Getting started with Conda and Nextflow

Week 4 - Workflow Management Training Workshop

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Note! Switching things up this week

Conda and Nextflow are expansive topics

Mixing lecture with hands-on exercises

Please interrupt and ask questions

BIOCONDA®

CONDA

nextflow

nf-core

Topics for Today

Tentative Schedule

- Conda and Installation (~20 minutes)
- Nextflow and Example Runs (~30 minutes)
- Break (~10 minutes)
- Nextflow Channels & Processes (~20 minutes)
- Nextflow DSL1 vs DSL2 (~20 minutes)
- Additional Exercises and Discussion
- Wrap-up (Final ~15 minutes)

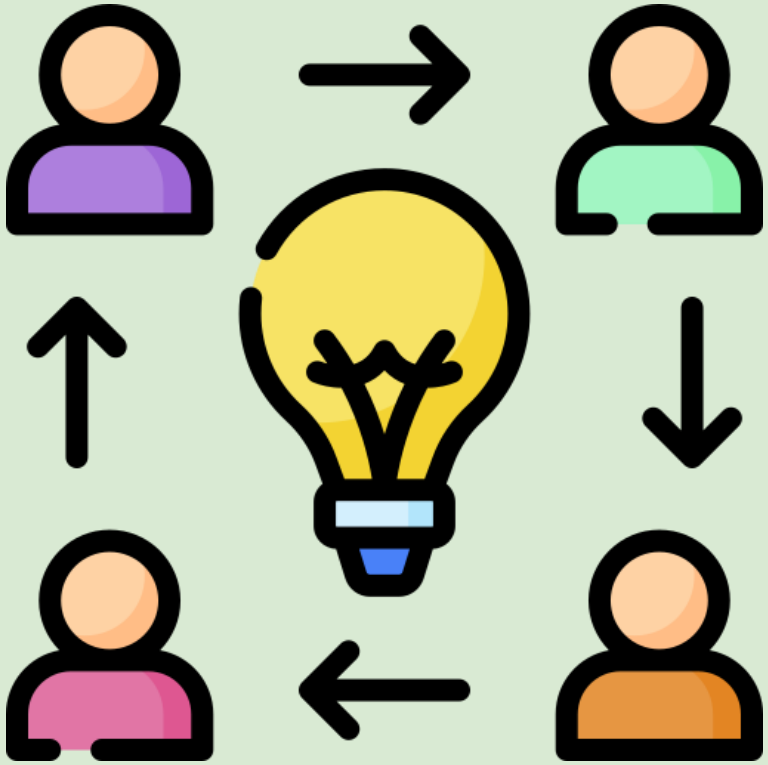
CONDA

- A package manager for installing 1000s of tools
- Available on Windows, Mac, and Linux
  - Windows has fewer available packages
- Packages are grouped into channels
  - conda-forge – 18k+ general, non-domain specific tools
  - Bioconda – 4k+ bioinformatic tools and libraries
  - Can even set up a personal channel

```
conda create -n fastq-scan fastq-scan
conda activate fastq-scan
fastq-scan -h
Usage: cat FASTQ | fastq-scan [options]
Version: 1.0.0

Optional arguments:
    -g INT   Genome size for calculating estimated
                 sequencing coverage. (Default 1)
    -p INT   ASCII offset for input quality scores,
                 can be 33 or 64. (Default 33)
    -q       Print only the QC stats, do not print
                read lengths or per-base quality scores
    -v       Print version information and exit
    -h       Show this message and exit
```

BIOCONDA® for all your bioinformatic tools



- Makes bioinformatics accessible
  - Easy installs, dependency handling
- Downstream containerization*
  - Docker – Biocontainers
  - Singularity Images - Galaxy Project
- Truly a community driven repository
  - More than 1,300 people have contributed
- Currently 4,000+ recipes are available
- Learn more at bioconda.github.io

Exercise 1: Conda

Exercise 1: Install Conda and Serotype a Shigella genome

- Head on over to GitHub: Exercise 1 - Conda

- Together we will:
  - Install Miniconda3
  - Install Mamba
  - Create a “Shigatyper” environment
  - Serotype and Shigella genome

