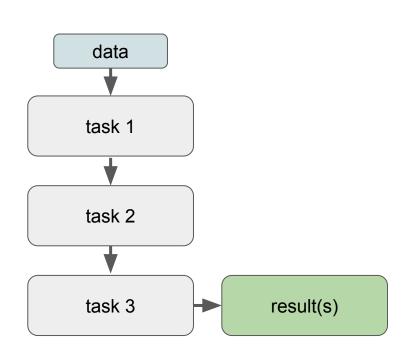
Pipelines with Cit flow

Maxime Borry, Quentin Letourneur

Why do you need a pipeline language?

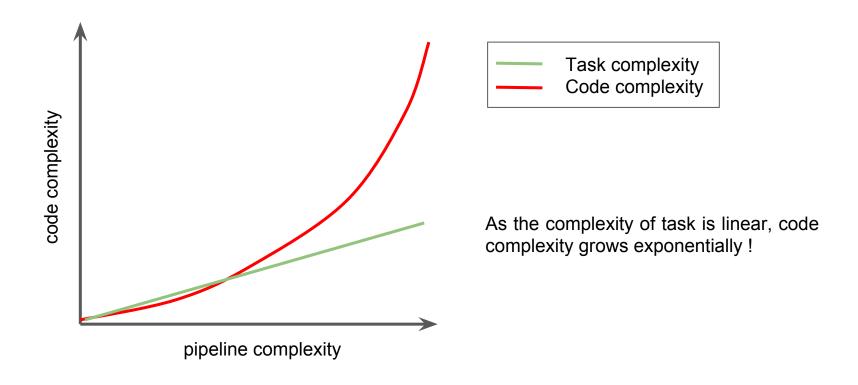


"Easy, I can write a script in ** to do that"

**insert programming language here

- Runtime optimisation
- Reporting
- Code Readability
- Share-ability
- Versioning
- Dependencies
- Scalability

Pipeline vs code complexity



A solution: workflow managers











nextflow.io

Di Tommaso, Paolo, et al. "Nextflow enables reproducible computational workflows." Nature biotechnology 35.4 (2017): 316.

Snakemake vs Nextflow

	Nextflow	Snakemake
Language	Groovy / JVM	Python
Tasks connection	Channels	File name
Asynchronous job gestion	+++	++
Scheduler flexibility	+++	+
HTML reports (results)	N	Υ



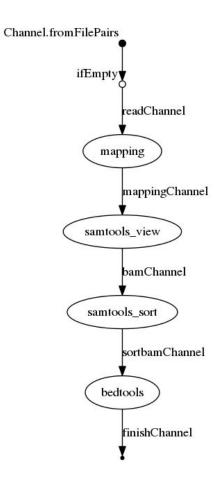
Anatomy of Nextflow pipeline

What is a channel?

How to give inputs?

How to define a process?

How to define arguments/parameters?



Channels

A First in First out (FiFo) pipe that allows processes to communicate (pass files) between themselves

Channel factory

```
myChannel=Channel.fromPath("/home/data")
        [/my/data/SRR493366_1.fastq]

myChannel=Channel.fromFilePairs("/path/to/paired_{1,2}_data")
        [SRR493366, [/my/data/SRR493366 1.fastq, /my/data/SRR493366 2.fastq]]
```

https://www.nextflow.io/docs/latest/channel.html

Processes

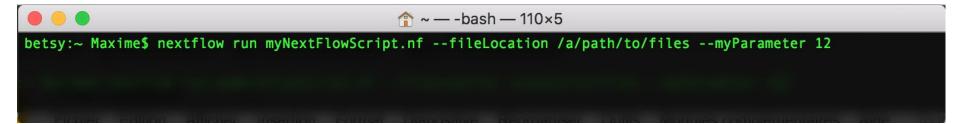
```
process toto {
     input:
     file (myFile) from myInputChannel
     output:
     file("myOutput.txt") into myOutputChannel
     script:
     11 11 11
     myscript $myFile
     11 11 11
```

```
input:
     <input qualifier> <input name> [from <source channel>] [attributes]
output:
     <output qualifier> <output name> [into <target channel>[,channel,..]] [attribute
[,..]]
```

Parameters

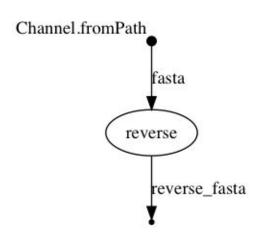
Avoid hardcoded path and parameters!

```
params.fileLocation = "/default/path"
params.myParameter = 8
```

