Big Data analytics mit Nextflow und nf-core

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apeltzer.github.io

Slides: http://bit.ly/nf-core-tuebix

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Challenges: Big Data

- Data in computational (biology, physics, chemistry ...) is
  - big (PB scale)
  - diverse (e.g. sequencing, proteomics, ...)
  - erroneous (e.g. contains sequencing errors)

We need methods and tools to analyze such data!

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Challenges: Software dependencies

Workflows / Pipelines consist of

- different tools
- dozens of individual methods

Complex dependency trees and configuration requirements!

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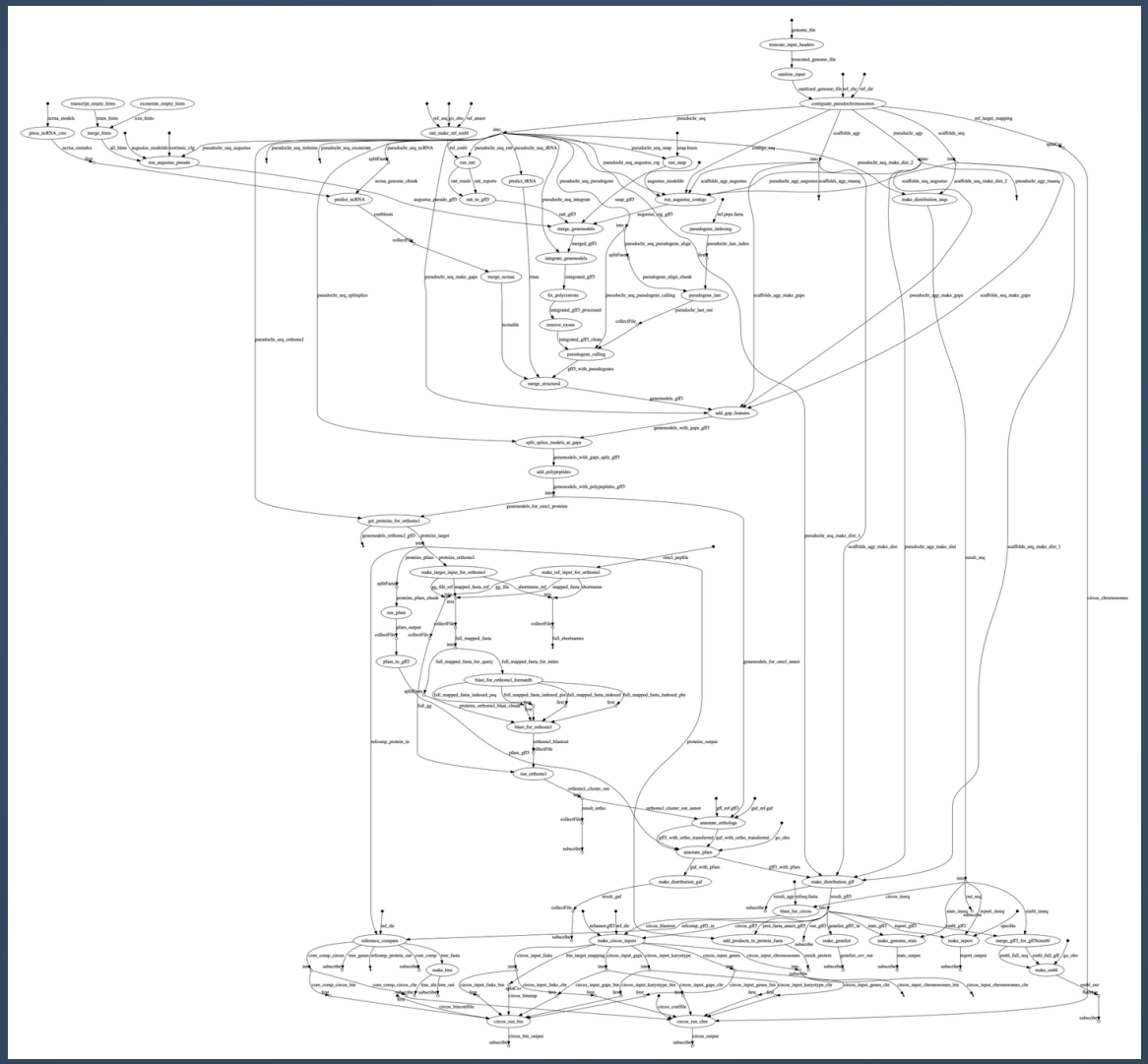

