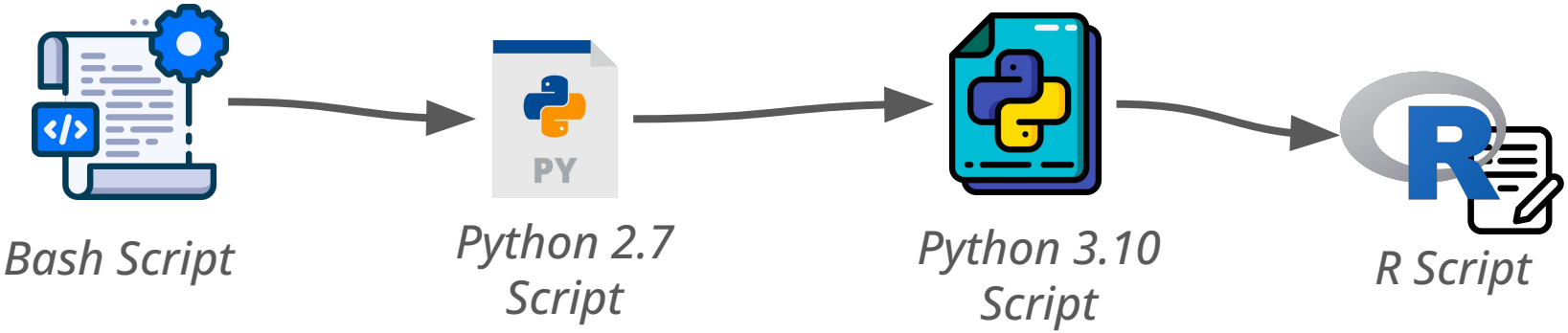
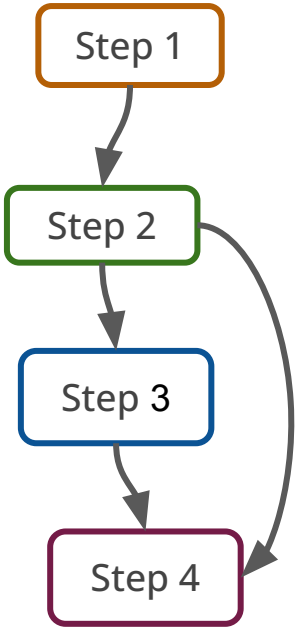


Objectives

- Acquiring basic **workflow concepts**
- Understanding the **capabilities of workflow management systems** in encapsulating heterogeneous code, scalability, software environment management, and computational resource management
- Learning how to **implement** simple workflows

1. Introduction to (Nextflow) Workflows (~1h)
    a. Motivational Example
    b. Objectives
    c. **Scientific Workflows**
    d. Software Containers
    e. Nextflow Workflows
    f. Presentation of the “Project”
2. Practical Work (~1h30)
3. Reproducibility Consensus (~30min)

Scientific Workflows



A **set of data analysis steps** that are **linked** together to form a more **complex** task

Workflow management system:

Apache Taverna

Galaxy PROJECT

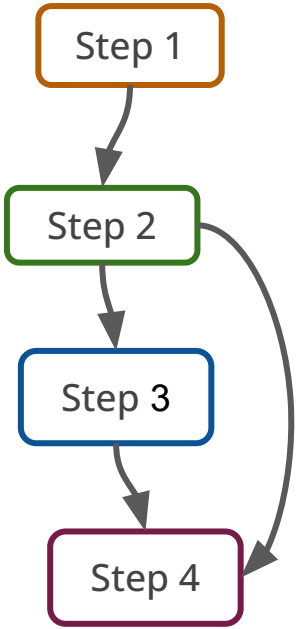
Drag and drop programming

nextflow

snakemake

Code based programming

Scientific Workflows



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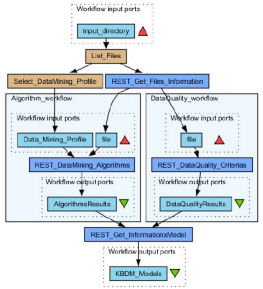
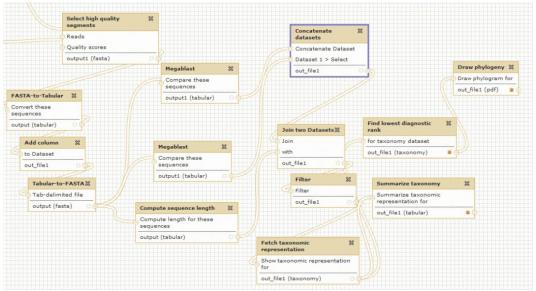
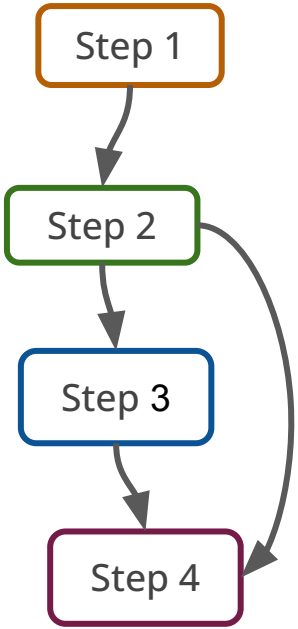




Scientific Workflows



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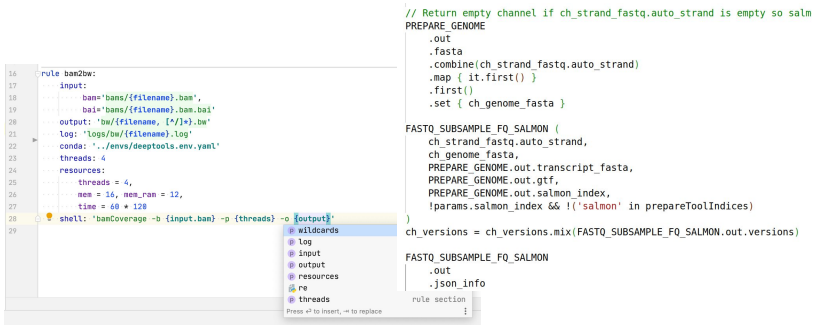

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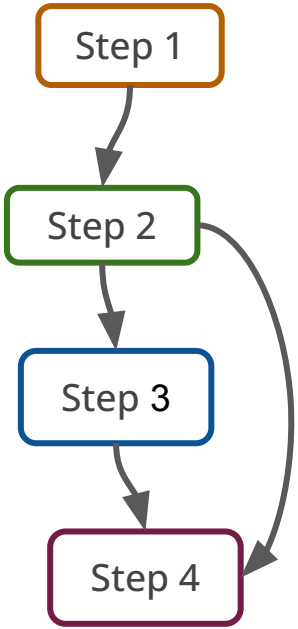

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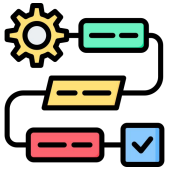
Share