- Wrap up the exercise

When to use and not use CONDA

- Use Conda:
  - Rapid prototyping
  - Need a quick answers
  - Personal systems

- Skip Conda:
  - Production should use containers (Docker or Singularity)
  - HPC and Cloud environments
  - Using Windows only (*e.g., not using WSL2*)

Conda “best practices”

- Keep the initial “base” environment clean
  - Mamba is an exception
- Use “conda create” for isolated environments
  - Treat these environments as disposable
- Channel priority is important
  - Prefer conda-forge before bioconda

Common Conda issues to keep in mind

- “Unable to solve environment”

- Automated docker builds can be problematic
  - If a StaPH-B Docker container is available, use it
    - Rigorous manual builds that are verified to be working
  - Curtis Kapsak is an expert for using Docker for bioinformatics

- Conda is can be fragile if misused
  - Fragility increases as “base” environment grows
  - If all else fails, just reinstall it

Questions or comments?

Introduction to Nextflow

nextflow

```
nextflow.enable.dsl=2


process sayHello {
  input:
    val cheers
  output:
    stdout

  """
  echo $cheers
  """
}

workflow {
  channel.of('Ciao','Hello','Hola') | sayHello | view
}
```

- A popular workflow manager in Bioinformatics
- Enables scalable and reproducible pipelines, with built in resumability
- Supports Conda, Docker, and Singularity
- Seamlessly move between local resources, HPC, and major cloud providers
- Regularly solicits user feedback to guide future developments

nextflow is platform independent

- Execute on a laptop of the cloud, with a simple parameter change
- Available on:
  - Bioconda, Docker, Singularity
  - Google Cloud Platform
  - Amazon Web Services
  - Microsoft Azure
  - HPC Schedulers
- Executable from:
  - Nextflow Tower

kubernetes

Google Cloud

GRID ENGINE

aws

slurm
workload manager

Microsoft Azure

IBM Spectrum LSF

nextflow tower

nf-core pushing Nextflow to the limits

- Community effort to collect curated Nextflow pipelines
  - 2400 Slack users, 1000+ GitHub contributors
- Includes 60+ hi-quality bioinformatic pipelines
  - rnaseq, mag, bactmap, many more
- nf-core/modules has 400+ DSL2* modules available
- Standardized guidelines for developers
- Thorough review process produces robust pipelines

Web platforms that support Nextflow

- Freely available web-platforms for the execution of bioinformatic pipelines
- No command-line knowledge required, allowing users to do more science
- Platforms:
  - Nextflow Tower from Seqera Labs
    - Supports workflows written in Nextflow
    - Platform agnostic and supports many providers
      - HPC, Google Cloud, Microsoft Azure, Amazon Web Services
    - Community showcase of curated pipelines
  - Terra from the Broad Institute
    - Nextflow executed inside Jupyter notebooks
    - Limited to Google Cloud Platform
  - CGC from Seven Bridges
    - Extensive API for executing workflows
    - Limited to Amazon Web Services

Exercise 2: Nextflow Introduction

Executing Nextflow Pipelines

- Use "nextflow run" to execute pipelines

```
nextflow run main.nf
```

- Can also run from GitHub repository

```
nextflow run nf-core/rnaseq
```

- "-resume" allows pipelines to be resumed

```
nextflow run nf-core/rnaseq -resume
```

- Many command-line arguments available, and additional sub-commands

Exercise 2: Install Nextflow and run a few workflows

- Head on over to GitHub: Exercise 2 – Nextflow Introduction

- Together we will:
  - Create a “Nextflow” environment
  - Execute Hello World
  - Execute Bactopia/nf-core test workflows
  - Browse Nextflow outputs

