

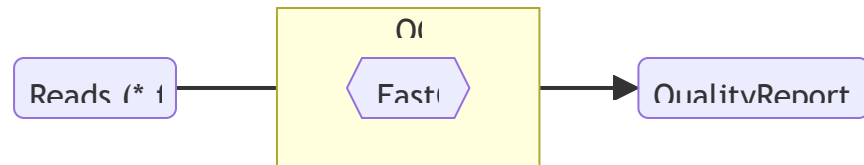
CWL in ARCs

DataPLANT Data Steward Circle – Feb 5th, 2025

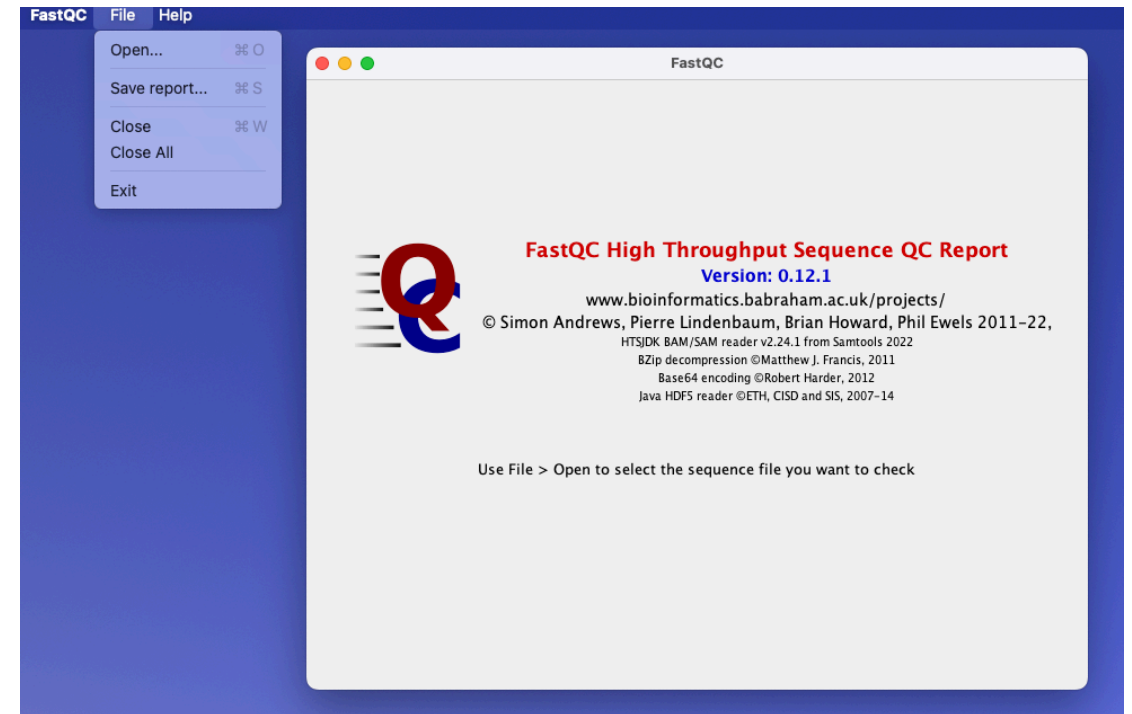
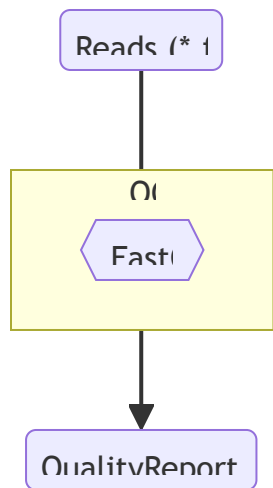
Dominik Brilhaus

Example tool: FastQC

First step in RNASeq data analysis: QC of read files (e.g. *.fastq)



FastQC has a GUI



Are we **FAIR** yet?