Describe

Execute

While guaranteeing a better **reproducibility** of analyses

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    a. Motivational Example
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    d. **Software Containers**
    e. Nextflow Workflows
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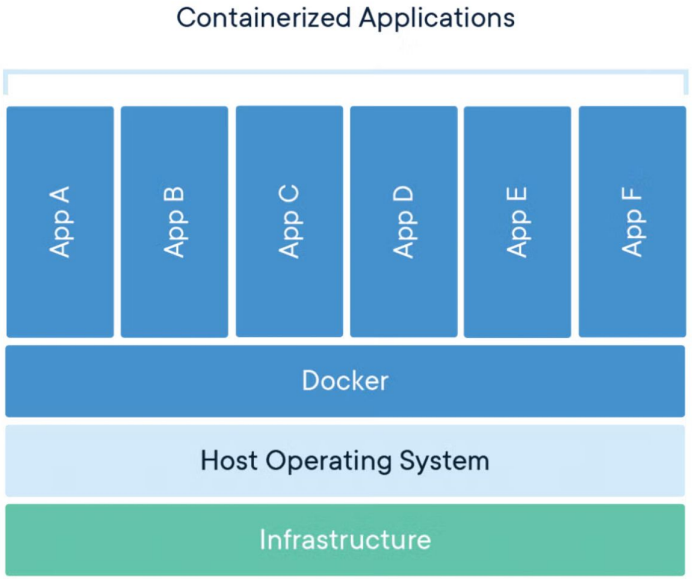
2. Practical Work (~1h30)
3. Reproducibility Consensus (~30min)

Software Containers

- Are lightweight, standalone, and executable software packages that **include everything needed to run a piece of software**
- Are **lightweight**, **reproducible** and **consistent**
- Are totally **independent** to the host system and other software installed on the machine



docker.com

docker

Apptainer

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Nextflow Workflows

- Are composed of **many simple tasks** which are chained together to form a more **complex pipeline**
- Can be composed of **steps written is mostly any programming language**:
  - Bash, Perl, Ruby, Python, etc...
- Are **flexible**, **scalable** and **reproducible**

```
// Script parameters
params.query = "/some/data/sample.fa"
params.db = "/some/path/pdb"

process blast_search {
  input:
  path query
  path db

  output:
  path "top_hits.txt"

  script:
  """
  blastp -db $db -query $query -outfmt 6 > blast_result
  cat blast_result | head -n 10 | cut -f 2 > top_hits.txt
  """
}

process extract_top_hits {
  input:
  path top_hits
  path db

  output:
  path "sequences.txt"

  script:
  """
  blastdbcmd -db $db -entry_batch $top_hits > sequences.txt
  """
}

workflow {
  def query_ch = channel.fromPath(params.query)
  blast_search(query_ch, params.db)
  extract_top_hits(blast_search.out, params.db).view()
}
```

Processes

- Are the **steps of the workflow**
- Are **user defined**
- Are **composed of different sections**

```
process example_process {
    label 'example'

    input:
        <input qualifier> <input name>

    output:
        <output qualifier> <output name> [, <option>: <option value>]

    '''
    echo "This is an example process!"
    '''
}
```