- Wrap up the exercise

A few things to keep in mind about Nextflow

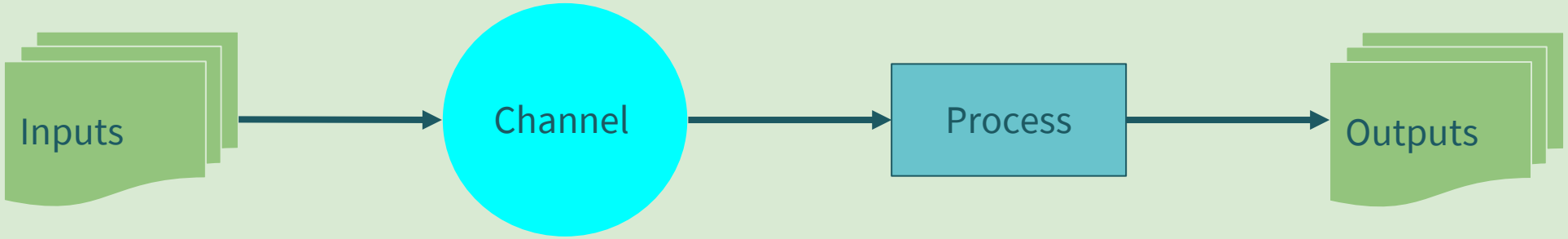
- Missing features:
  - Command line argument parser
    - nf-core has a library to handle this
  - Dry run feature
    - "stub runs" are a decent alternative
- Error messages can sometimes be hard to decipher
- By default, Nextflow uses all available resources

Questions or Comments?

Break Time ~10 minutes

Exercise 3: Nextflow Channels, Operators, and Processes

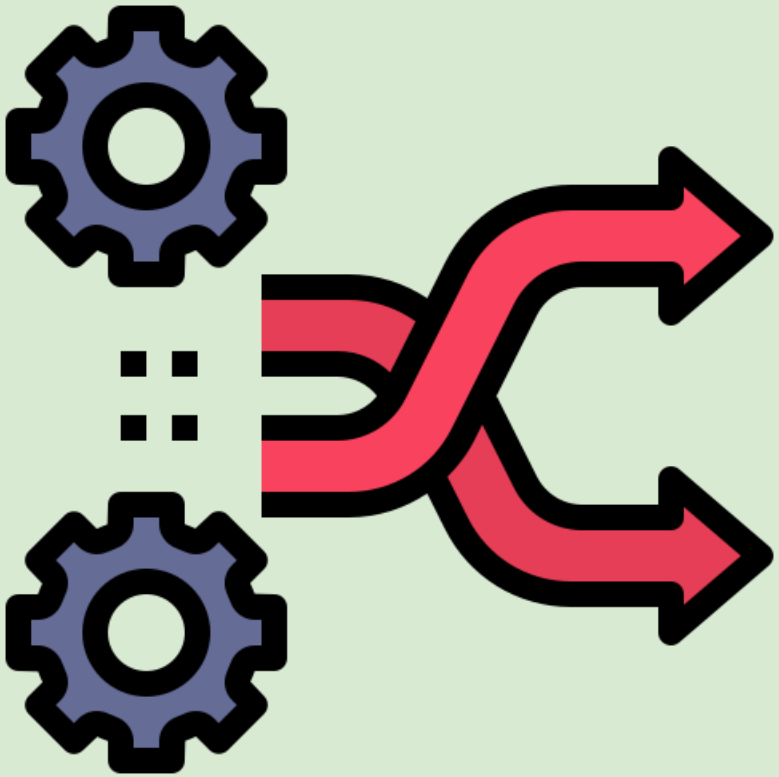
Nextflow Basic Structure



- Channel
  - Queue Channel
    - "*First-in, First-out*" (FIFO) connecting processes and operators
  - Value Channel
    - Stores a single value (*e.g., genome size*)
    - Can be a named list (*e.g., ["id": "my_sample", "genome_size": 360000]*)

- Channels can be used by Operators and Processes

Channel Operators



- Methods to connect channels, or transform values of channels
  - Filtering
  - Transforming
  - Splitting
  - Combining
  - Forking
  - Math

- More than 50 Operators available to use

Processes

- The basic unit for executing user scripts
- 30+ directives adjust optional settings
  - Can be dynamic
- Inputs and outputs are channels
  - Can be optional
- Conditional executions using ‘when’
- The script block executes user code

```
process < name > {

   [ directives ]

   input:
    < process inputs >

   output:
    < process outputs >

   when:
    < condition >

   [script|shell|exec]:
   < user script to be executed >

}
```