Command line tool

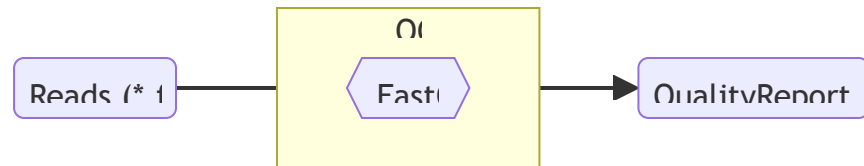
- Some tool that you can run ... on the command line
- Example:
 - CLI: **ARC Commander**
 - (GUI: **ARCitect**)
- Takes arguments or parameters as **inputs**
- Generates **outputs**

FastQC via command line

```
fastqc --version  
fastqc --help
```

FastQC via command line

```
fastqc assays/rnaseq/dataset/blau1_CGATGT_L005_R1_002.fastq.gz
```



Materials & Methods

```
fastqc assays/rnaseq/dataset/sample1  
fastqc assays/rnaseq/dataset/sample2  
fastqc assays/rnaseq/dataset/ ...
```

"FastQC v0.12.1 was employed for read quality control using default parameters."

Installing bioinformatic tools

- From source:

<https://www.bioinformatics.babraham.ac.uk/projects/download.html#fastqc>

- Docker: `docker pull quay.io/biocontainers/fastqc:0.11.9--hdfd78af_1`
- Conda: `conda install fastqc`

Why CWL and ARCs

- Reproducibility / Replicability **of the data**
 - Rerunning the same analysis on the **same** dataset
- Reusability **of the analysis**
 - Applying the same (type of) analysis on **another** dataset

Some factors affecting reproducibility & reusability

- Operating system (linux, win, mac) and version
- Version of tool / software
- Version of package/library and interpreter (python, R, F#, etc.)
- ...

Approaches towards CWL in ARCs

1. Wrap a script
2. Wrap a CLI tool
3. Reuse an existing CWL document (command line tool or full workflow)
4. ...

Demo: CWL-Wrapping the CommandLineTool FastQC

Step 1

- Without in/out
- **Local tool installed**

```
#!/usr/bin/env cwl-runner
cwlVersion: v1.2
class: CommandLineTool

baseCommand: ["fastqc", "--help"]

inputs: []

outputs: []
```

Step 2: Add a docker container

```
#!/usr/bin/env cwl-runner
cwlVersion: v1.2
class: CommandLineTool

hints:
  DockerRequirement:
    dockerPull: quay.io/biocontainers/fastqc:0.11.9--hdfd78af_1

baseCommand: ["fastqc", "--help"]

inputs: []

outputs: []
```

Step 3: Define inputs

```
#!/usr/bin/env cwl-runner
cwlVersion: v1.2
class: CommandLineTool

hints:
  DockerRequirement:
    dockerPull: quay.io/biocontainers/fastqc:0.11.9--hdfd78af_1

baseCommand: ["fastqc"]

inputs:
  reads:
    type: File[]
    inputBinding:
      position: 1

arguments:
  - valueFrom: $(runtime.outdir)
    prefix: "-o"

outputs: []
```


Step 4: Define outputs

```
#!/usr/bin/env cwl-runner
cwlVersion: v1.2
class: CommandLineTool

hints:
  DockerRequirement:
    dockerPull: quay.io/biocontainers/fastqc:0.11.9--hdfd78af_1

baseCommand: ["fastqc"]

inputs:
  reads:
    type: File[]
    inputBinding:
      position: 1

arguments:
  - valueFrom: $(runtime.outdir)
    prefix: "-o"

outputs:
  fastqc_out:
    type: File[]
    outputBinding:
      glob:
        - "*_fastqc.zip"
        - "*_fastqc.html"
```

Step 4: Define outputs

```
#!/usr/bin/env cwl-runner
cwlVersion: v1.2
class: CommandLineTool

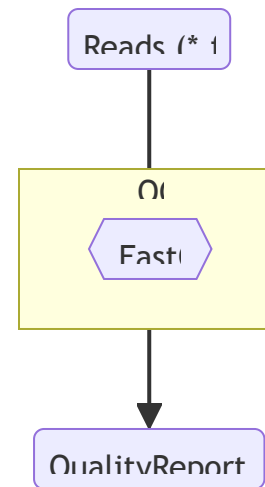
hints:
  DockerRequirement:
    dockerPull: quay.io/biocontainers/fastqc:0.11.9--hdfd78af_1

baseCommand: ["fastqc"]

inputs:
  reads:
    type: File[]
    inputBinding:
      position: 1

arguments:
  - valueFrom: $(runtime.outdir)
    prefix: "-o"

outputs:
  fastqc_out:
    type: File[]
    outputBinding:
      glob:
        - "*_fastqc.zip"
        - "*_fastqc.html"
```