Steinbiss et al., "*Companion*: a web server for annotation and analysis of parasite genomes", NAR 2016

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Challenges: Software dependencies

Workflows / Pipelines consist of

- different tools
- dozens of individual methods

"[...] of the tools selected for our comprehensive and systematic usability test, **49% were deemed "difficult to install," and 28% of the tools failed to be installed** [...]."

- *Mangul et al, biorxiv preprint, October 25 2018*

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Challenges: Reproducibility

- Large-scale projects more common today
  - 1,000 Genomes Project
  - 100,000 Genomes Project UK
  - (EU 1,000,000 Genomes Project)
- Reproduce results with older data / integrate with newer data

Many paper results are not reproducible at all

or require a lot of effort !

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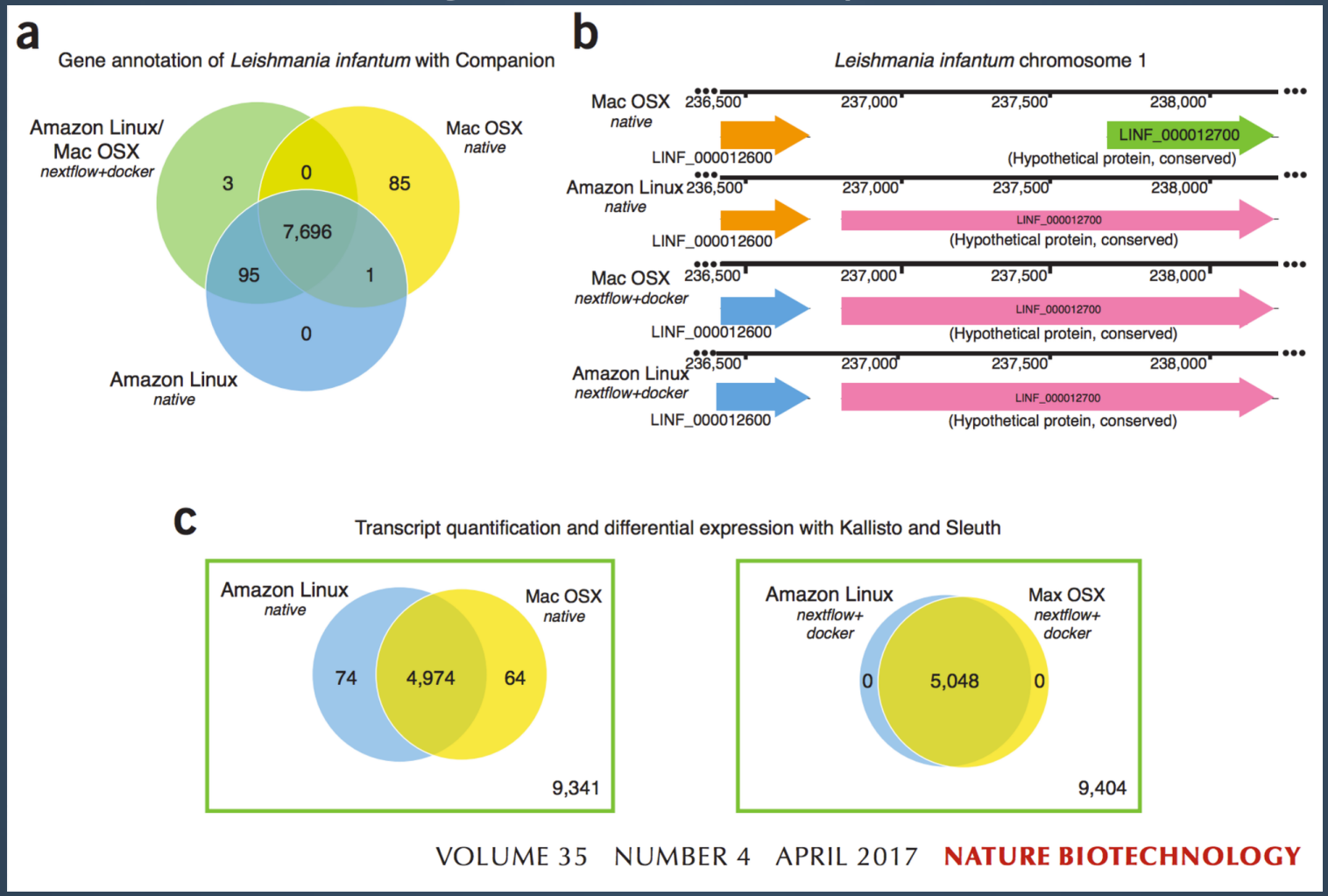
Challenges: Environmental stability

