seqeralabs

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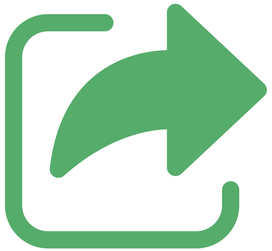
Reproducible bioinformatics for everyone:

Nextflow & nf-core

MDC / FMP PhD Retreat 2023

Reproducible bioinformatics

Get the same results
every time



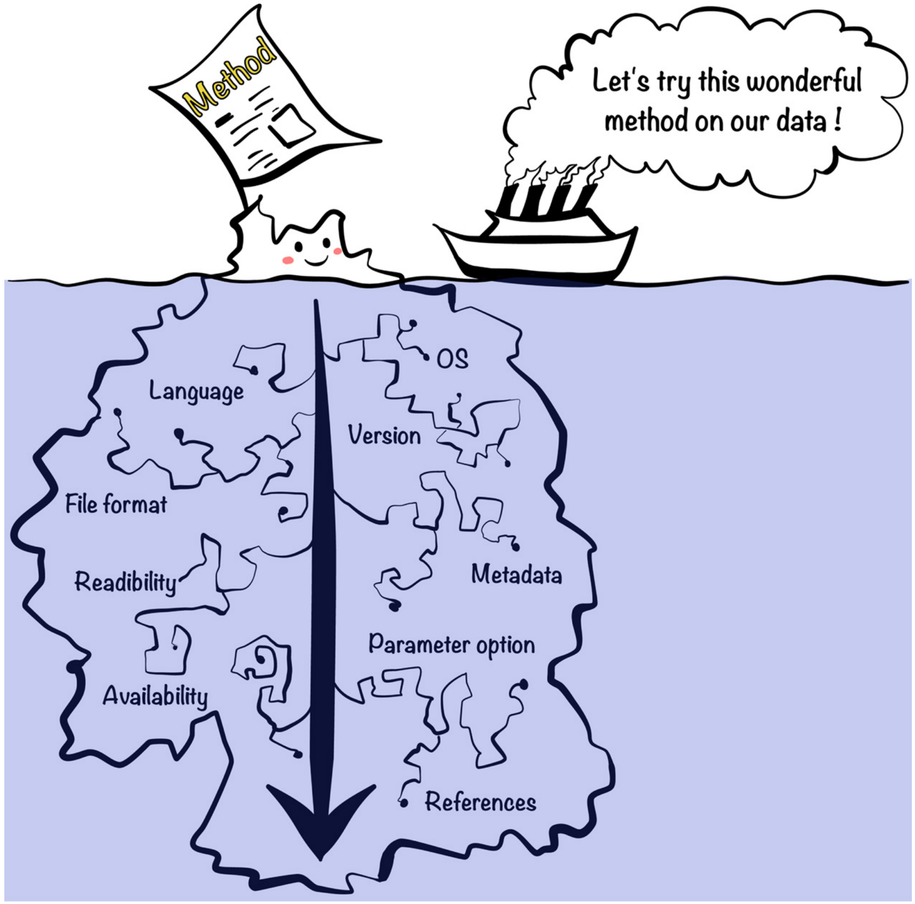
Other people also
get the same results

Others can replicate
your findings with
their data

Reproducible bioinformatics

Sharing your code is not enough

~~Reproducible~~ bioinformatics

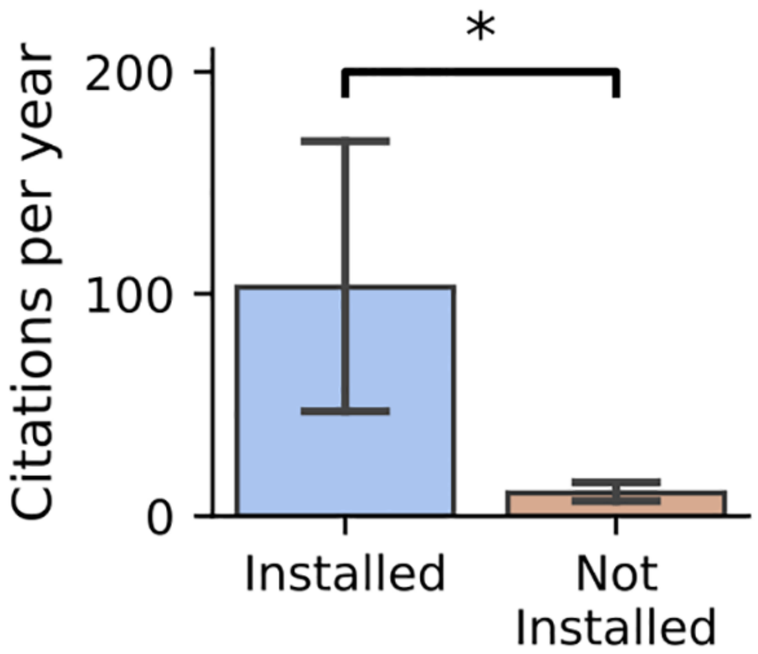


> First, we **tried** to re-run the analysis with the code and data provided by the authors.