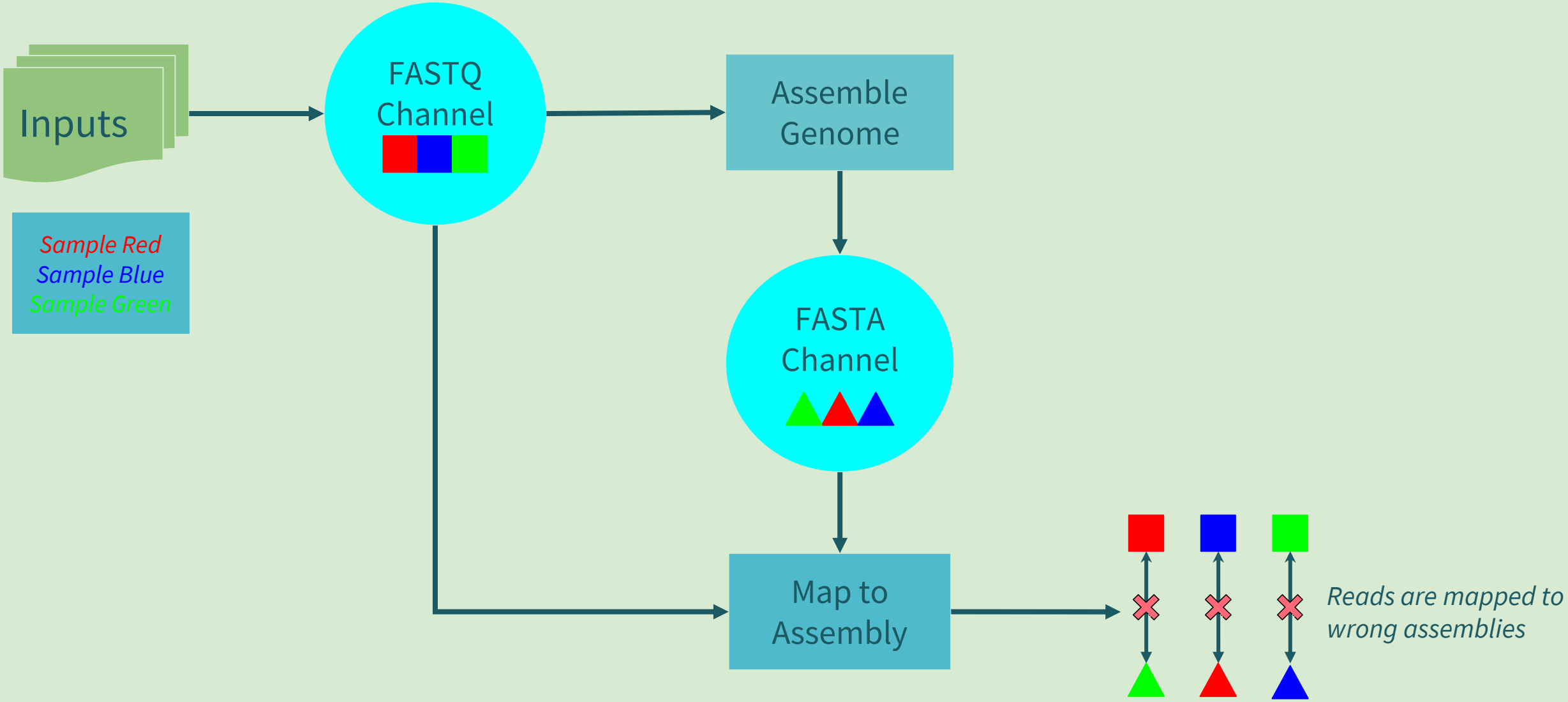
Exercise 3: Nextflow Channels and Processes