- Portability and stability of code between different OS should be ensured
- Are results different? Yes, they are ...

Challenges: Software dependencies



Di Tommaso et al., 2017, Nature Biotechnology

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All of this is a requirement for:

FAIR Data Sharing

- **Findable**
- **Accessible**
- **Interoperable**
- **Reproducible**

Strong move towards FAIR-Sharing, FAIR-Processing in scientific disciplines!

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Nextflow

- Custom DSL (domain-specific language) for
  - fast prototyping
  - enabling task composition
  - easy parallelization
- Self-contained: Containerize tasks (e.g. with Docker)
- Isolation of dependencies: Keep container - rerun analysis at any point!

Automated

Parallelizable

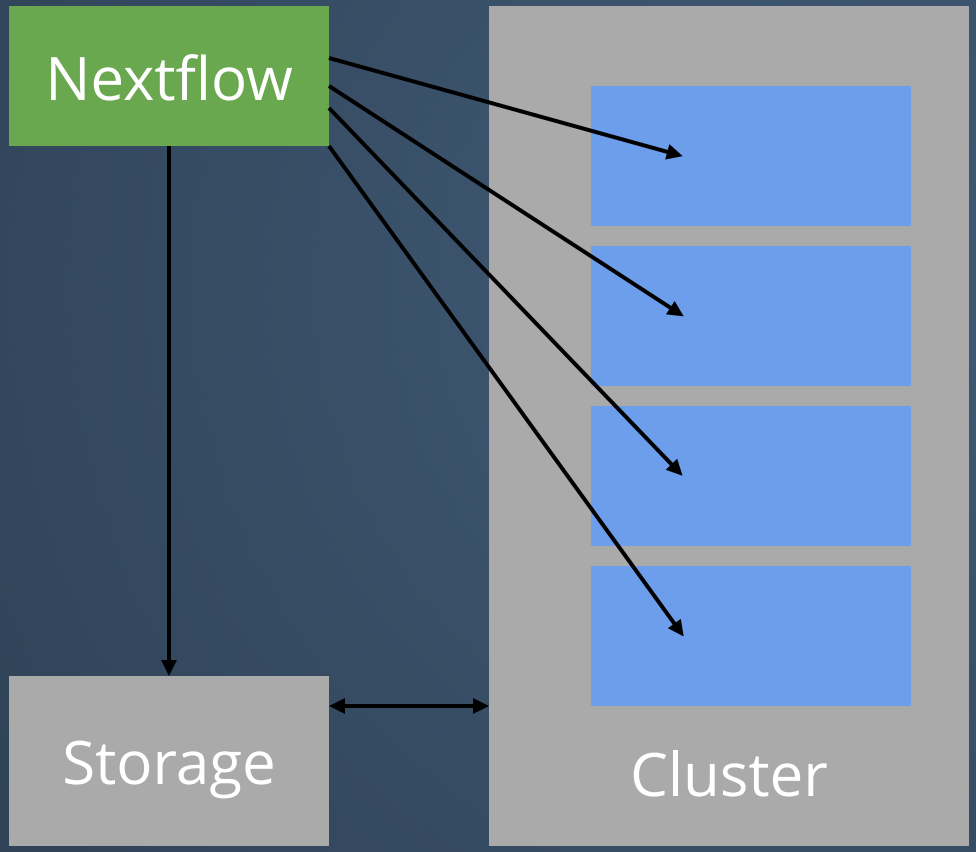
Reliable

Easy for others to run

Reproducible results

nextflow

Nextflow: Centralised Orchestration



- Submit jobs to cluster nodes
- Store data on shared storage

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Nextflow: Executor abstraction

```
#Run script locally
process.executor = 'local'

#Run script on PBS/Torque
process.executor = 'pbs'

#Run script on Kubernetes cluster
process.executor = 'k8s'

#Run script on AWS Batch
process.executor = 'awsbatch'
```