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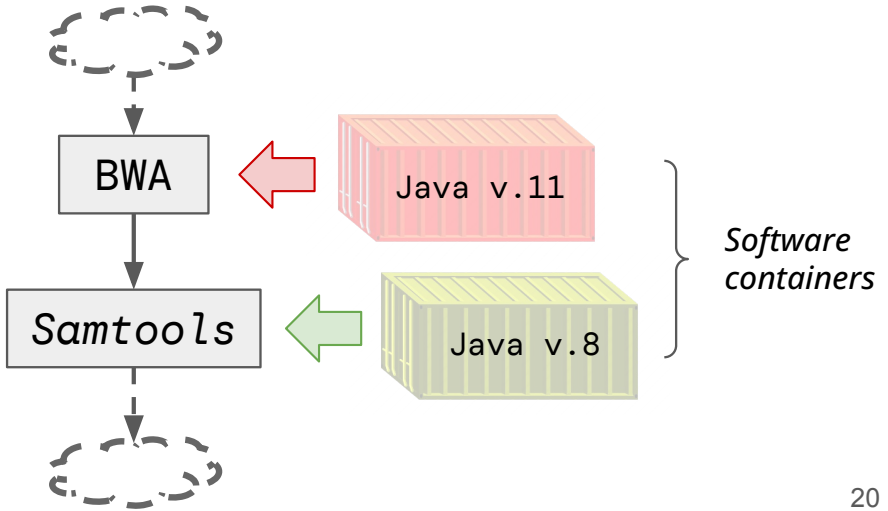
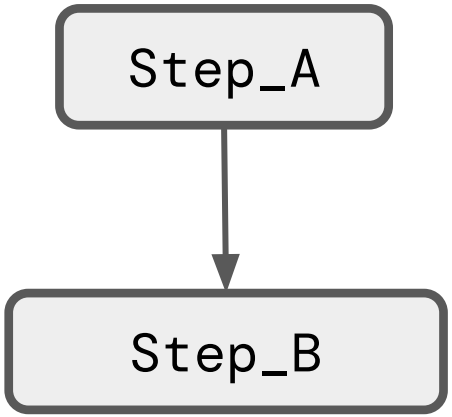
```

- Have **independent software environments** to one another (thanks to software containers)
- Are **chained together** to form the more complex pipeline



Channels and Operators

- Channels allow **to exchange data between the processes** of the workflow
- Channels can considered as **FIFO queues**



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- Channels allow **to exchange data between the processes** of the workflow
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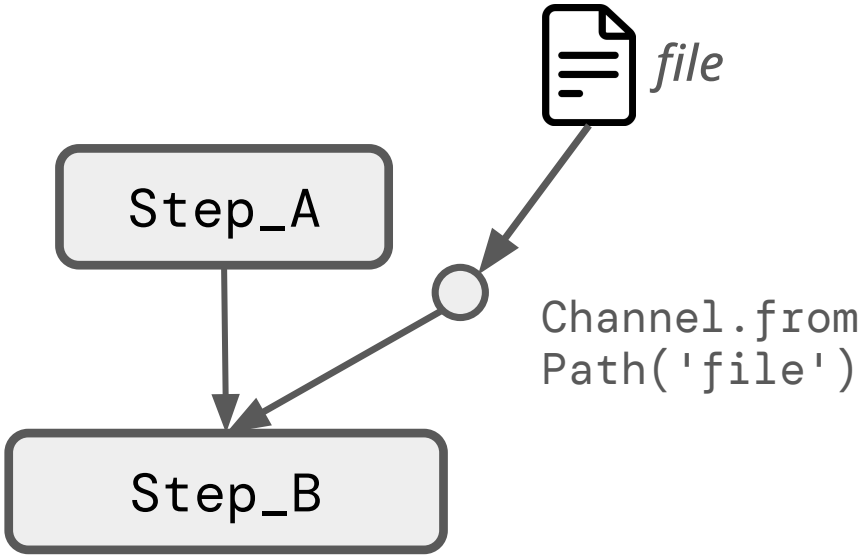
- Operators allows to **manipulate** channels, by
  - creating them, merging them, filtering them, etc...
- Operators are **pre-defined by Nextflow**
- There are **many different types of operators** (*today we are only gonna focus on the simplest ones*)