- Head on over to GitHub: Exercise 3 - Nextflow Channels and Processes

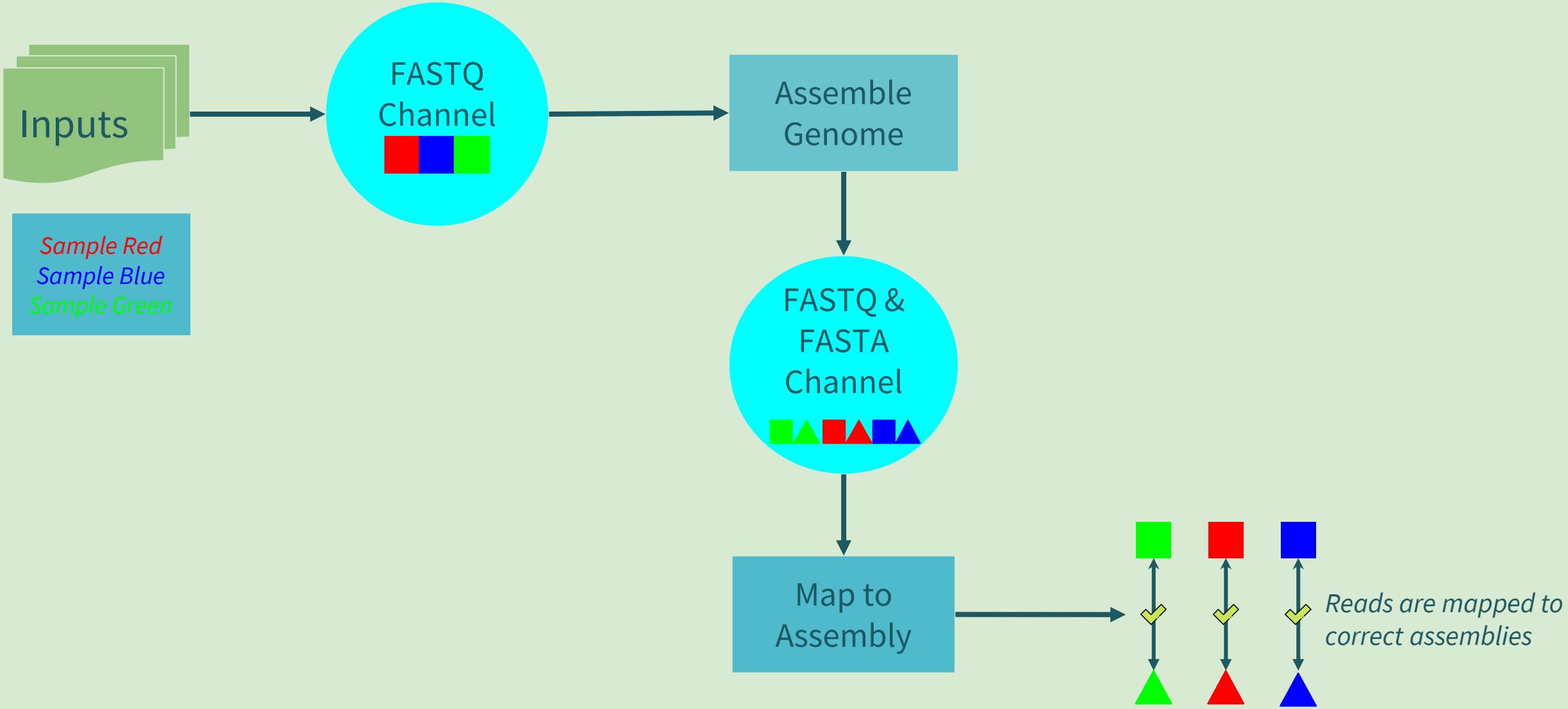
- Together we will:
  - Demonstrate Operators
  - Demonstrate FIFO nature of Channels
  - Pass Channels between Processes
  - Create Channels from Process outputs

- Wrap up the exercise

FIFO Can Cause "*Unexpected*" Results



One Solution: Carry Inputs Across Processes



Questions or Comments?