=> Improves code portability

nextflow

```
#!/usr/bin/env nextflow
input = Channel.fromFilePairs(params.reads)

process fastqc {
  input:
  file reads from input

  output:
  file "*_fastqc.{zip,html}" into results

  script:
  """
  fastqc -q $reads
  """
}
```

nextflow

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}
```

```
nextflow run main.nf --reads "*.fastq.gz"
```

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- Community effort to collect production ready analysis pipelines
- Save time in development, more testing, more updates
- https://nf-co.re


Phil Ewels


Alex Peltzer


Harshil Patel


Maxime Garcia


Sven Fillinger


Andreas Wilm

+ many others!

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- Initially supported by SciLifeLab, QBiC and A*Star Genome Institute Singapore

SciLifeLab

QBiC

A*STAR Genome Institute of Singapore

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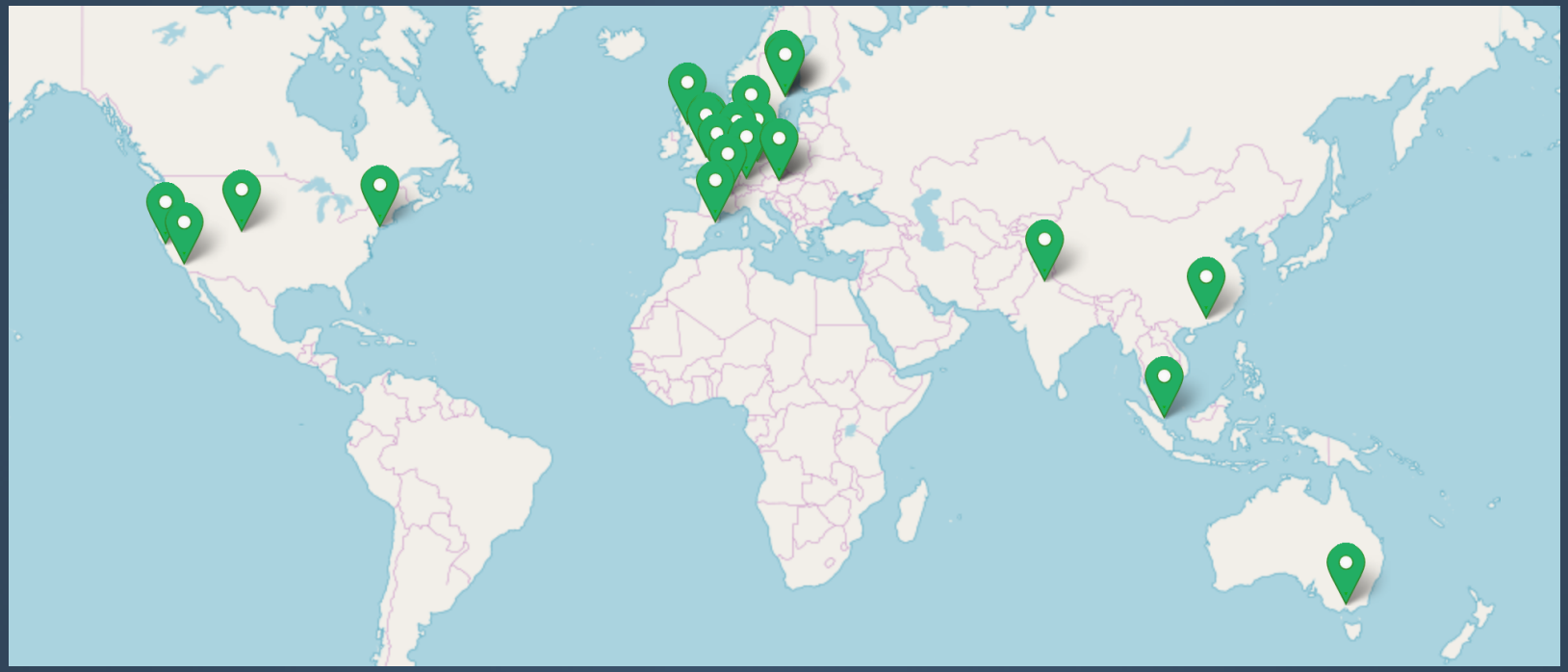

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nextflow

conda-forge

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Twitter

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Slack

Google Group

nf-co.re

GitHub

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All pipelines adhere to requirements

- Nextflow based
- MIT license
- Software bundled in Docker / Singularity
- Continuous integration testing (e.g. Travis CI)
- Stable release tags
- Common pipeline usage and structure
- Software bundled in bioconda

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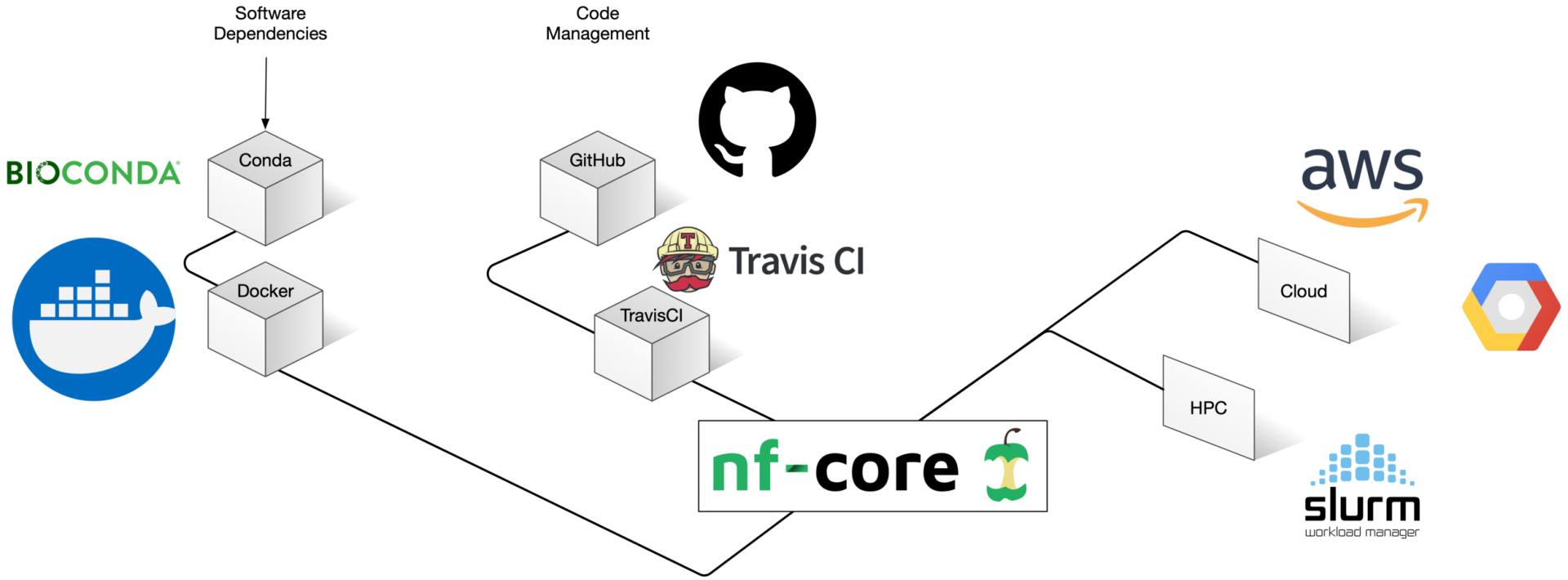
Software Dependencies
Code Management
BIOCONDA