Second, **we reimplemented the whole method** in a Python package...

> Experimenting with reproducibility:
> a case study of robustness in bioinformatics
> *Kim et al.*, GigaScience (2018).
> https://doi.org/10.1093/gigascience/giy077

~~Reproducible~~ bioinformatics



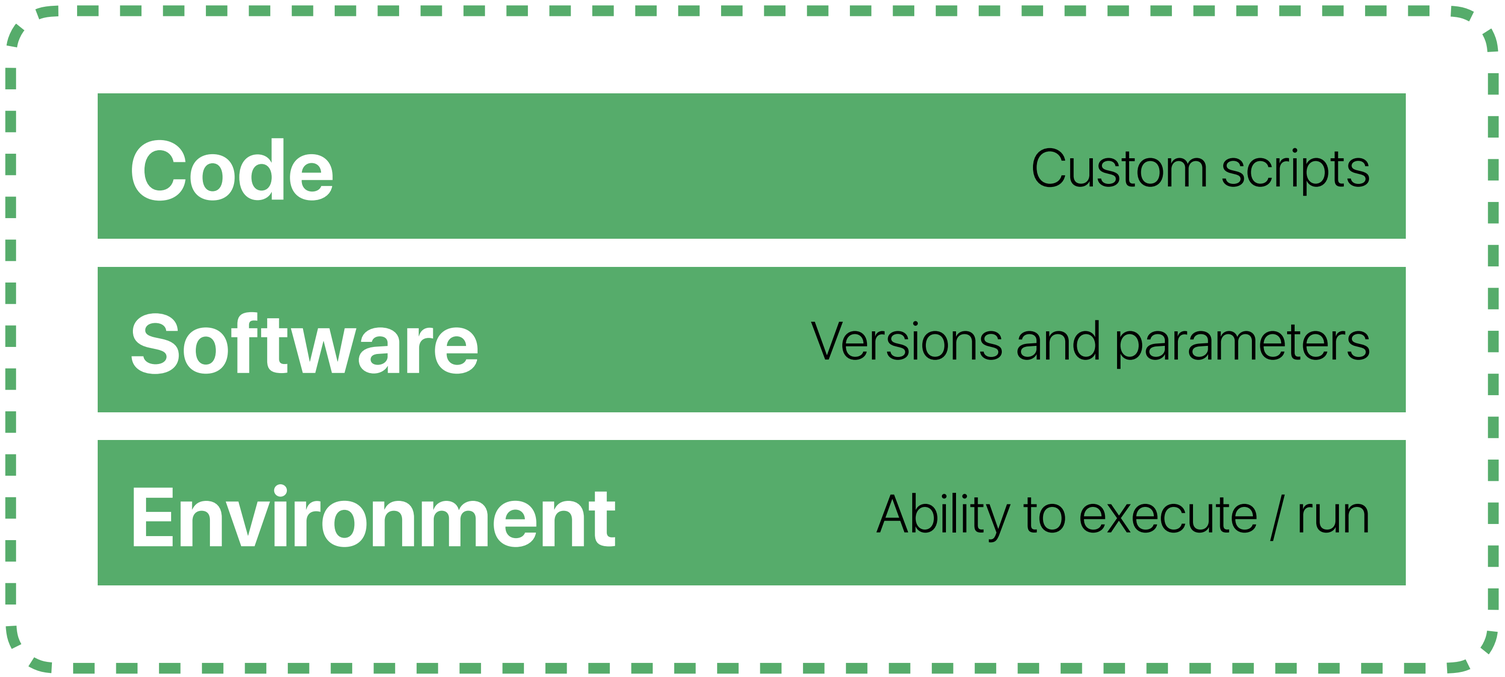
> We found that **28%** of all omics software resources are currently **not accessible** through URLs published in the paper.
>
> Among the tools selected, 49% were **difficult to install** or **could not be installed at all**.