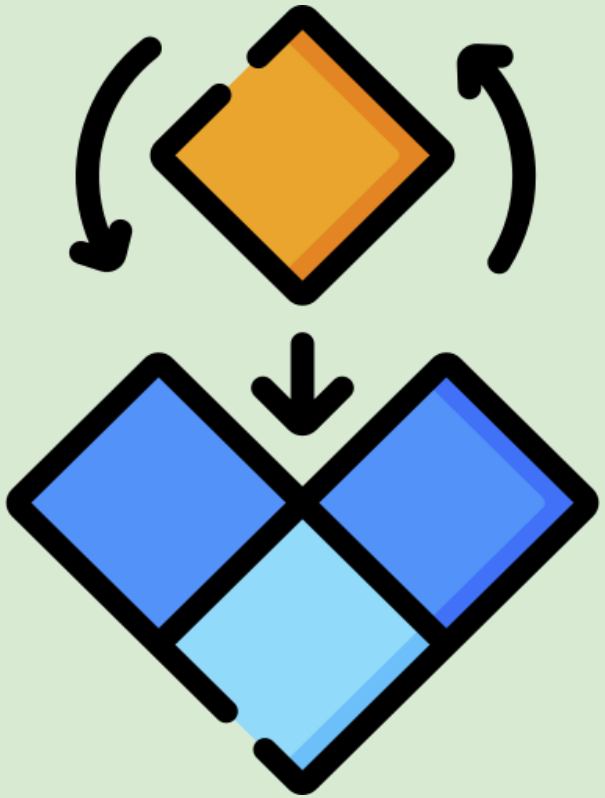
Exercise 4: Nextflow DSL1 vs DSL2

nextflow DSL1

- The original syntax for Nextflow language
- Pipelines were written in a single script
  - Increased maintenance burden as pipeline grew
- Pipelines were not modular
  - Difficult to reuse pieces from one pipeline in another
- Data channels were one-time use
  - Required channels to be duplicated

nextflow DSL2

- Major evolution in the Nextflow language
- Introduced true modularization in Nextflow workflows
  - Modules – A ***reusable*** Nextflow script with a process definition
  - Subworkflows – Multiple modules linked together
- Modules are portable and easily shared between workflows
- Data channels can be used more than once



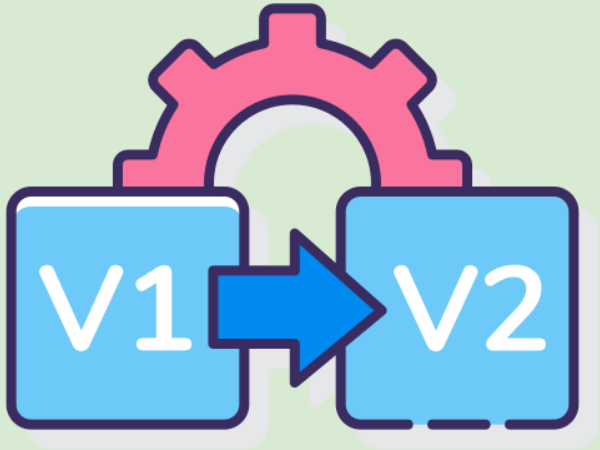
Exercise 4: Nextflow DSL1 vs DSL2

- Head on over to GitHub: Exercise 4 - Nextflow DSL1 vs DSL2

- Together we will:
  - Demonstrate config file usage
  - Walk through “scan-n-trim” DSL1 pipeline
  - Walk through “scan-n-trim” DSL2 pipeline
  - Alter command-line arguements

- Wrap up the exercise

Choose DSL2 Going Forward



- As of v22.04 DSL2 is now the default in Nextflow
  - DSL1 pipelines must tell Nextflow to use DSL1
- New pipelines should be written in DSL2
- nf-core/modules has 500+ ready to use DSL2 modules
  - Rapid prototyping and pipeline building
  - Version controlled, extensive logging, supports Conda, Docker and Singularity

Questions or Comments?