Conda
Docker
GitHub
Travis CI
TravisCI
aws
Cloud
HPC
slurm
workload manager
nf-core

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Need help?

- nf-core Tools: To get a skeleton for new pipelines
  - Synchronization of best-practices across pipelines!
  - Linting app: To check what conforms with nf-co.re
- Slack: To communicate with the community!

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nf-core create: Create a pipeline from scratch

nf-core lint: Check pipeline conforms with best-practices

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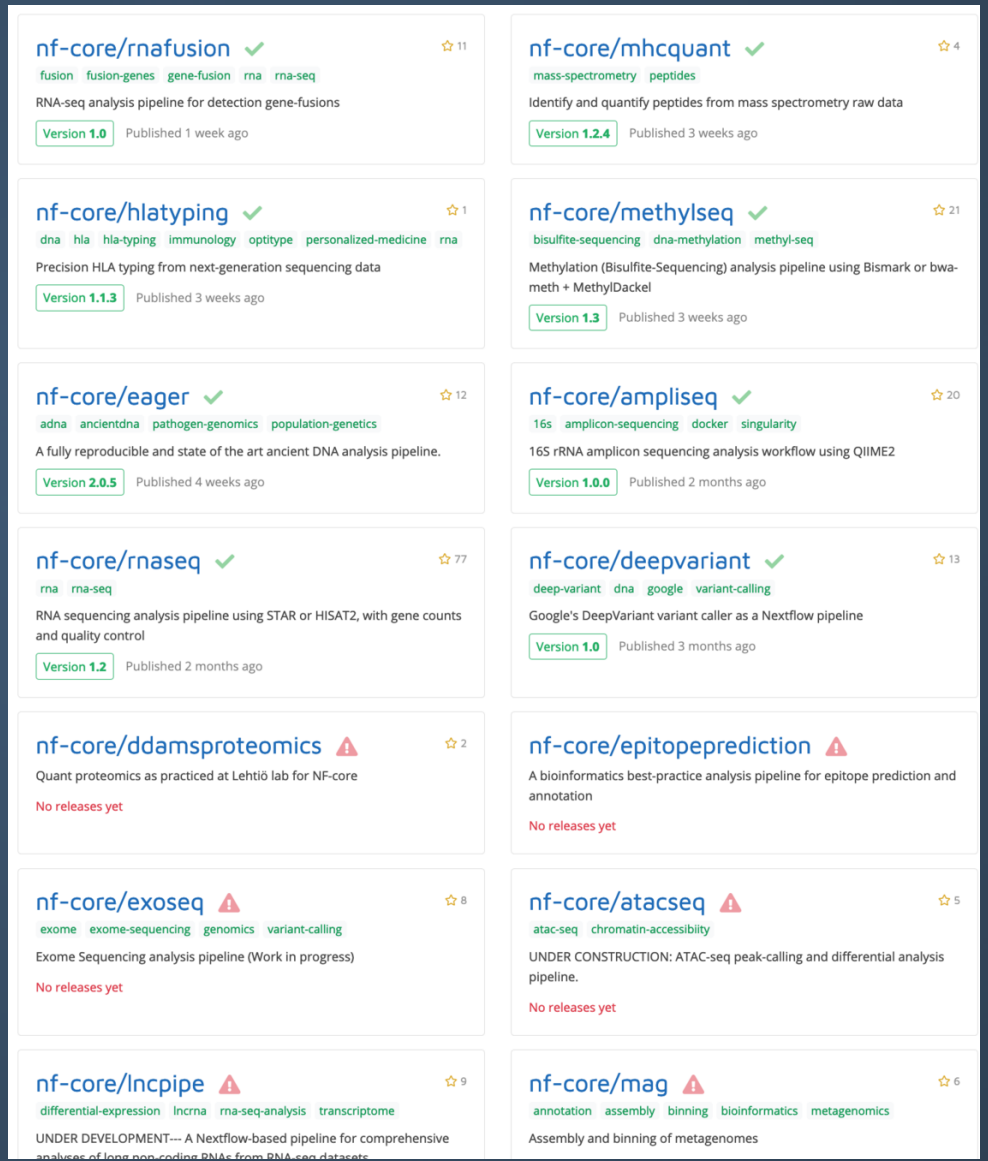
- 15 stable
- 15 in development

https://nf-co.re/pipelines



nf-core/rnafusion ✓ ☆ 11
fusion fusion-genes gene-fusion rna rna-seq
RNA-seq analysis pipeline for detection gene-fusions
Version 1.0 Published 1 week ago

nf-core/mhcquant ✓ ☆ 4
mass-spectrometry peptides
Identify and quantify peptides from mass spectrometry raw data
Version 1.2.4 Published 3 weeks ago

nf-core/hlatyping ✓ ☆ 1
dna hla hla-typing immunology optitype personalized-medicine rna
Precision HLA typing from next-generation sequencing data
Version 1.1.3 Published 3 weeks ago

nf-core/methylseq ✓ ☆ 21
bisulfite-sequencing dna-methylation methyl-seq
Methylation (Bisulfite-Sequencing) analysis pipeline using Bismark or bwa-meth + MethylDackel
Version 1.3 Published 3 weeks ago

nf-core/eager ✓ ☆ 12
adna ancientdna pathogen-genomics population-genetics
A fully reproducible and state of the art ancient DNA analysis pipeline.
Version 2.0.5 Published 4 weeks ago

nf-core/ampliseq ✓ ☆ 20
16s amplicon-sequencing docker singularity
16S rRNA amplicon sequencing analysis workflow using QIIME2