Workflow Main

- Is the **entry point of the workflow**
- It can be considered as the “main” as in generic programming (C, java, etc…)
- It is from this section **Processes can be called and Channels manipulated**

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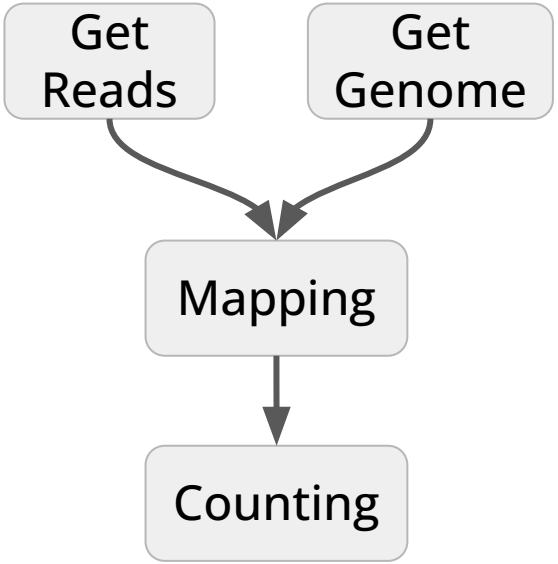
Configuration File

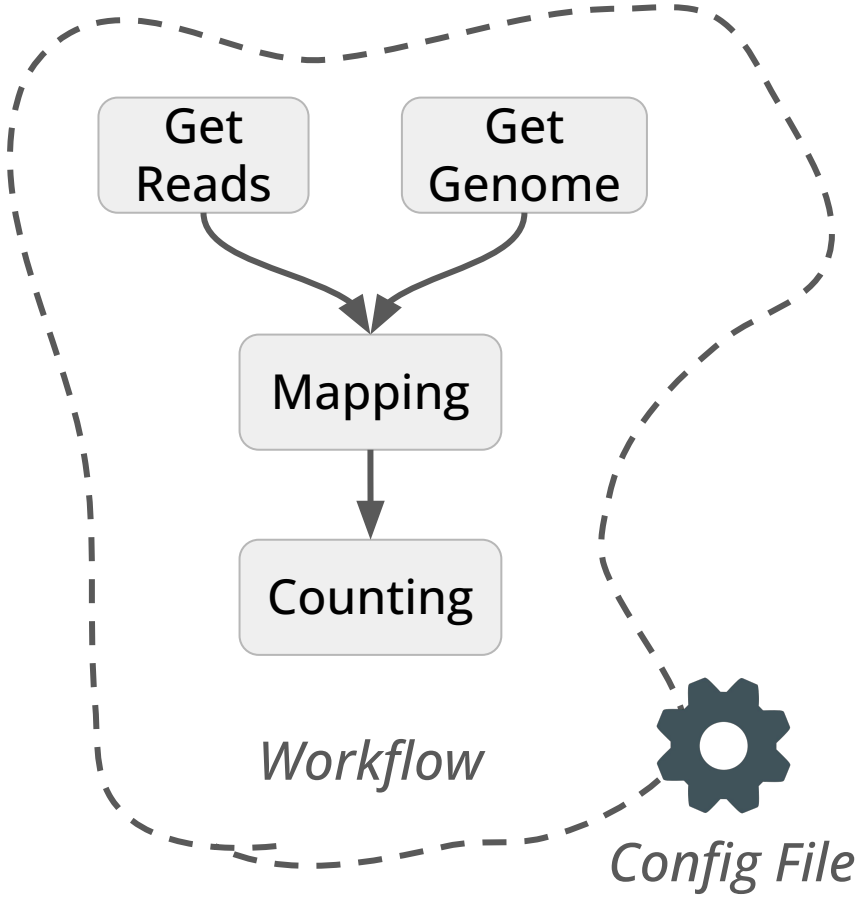
- Is **necessary to execute the workflow**



Workflow

Configuration File

- Is **necessary to execute the workflow**
- Defines the **configuration properties** of the workflow
- Is used to:
  - define which **executor to use**
  - the **process's environment variables**
  - **pipeline parameters**
  - etc...



Summary

- Nextflow allow to develop **flexible**, **scalable** and **reproducible** workflows

- Nextflow workflows are composed of:
  - **Processes**