Additional Exercise Ideas

Additional Exercise Ideas

- Use “publishDir” to adjust how files are output
- Use “label” to adjust runtime requirements
- Create a “config profile” to switch between Conda and Docker
- Create a DSL2 pipeline using modules from nf-core

Additional Nextflow Resources

Nextflow and Bioconda specific support channels

- Nextflow Slack
  - General Nextflow Support
  - Nextflow devs regularly helping users
- Nf-core Slack
  - Nf-core and Nextflow devs regularly helping users
- Bioconda Gitter
  - Mostly related to submitting Bioconda recipes
- StaPH-B Slack
  - Many users from the state public health labs

Nextflow Continuing Education

- Nextflow Training Workshop
  - 10+ hour Nextflow course given by Seqera Labs
- Nextflow and nf-core
  - 10+ hour course being developed by nf-core members available from Software Carpentries
- Reproducible, scalable, and shareable analysis workflows with Nextflow
  - 10+ hour Nextflow course by Sateesh Peri, Michael Cipriano, and Matthew Hunter Seabolt

Useful Nextflow Links

- Nextflow Documentation
  - Extensive documentation of Channel operators, Process directives, executors, and many other Nextflow features
- Awesome Nextflow
  - A curated list of Nextflow pipelines
  - Presentations, tutorials, videos, etc…
- Nextflow Patterns
  - A repository of ways to do things in Nextflow

Useful nf-core Links

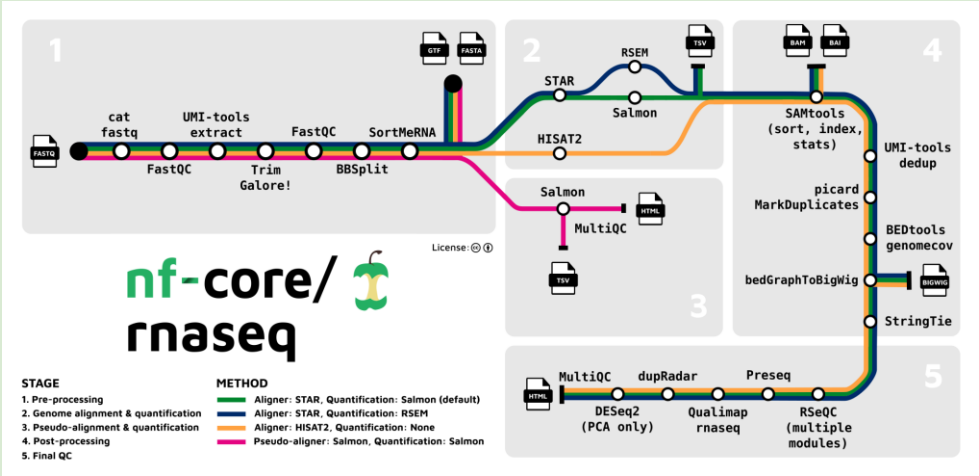
- nf-core
  - Nf-core's main website, includes documentation for each pipeline, module documentation, etc…
- nf-core bytesize Talks
  - 20-minute videos covering all things nf-core, Nextflow, and best practices
- nf-core/modules
  - More than 400 ready-to-use DSL2 modules
- nf-core/configs
  - Numerous (80+) Nextflow configs for inspiration
- nf-core/tools
  - Python package with helper tools for the nf-core community.