Version 1.0.0 Published 2 months ago

nf-core/rnaseq ✓ ☆ 77
rna rna-seq
RNA sequencing analysis pipeline using STAR or HISAT2, with gene counts and quality control
Version 1.2 Published 2 months ago

nf-core/deepvariant ✓ ☆ 13
deep-variant dna google variant-calling
Google's DeepVariant variant caller as a Nextflow pipeline
Version 1.0 Published 3 months ago

nf-core/ddamsproteomics ⚠ ☆ 2
Quant proteomics as practiced at Lehtiö lab for NF-core
No releases yet

nf-core/epitopeprediction ⚠
A bioinformatics best-practice analysis pipeline for epitope prediction and annotation
No releases yet

nf-core/exoseq ⚠ ☆ 8
exome exome-sequencing genomics variant-calling
Exome Sequencing analysis pipeline (Work in progress)
No releases yet

nf-core/atacseq ⚠ ☆ 5
atac-seq chromatin-accessibiity
UNDER CONSTRUCTION: ATAC-seq peak-calling and differential analysis pipeline.
No releases yet

nf-core/lncpipe ⚠ ☆ 9
differential-expression lncrna rna-seq-analysis transcriptome
UNDER DEVELOPMENT--- A Nextflow-based pipeline for comprehensive

nf-core/mag ⚠ ☆ 6
annotation assembly binning bioinformatics metagenomics
Assembly and binning of metagenomes

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Comes with interactive reports!

https://multiqc.info/examples/wgs/multiqc_report.html

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Comes with proper documentation!

Pipeline overview

The pipeline is built using Nextflow and processes data using the following steps:

- FastQC - read quality control
- TrimGalore - adapter trimming
- STAR - alignment
- RSeQC - RNA quality control metrics
  - BAM stat
  - Infer experiment