  - **Channels** (which can be manipulated thanks to **Operators**)
  - **Workflow Main**
  - **Configuration File**

- For more information regarding Nextflow workflows, check out its documentation and tutorial https://www.nextflow.io/

Returning to the Motivational Example

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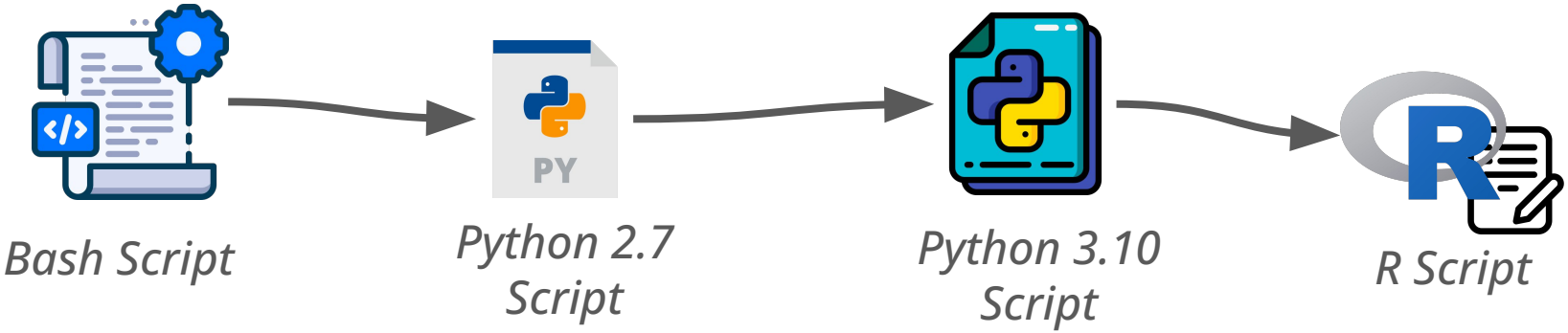

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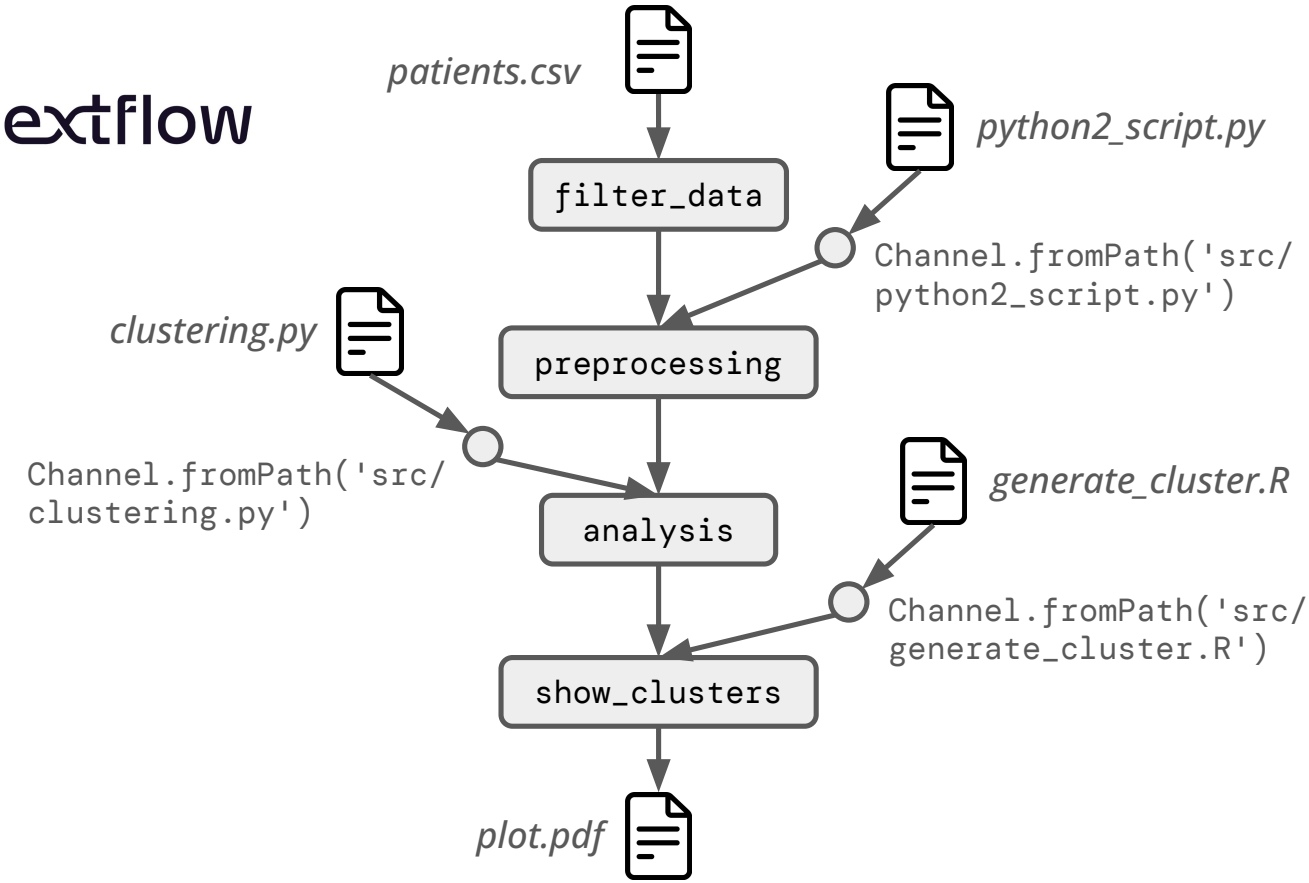

Returning to the Motivational Example

- Link to workflow implementation:
  - https://github.com/George-Marchment/acmrep25/tree/main/example_use_case

- Command to run the workflow:

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nextflow workflow.nf
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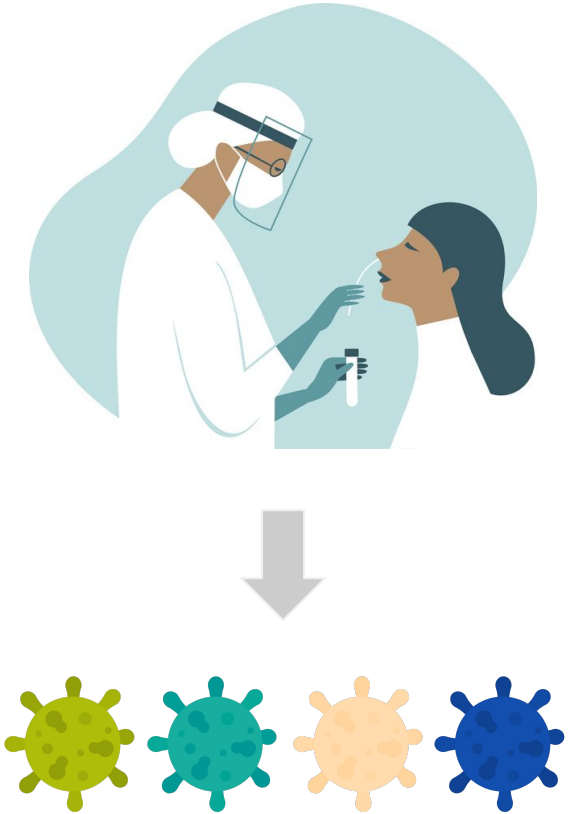
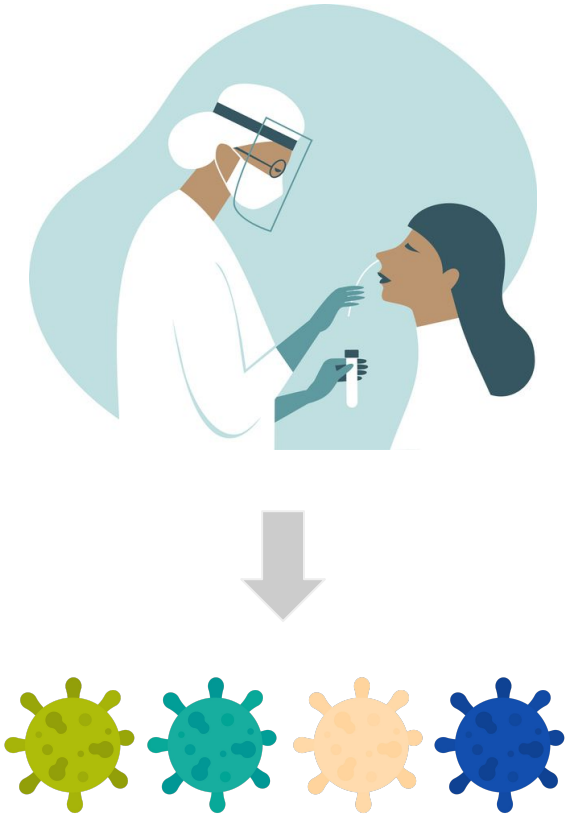