Challenges and recommendations to improve the installability and archival stability of omics computational tools
Serghei Mangul, et al. PLOS Bio (2019).
https://doi.org/10.1371/journal.pbio.3000333

Reproducible bioinformatics

Code	Custom scripts
Software	Versions and parameters
Environment	Ability to execute / run

Reproducible bioinformatics



Workflow

nextflow

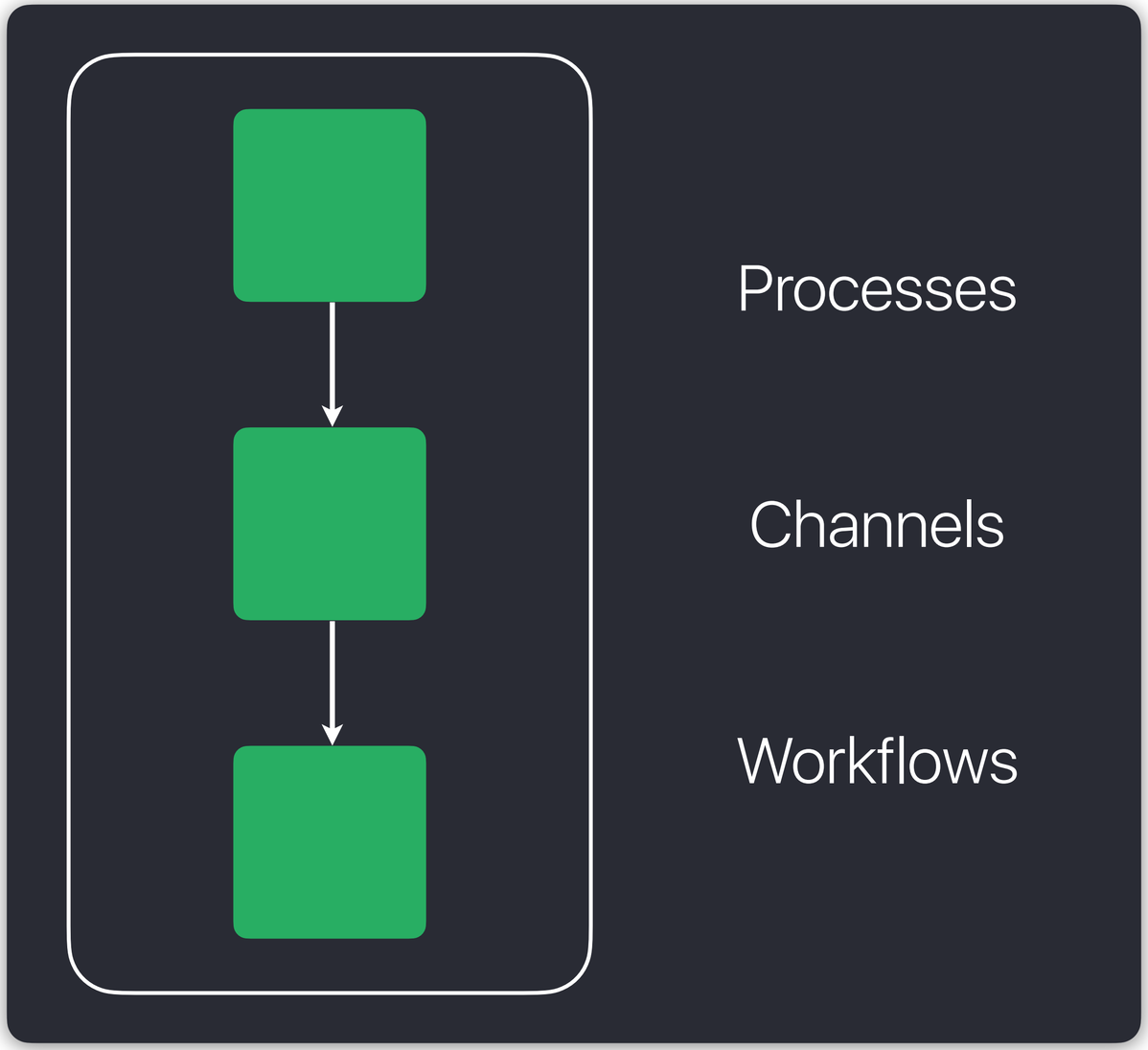