Run the workflow

You can provide arguments via another file:

```
run.yml
```

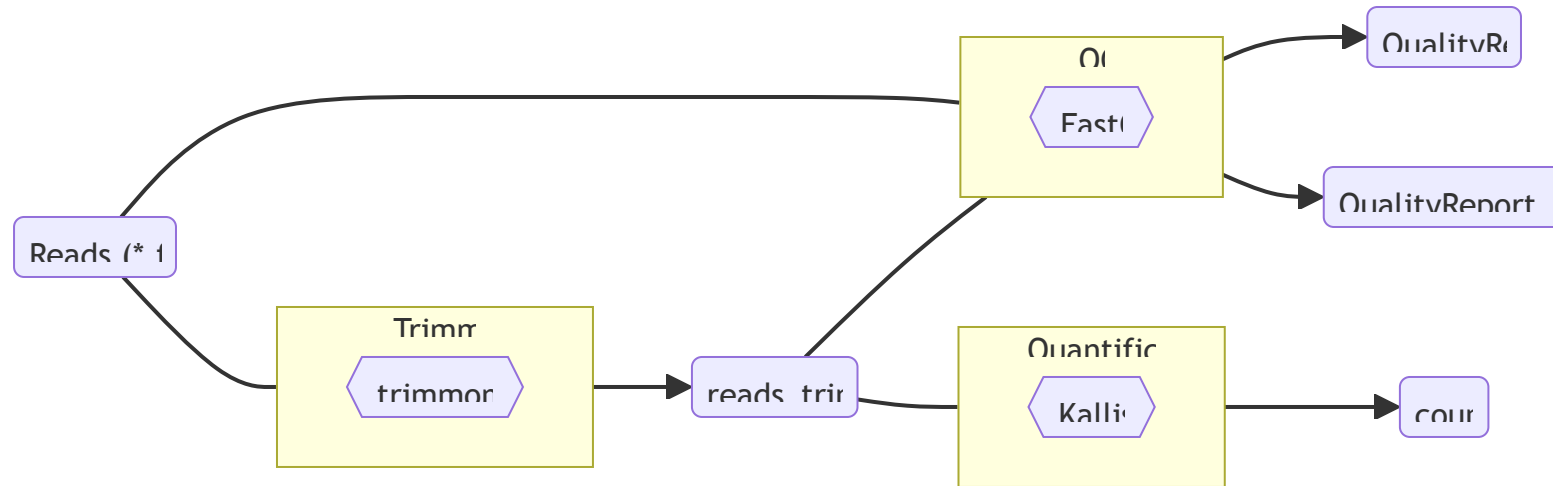
```
reads:
```

- class: File
path: ../../assays/rnaseq/dataset/blau1_CGATGT_L005_R1_002.fastq.gz
- class: File
path: ../../assays/rnaseq/dataset/blau2_TGACCA_L005_R1_002.fastq.gz

Reusability: Simply import an existing CWL

- e.g. from one ARC to another

Example workflow: First steps RNASeq pipeline



CWL is a time investment at first

There's a *tiny* learning curve and some dependencies

- JavaScript
- Docker
- Conda and the cwltool (reference runner)

Resources

- Specification v1.2: <https://www.commonwl.org/v1.2/CommandLineTool.html>
- Published Workflows: <https://view.commonwl.org/workflows>
- CWL repos: <https://www.commonwl.org/repos/>
- bio-cwl-tools: <https://github.com/common-workflow-library/bio-cwl-tools/tree/release>
- EBI-Metagenomics: <https://github.com/EBI-Metagenomics/workflow-is-cwl/tree/master/tools>
- Scatter example: https://github.com/Gibbsdavidl/CWL_scatter_example
- CWL tool: <https://github.com/common-workflow-language/cwltool>