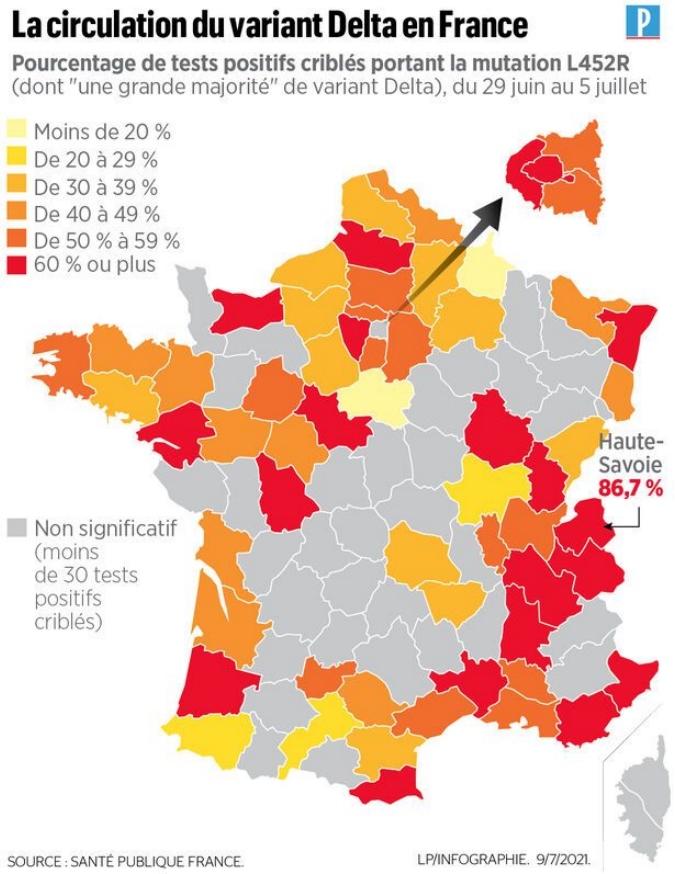


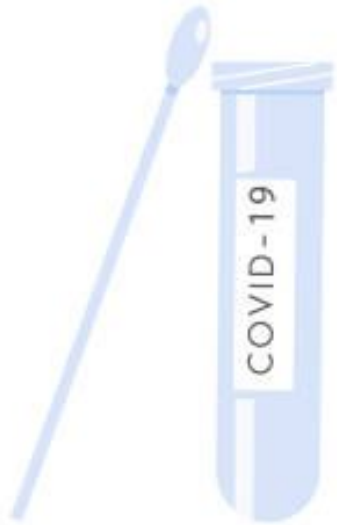
Identification of the **variant** in a person infected with the virus



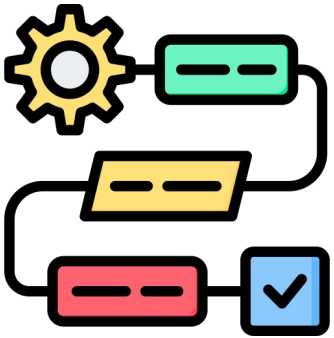


https://www.leparisien.fr/societe/sante/covid-19-et-variant-delta-en-france-ces-departements-ou-lepidemie-repart-09-07-2021-TJ3DDB7UXRC4TF23FRAB4TBAAY.php

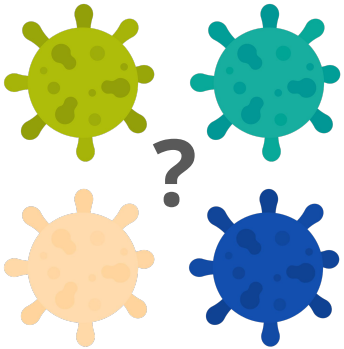
Goal of the “Project”



Sample

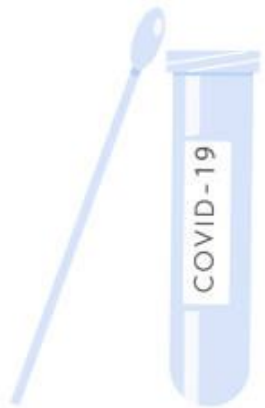


Workflow



Variant

Biology 101



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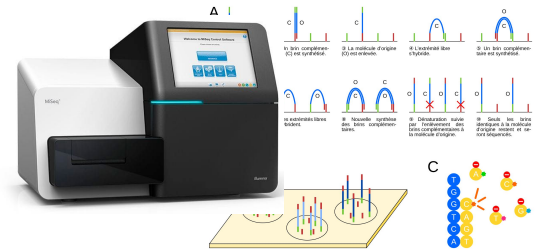
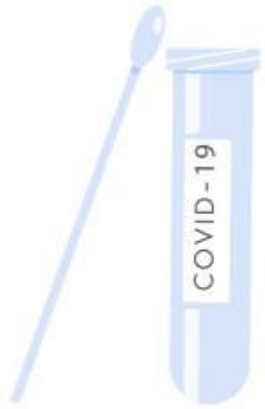


Sequencer

Genetic Code

Biology 101



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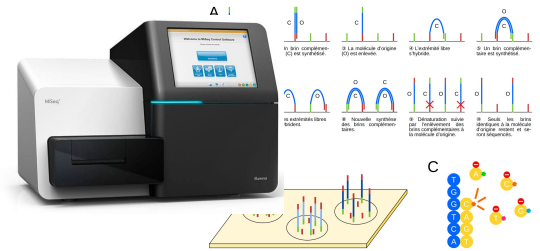

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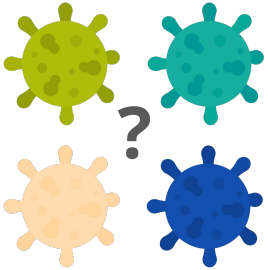