Language

Software

Compute

Language

nextflow



nextflow

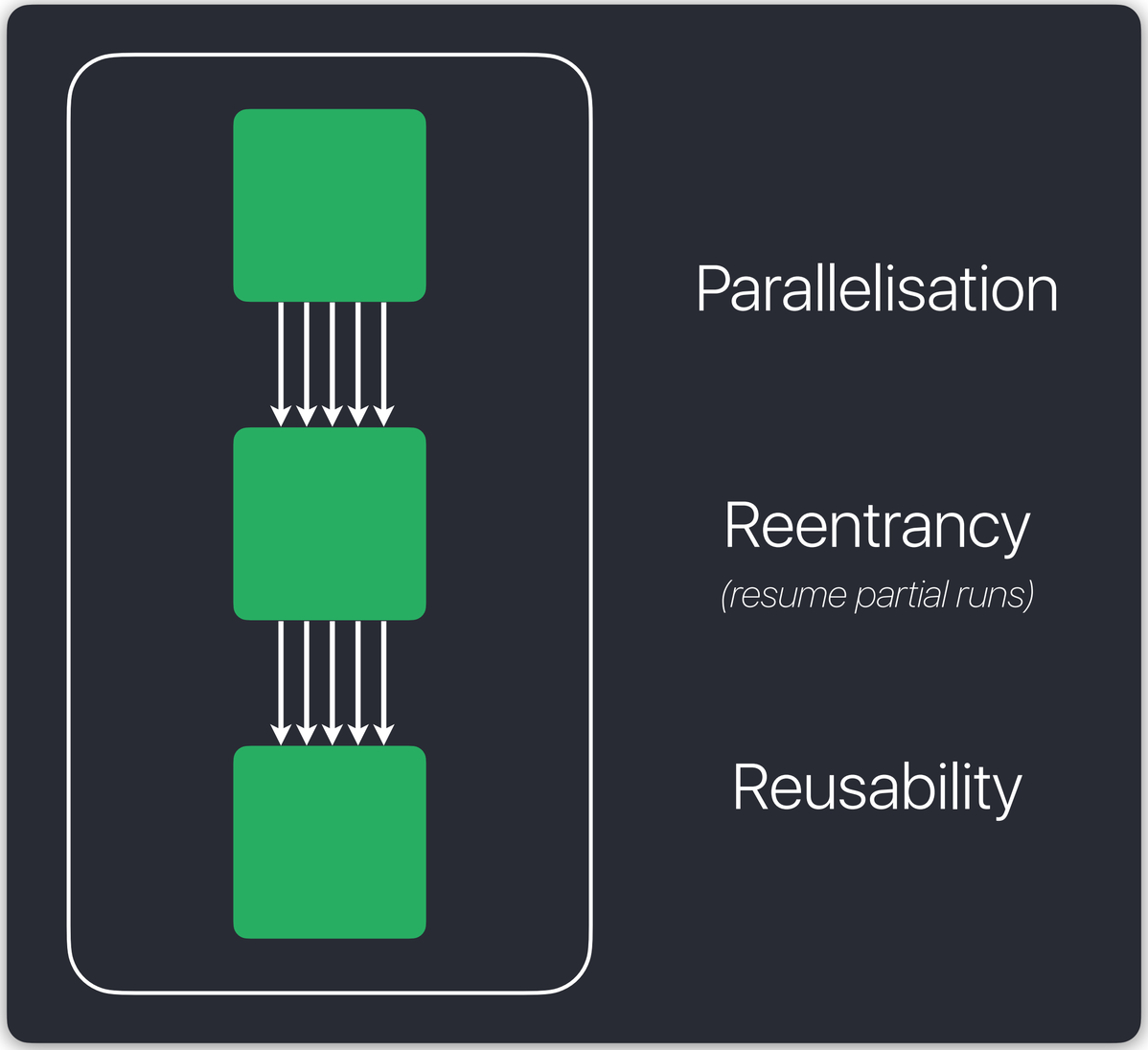
```
#!/usr/bin/env nextflow
process fastqc {
  input:
  path input

  output:
  path "*_fastqc.{zip,html}"

  script:
  """
  fastqc -q $input
  """
}

workflow {
  Channel.fromPath("*.fastq.gz") | fastqc
}
```

nextflow



Parallelisation

Reentrancy

(resume partial runs)