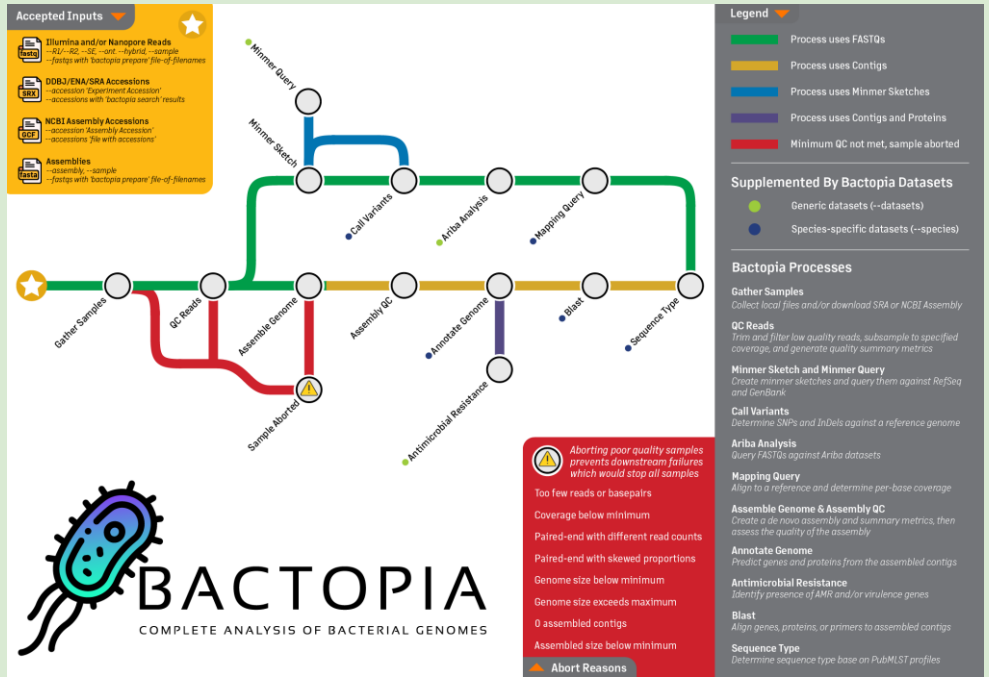
Nextflow DSL2 pipelines for inspiration

- Make use of them, or use their source code for ideas

- nf-core/rnaseq
  - RNA sequencing analysis pipeline with gene counts and extensive QC
  - Cutting-edge on Nextflow features

- Bactopia *(shameless plug)*
  - For the complete analysis of bacterial genomes
  - Illumina and Nanopore support, 130+ bioinformatic tools, 30+ additional workflows





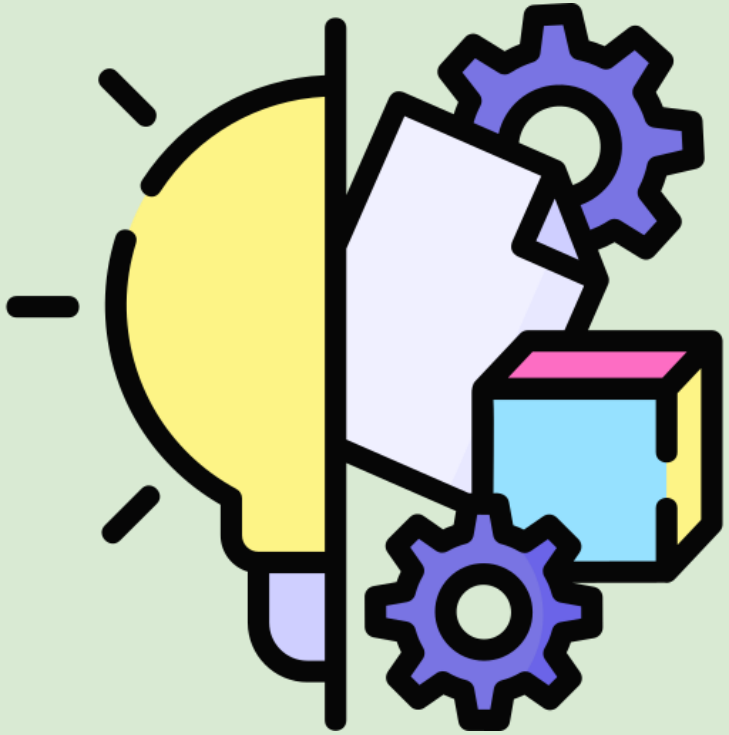
Final Wrap Up

Workflow managers make bioinformatics manageable

- Manages the execution of pipelines
  - Linking inputs/outputs of bioinformatic tools
  - Queuing jobs locally, on clusters, or the cloud
  - Logging, errors, audit trails
- Promote reproducible and reusable science
- Common workflow languages:
  - Nextflow, WDL, and Snakemake
- Pick one that works for you

The *beginnings* of a strong bioinformatic skill set

- Accessibility and Portability
  - Docker
  - Conda
- Reproducibility
  - Workflow Description Language (WDL)
  - Nextflow
- Bioinformatic Platforms
  - Terra.bio
  - Nextflow Tower



But don’t let it end here!

- *This has only been the <u>beginnings</u> of a strong bioinformatic skill set*
- Practice, practice, practice
- Make mistakes, break things, debugging error messages is a top-tier skill
- Try to figure things out, but don’t hesitate to ask questions

Questions or Comments?