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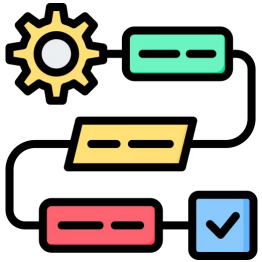
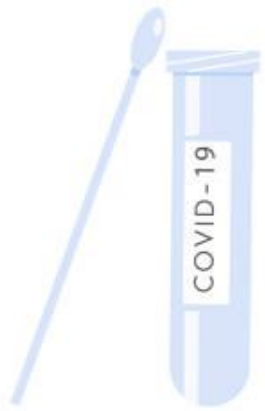
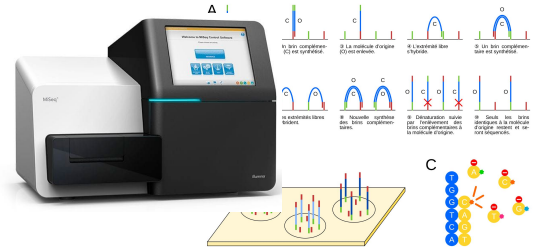


Workflow

Biology 101

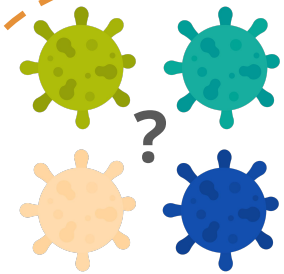


Sample

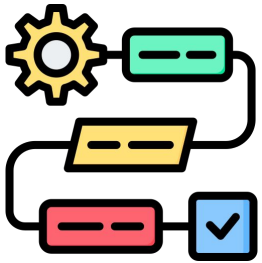


Sequencer

Genetic Code

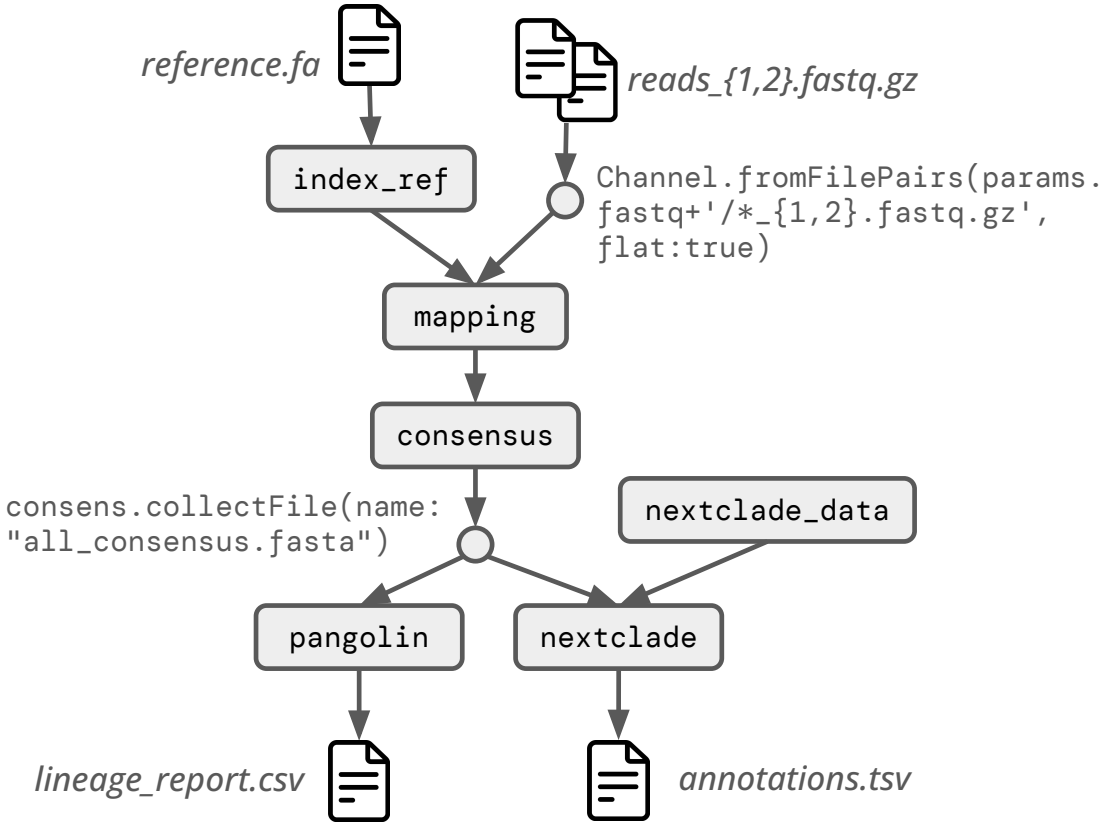


Variant



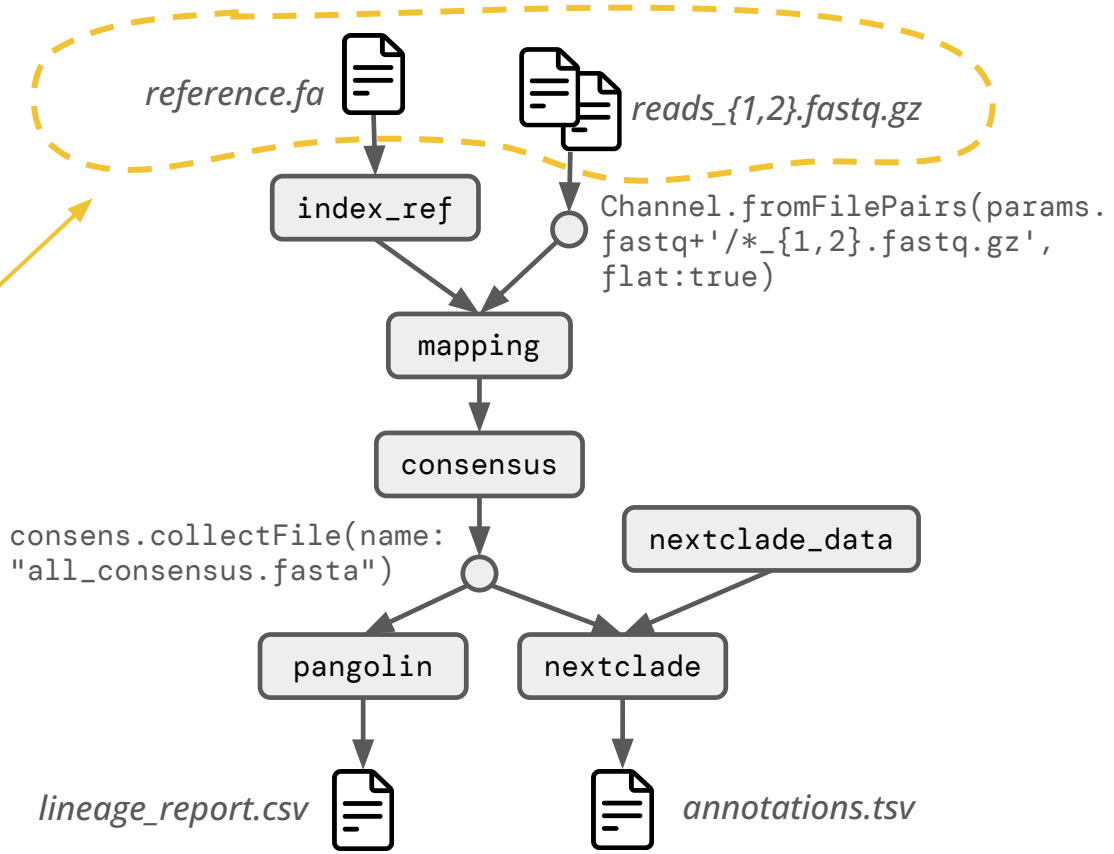
Workflow

The Workflow



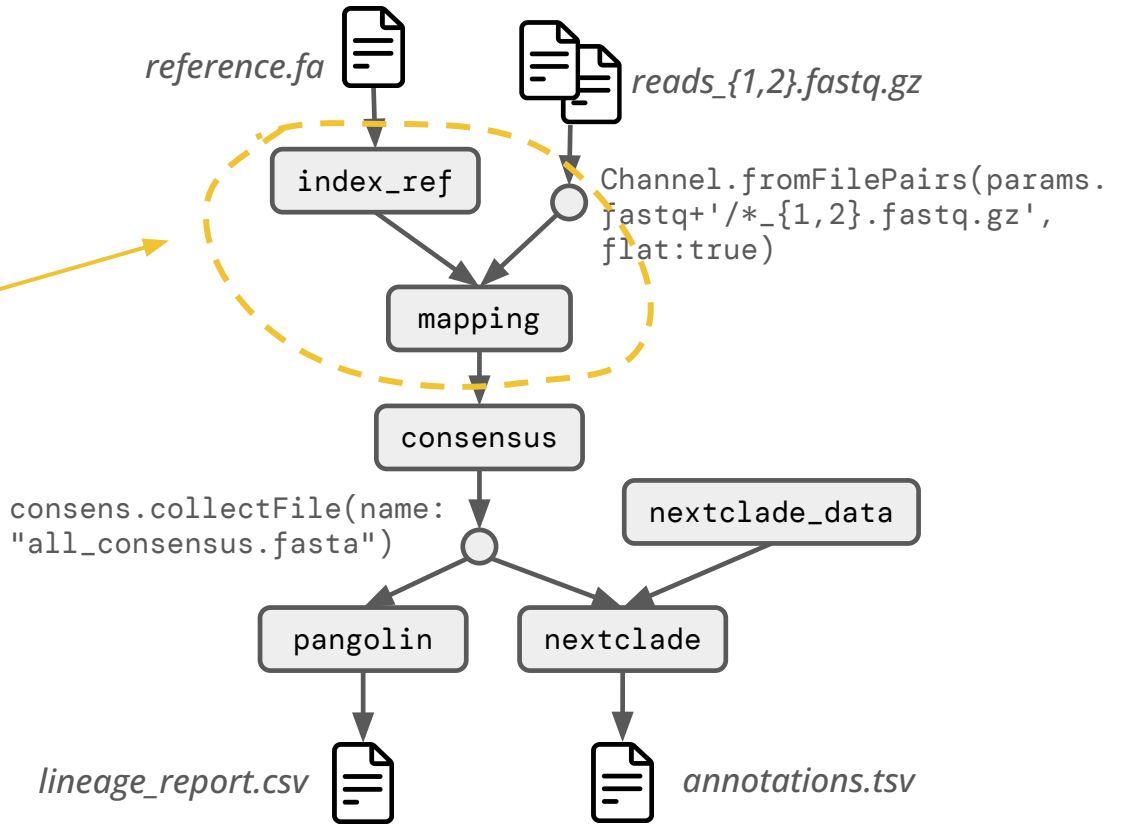
The Workflow

- Inputs:
  - Two compressed fastq files from the SARS-CoV2 sample
  - The reference genome to map



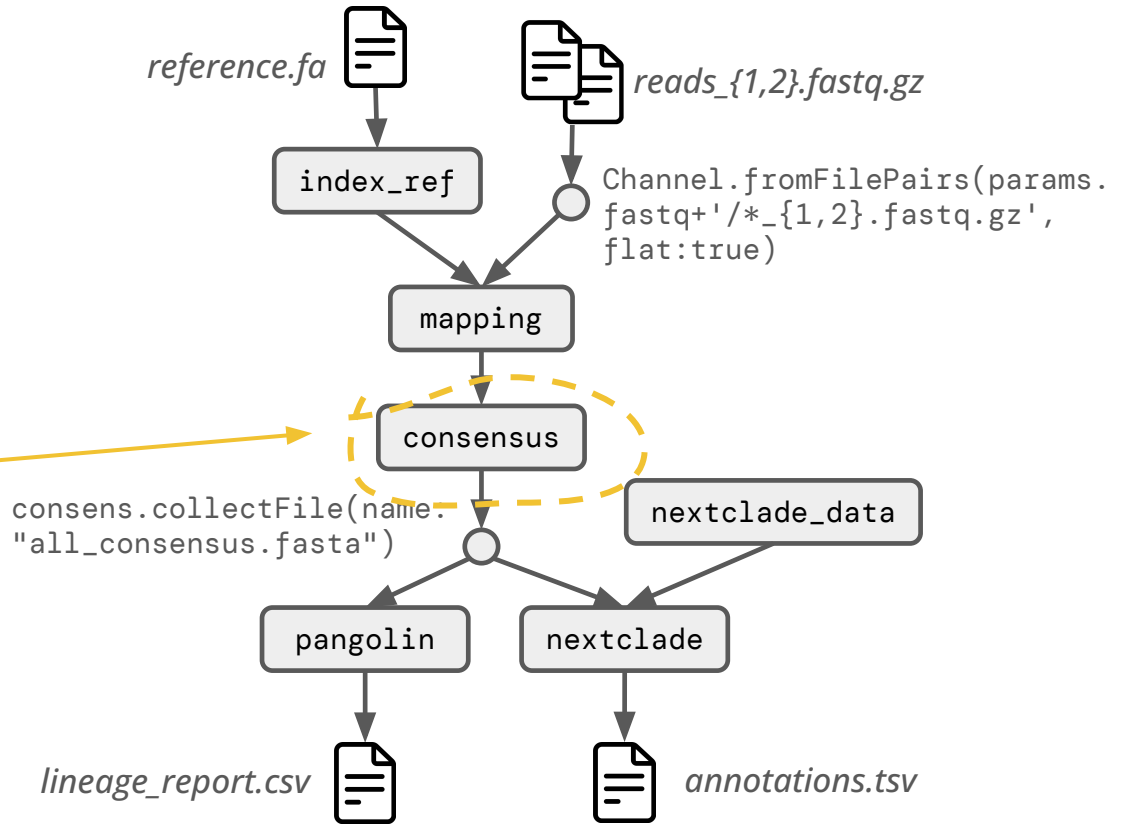
The Workflow

- Step 1:
  - Mapping the reads on a reference genome



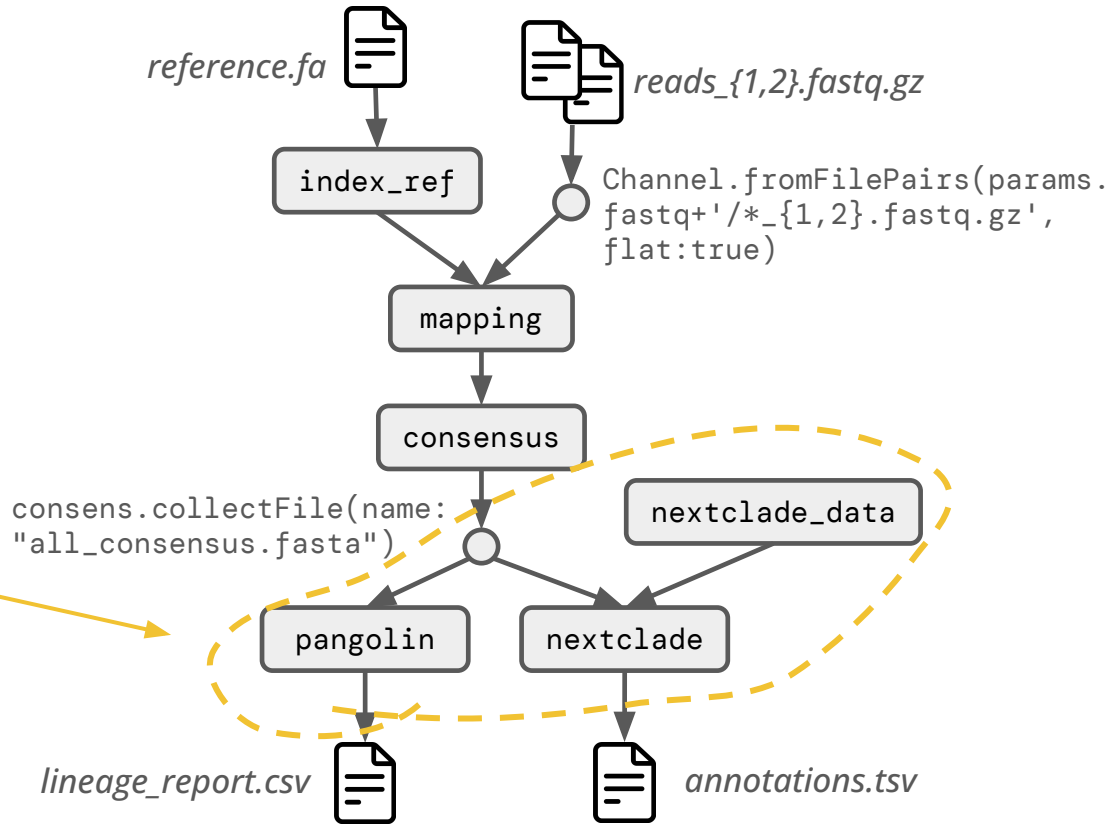
The Workflow

- Step 2:
  - Building consensus sequence



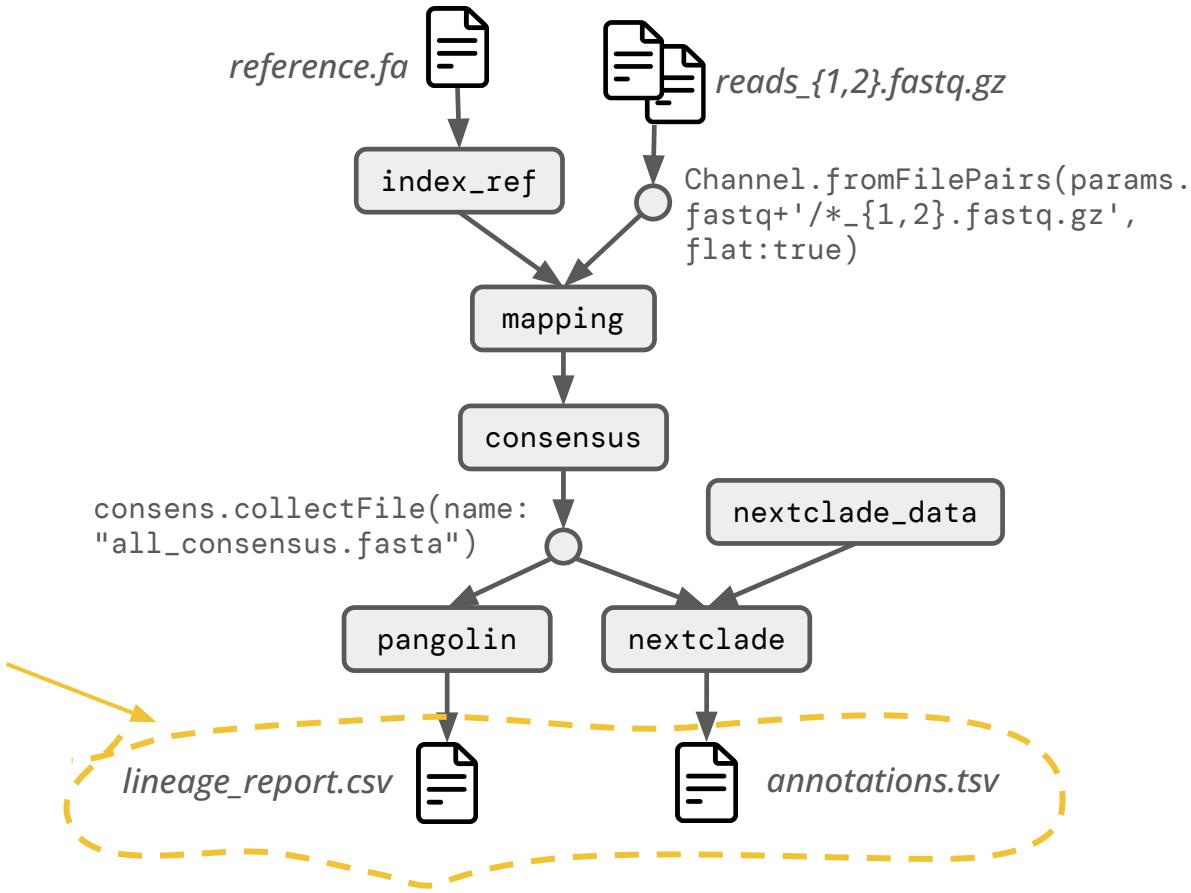
The Workflow

- Step 3:
  - Detecting clade