Reusability

Language

nextflow

Language

Software

Compute

nextflow

AWS CodeCommit

Azure Repos

Software

Compute

nextflow

git

GitHub

Bitbucket

GitLab

Gitea

AWS CodeCommit

Azure Repos

docker

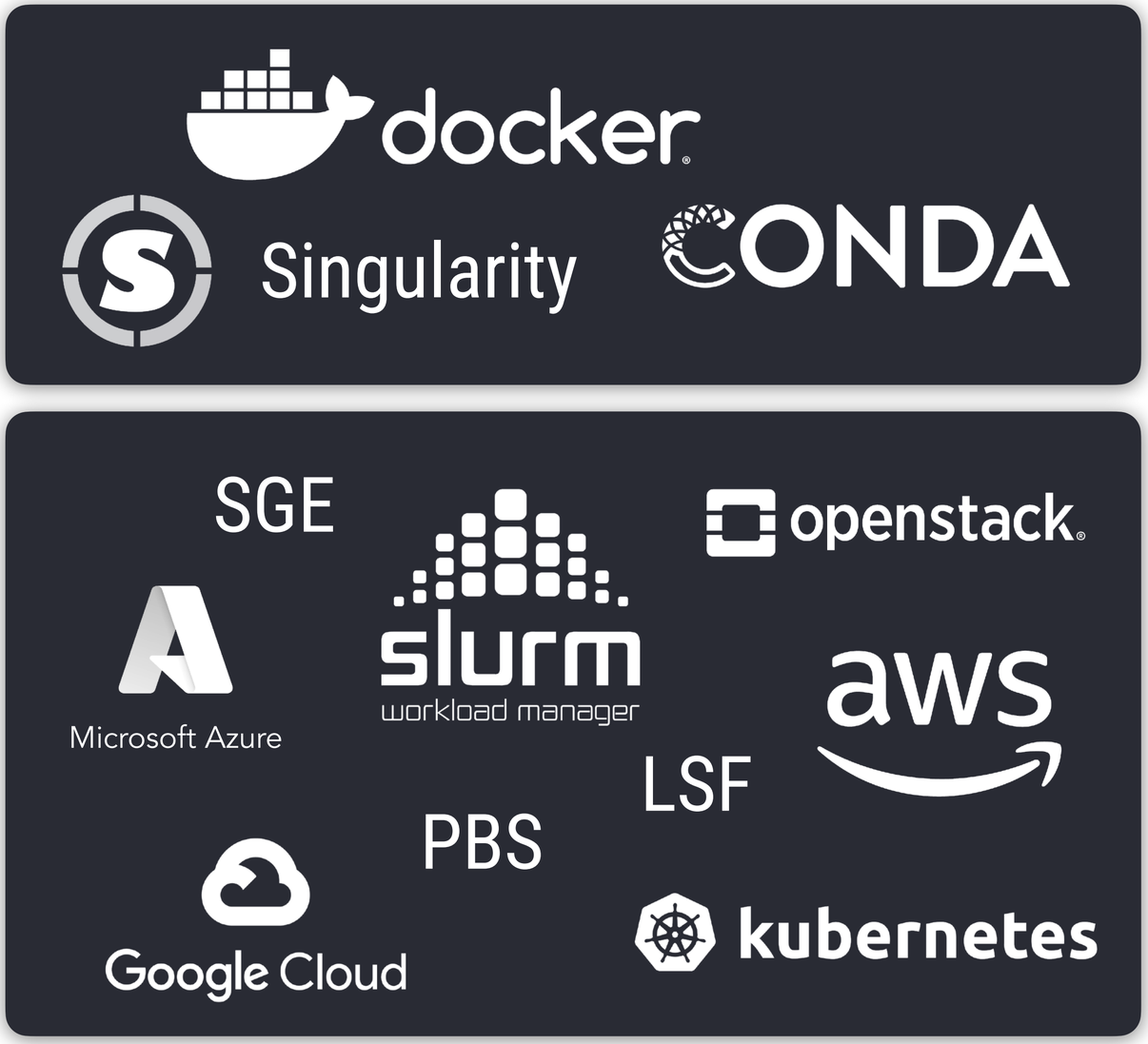
Singularity

CONDA

Compute

nextflow


git
GitHub
Bitbucket
GitLab
Gitea
AWS CodeCommit
Azure Repos


docker
Singularity
CONDA
SGE
Microsoft Azure
slurm
workload manager
openstack
aws
LSF
PBS
Google Cloud
kubernetes

nextflow

```
#!/usr/bin/nextflow
process fastqc {
  container "biocontainers/fastqc"

  input:
  path input

  output:
  path "*_fastqc.{zip,html}"

  script:
  """
  fastqc -q $input
  """
}

workflow {
  Channel.fromPath("*.fastq.gz") | fastqc
}
```

```
docker {
    enabled = true
}
```


```
nextflow run main.nf -c ~/mylocal.conf
```

nextflow

```
#!/usr/bin/nextflow
process fastqc {
  container "biocontainers/fastqc"

  input:
  path input

  output:
  path "*_fastqc.{zip,html}"

  script:
  """
  fastqc -q $input
  """
}

workflow {
  Channel.fromPath("*.fastq.gz") | fastqc
}
```

```
process {
  executor = 'slurm'
}
singularity {
  enabled = true
}
```

Singularity

```
nextflow run main.nf -c ~/myhpc.conf
```

nextflow

```
#!/usr/bin/nextflow
process fastqc {
  container "biocontainers/fastqc"

  input:
  path input

  output:
  path "*_fastqc.{zip,html}"

  script:
  """
  fastqc -q $input
  """
}

workflow {
  Channel.fromPath("*.fastq.gz") | fastqc
}
```

```
process {
  executor = 'slurm'
  queue = { task.time < 3.h ? 'short' : 'long' }
  beforeScript = "module load singularity"
}
singularity {
  enabled = true
  cacheDir = "/resources/nxf/singularity"
}
params {
  max_cpus = 24
  max_memory = 240.GB
  max_time = 168.h
}
```

```
nextflow run main.nf -c ~/myhpc.conf
```