  - Junction saturation
  - RPKM saturation
  - Read duplication
  - Inner distance
  - Gene body coverage
  - Read distribution
  - Junction annotation
- dupRadar - technical / biological read duplication
- Preseq - library complexity
- featureCounts - gene counts, biotype counts, rRNA estimation.
- StringTie - FPKMs for genes and transcripts
- Sample_correlation - create MDS plot and sample pairwise distance heatmap / dendrogram
- MultiQC - aggregate report, describing results of the whole pipeline

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... and a lot more!

Documentation

Extensive documentation covering installation, usage and description of output files ensures that you won't be left in the dark.

CI Testing

Every time a change is made to the pipeline code, nf-core pipelines use continuous-integration testing to ensure that nothing has broken.

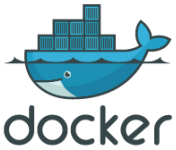
Travis CI

Stable Releases

nf-core pipelines use GitHub releases to tag stable versions of the code and software, making pipeline runs totally reproducable.

Docker

Software dependencies are always available in a bundled docker container, which Nextflow can automatically download from dockerhub.



Singularity

If you're not able to use Docker, built-in support for Singularity can solve your HPC container problems. These are built from the docker containers.

Bioconda

Where possible, pipelines come with a bioconda environment file, allowing you to set up a new environment for the pipeline in a single command.

Acknowledgements

NF-Core Team

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Evan Floden (CRG, Barcelona)