The Workflow

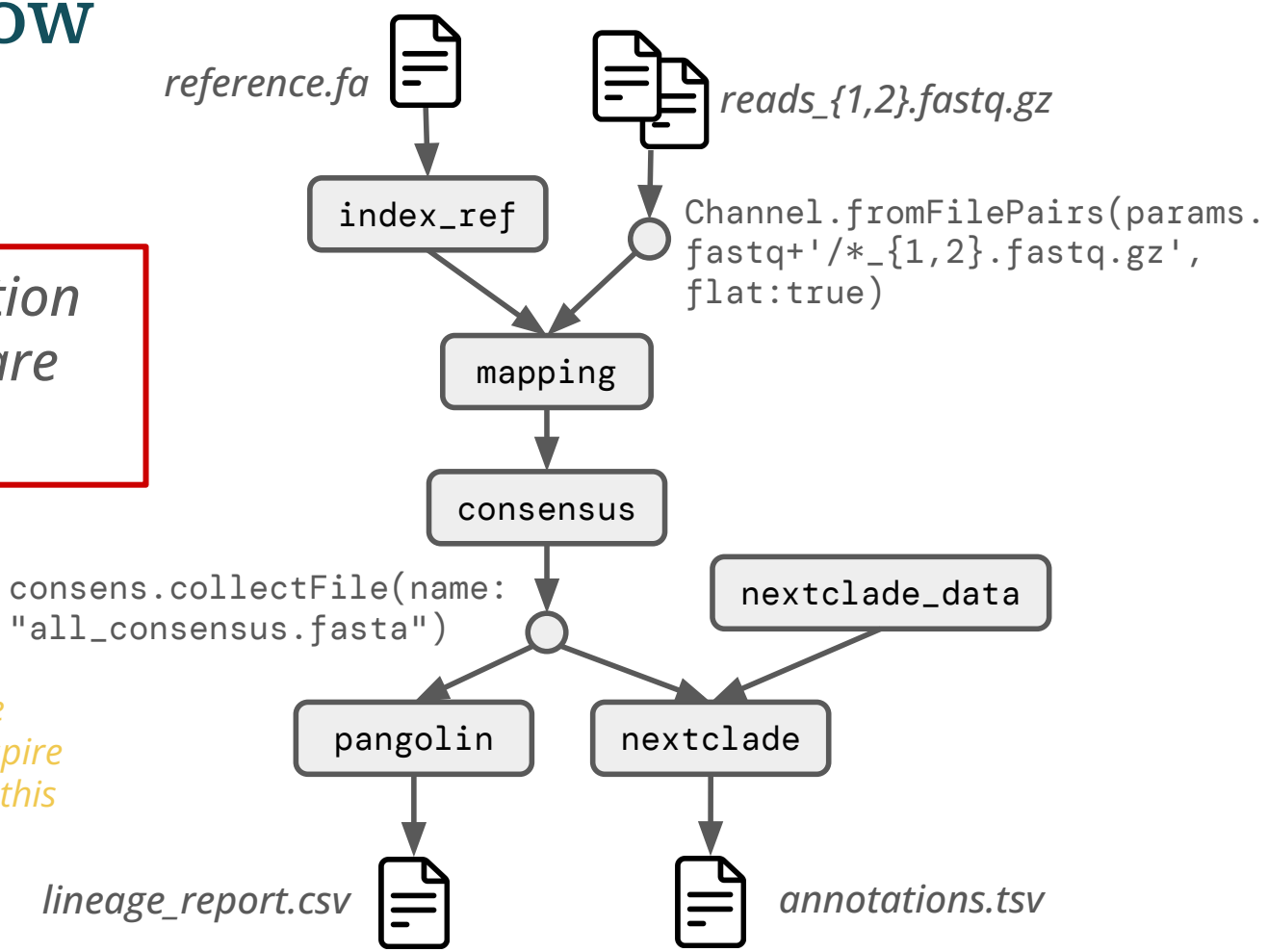
- Outputs:
  - annotations.tsv
  - lineage_report.csv



The Workflow

It's full specification and input data are described here

Use the correction of the use-case workflow to inspire your implementation of this workflow



1. Introduction to (Nextflow) Workflows (~1h)
    a. Motivational Example
    b. Objectives
    c. Scientific Workflows
    d. Software Containers
    e. Nextflow Workflows
    f. Presentation of the “Project”
2. **Practical Work (~1h30)**
3. Reproducibility Consensus (~30min)

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Reproducibility Consensus

- After implementing and running the workflow described above

- Please send the results of the workflow (the **`annotations.tsv`** as well as the **`lineage_report.csv`** file) to george.marchment[at]universite-paris-saclay.fr