nextflow

```
#!/usr/bin/nextflow
process fastqc {
  container "biocontainers/fastqc"

  input:
  path input

  output:
  path "*_fastqc.{zip,html}"

  script:
  """
  fastqc -q $input
  """
}

workflow {
  Channel.fromPath("*.fastq.gz") | fastqc
}
```

```
process {
  executor = 'awsbatch'
  queue = 'my-batch-queue'
}
aws {
  region = 'us-east-1'
}
```


```
nextflow run main.nf -c ~/mycloud.conf
```

nextflow

```
#!/usr/bin/nextflow
process fastqc {
  container "biocontainers/fastqc"

  input:
  path input

  output:
  path "*_fastqc.{zip,html}"

  script:
  """
  fastqc -q $input
  """
}

workflow {
  Channel.fromPath(params.input) | fastqc
}
```

```
params {
  input = "*.fastq.gz"
}
```

```
nextflow run main.nf --input "data/input*.fq"
```

nextflow

Reproducible

Between runs

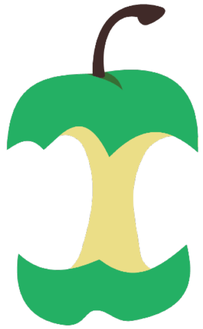
Portable

Between systems

nextflow

nf-core

nf-core



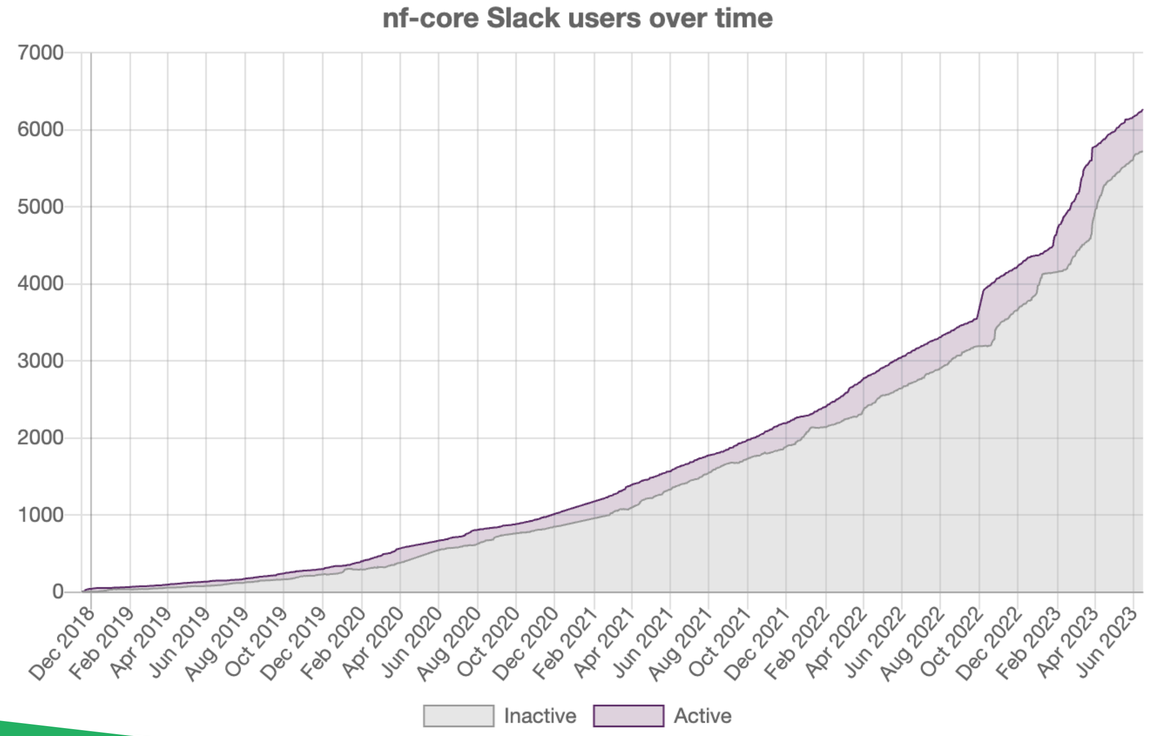
A community effort to collect a curated set of analysis pipelines built using Nextflow.