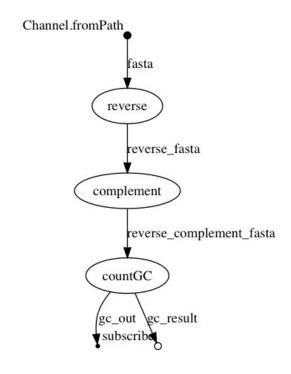


A simple Nextflow pipeline example

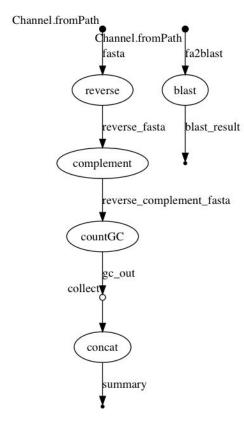
```
#!/usr/bin/env nextflow
params.fasta = "$baseDir/data/*.fasta"
params.results = "$baseDir/results"
fasta = Channel.fromPath(params.fasta)
process reverse {
    input:
    file(fa) from fasta
    output:
    file("*.reversed.fa") into reverse fasta
    script:
    11 11 11
    reverse.py $fa
    11 11 11
```



Other simple Nextflow examples

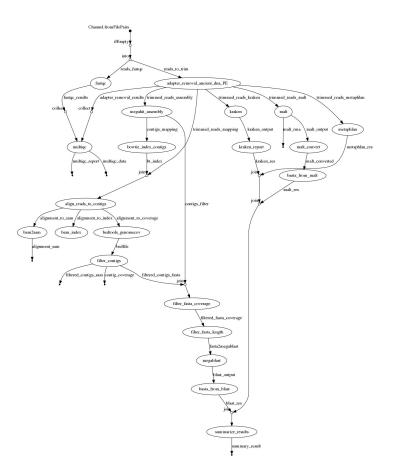


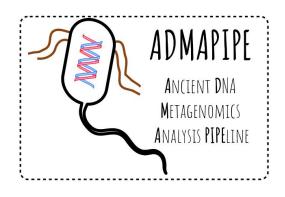
nf-example/example1.nf



nf-example/example2.nf

And more complicated pipelines...





github.com/maxibor/admapipe

Reproducibility

Can be used to run each step:

- Conda environment
- Singularity images
- Docker images



Conda is a package manager that lets you easily install programs into isolated environments

```
conda 'conda channel::package'
process blast {
     conda 'bioconda::blast'
     input:
     file(fa) from fa
     output:
     file("*.out") into blast result
     script:
     ** ** **
     blastn -db ${params.blastdb} -query $fa -out blast.out -outfmt 6
     11 11 11
```

Example of Singularity recipe file

```
Bootstrap: docker
                                                            header (always needed)
From: ubuntu:16.04
%files
    ~/genome.fasta /home
%post
    apt -y update
    apt -y install wget zlig1g bzip2 build-essential
    cd /home
                                                            sections (optional)
    wget https://github.com/samtools/samtools/
    releases/download/1.3/samtools-1.3.tar.bz2
    tar -xjf samtools-1.3.tar.bz2
    cd samtools-1.3
    ./configure
    make
    make install
```

https://www.sylabs.io/quides/2.6/user-quide/container_recipes.htm1

<u>In code</u>

```
process blast {
     container '/path/to/fasta.simg' local image
     input:
     file(fa) from fa
     output:
     file("*.out") into blast result
     script:
     11 11 11
     blastn -db ${params.blastdb} -query $fa
     -out blast.out -outfmt 6
     11 11 11
need to add -with-singularity to the command line
```

Limitations and benefits

Disk space usage (workdir)

Full potential used on computing clusters

No automated arguments/parameters check (yet ?)

Fast evolving (syntax change)

Now it's up to you!

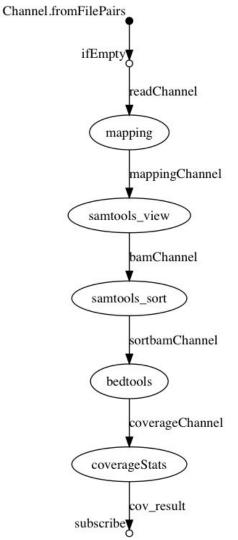
github.com/ParisDiderot-Bioinfo/nextflow-intro

Get Help:

Nextflow Documentation

maxime.borry@gmail.com

quentin.ltn92@gmail.com



First install Nextflow

With conda!

1- Install conda (if not already installed): conda.io/miniconda

2-conda install -c bioconda nextflow