https://nf-co.re

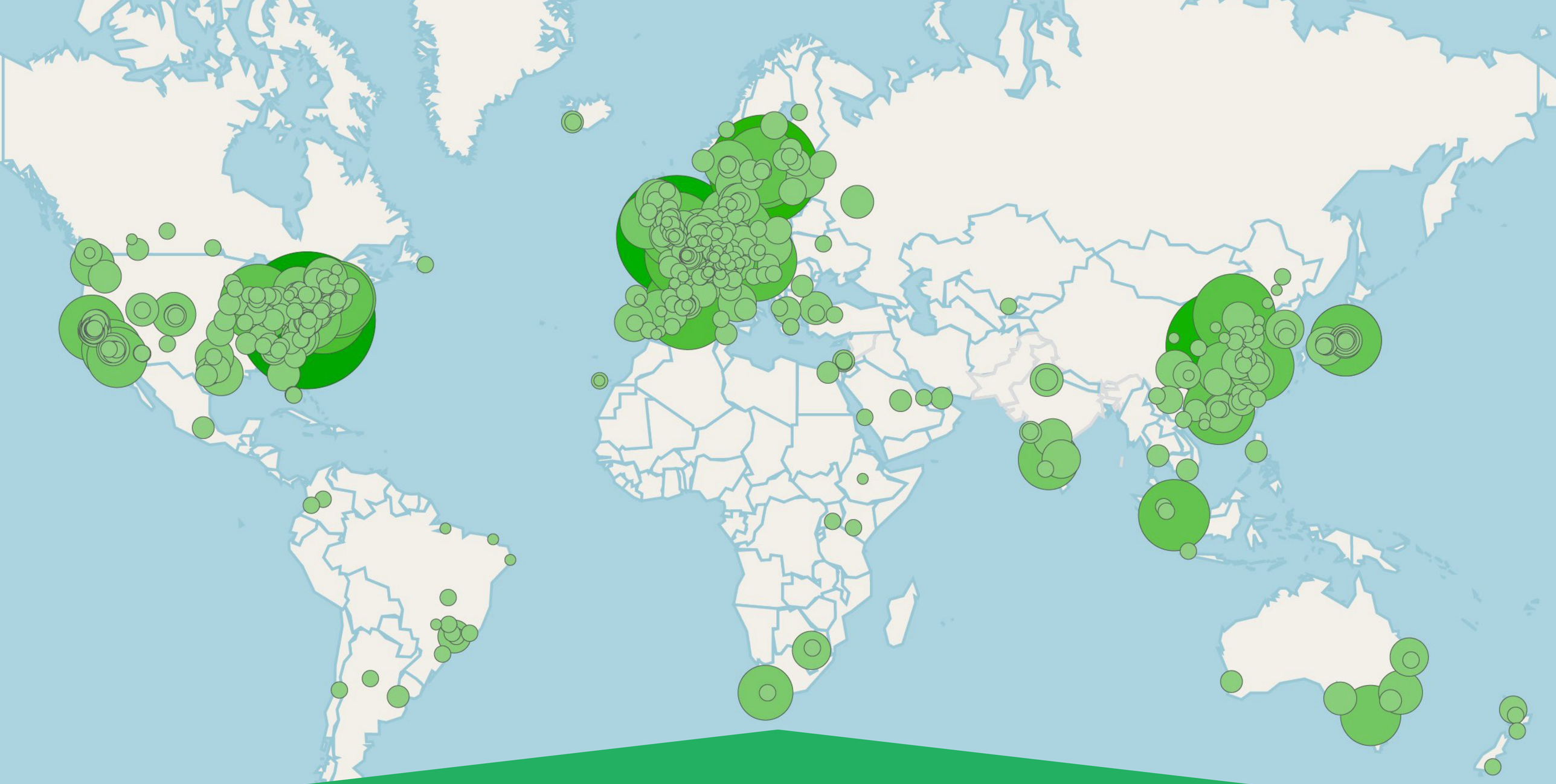
nf-core

> 6000 Slack members

> 2000 GitHub contributors

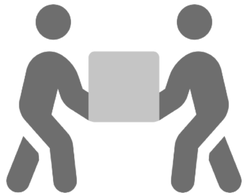


https://nf-co.re



https://nf-co.re

nf-core

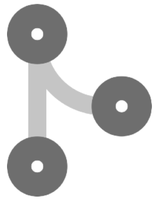


Cooperation

Develop with the community

Standards

Use a common template



Collaboration

Collaborate, don't duplicate

https://nf-co.re

nf-core

Framework

Tools built for everyone

Compatibility

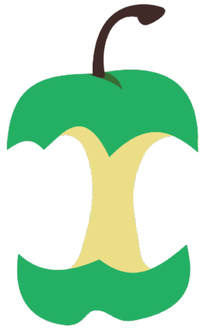
Works with any Nextflow pipeline

Components

Collaborate on components

https://nf-co.re

nf-core



82 Pipelines

Ready to use, covering most techniques in NGS

Helper tools

Running pipelines, writing pipelines, testing & automation

957 Modules

Tool process wrappers, with software and CI testing

44 Subworkflows

Shared subworkflows for common analysis pathways

https://nf-co.re

nf-core Pipelines

slamseq	SLAMSeq processing and analysis pipeline
circdna	Identification of extrachromosomal circular DNA (ecDNA)
scrnaseq	A single-cell RNAseq pipeline for 10X genomics data
spatialtranscriptomics	Spatially-resolved gene counts with spatial coordinates, image data, and scRNA-seq
rnaseq	RNA sequencing analysis pipeline with gene/isoform counts and extensive QC.
scflow	Complete analysis workflow for single-cell/nuclei RNA-sequencing data.

https://nf-co.re

nf-core Helper tools

Pipelines
Create from template, sync to get updates.

Subworkflows
Create, install and update.

Modules
Create, install, update, patch, test.

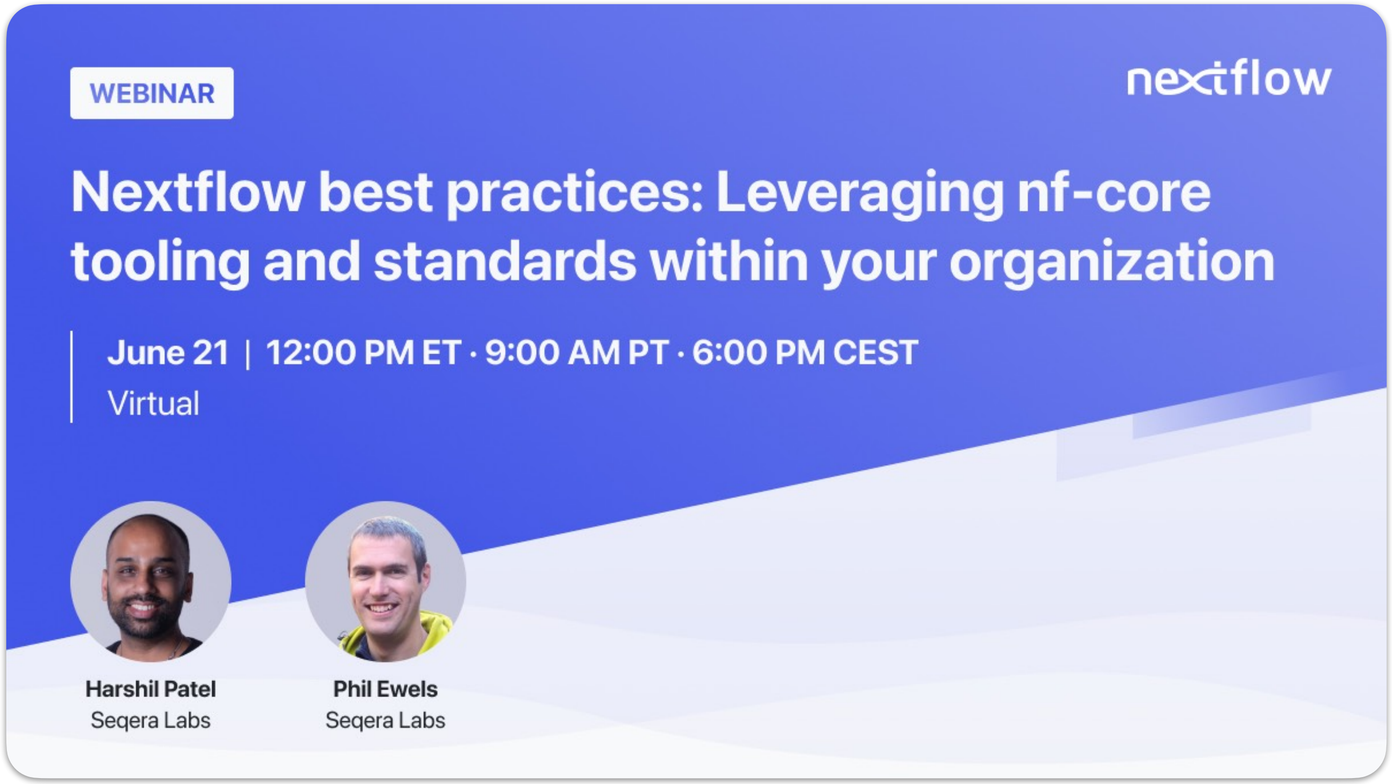
Schema
Build your pipeline schema with a GUI.

Linting
Test nf-core standards and best practices.

Download
Fetch with singularity images for offline use.

https://nf-co.re

nf-core Webinar



Building with nf-core

An introduction to nf-core components (pipelines, modules, sub workflows).

Follow along as Harshil creates a pipeline from scratch using nf-core tooling.

`https://seqera.io/webinar-nextflow-nf-core/`

`https://nf-co.re`

nature biotechnology

Correspondence | Published: 13 February 2020

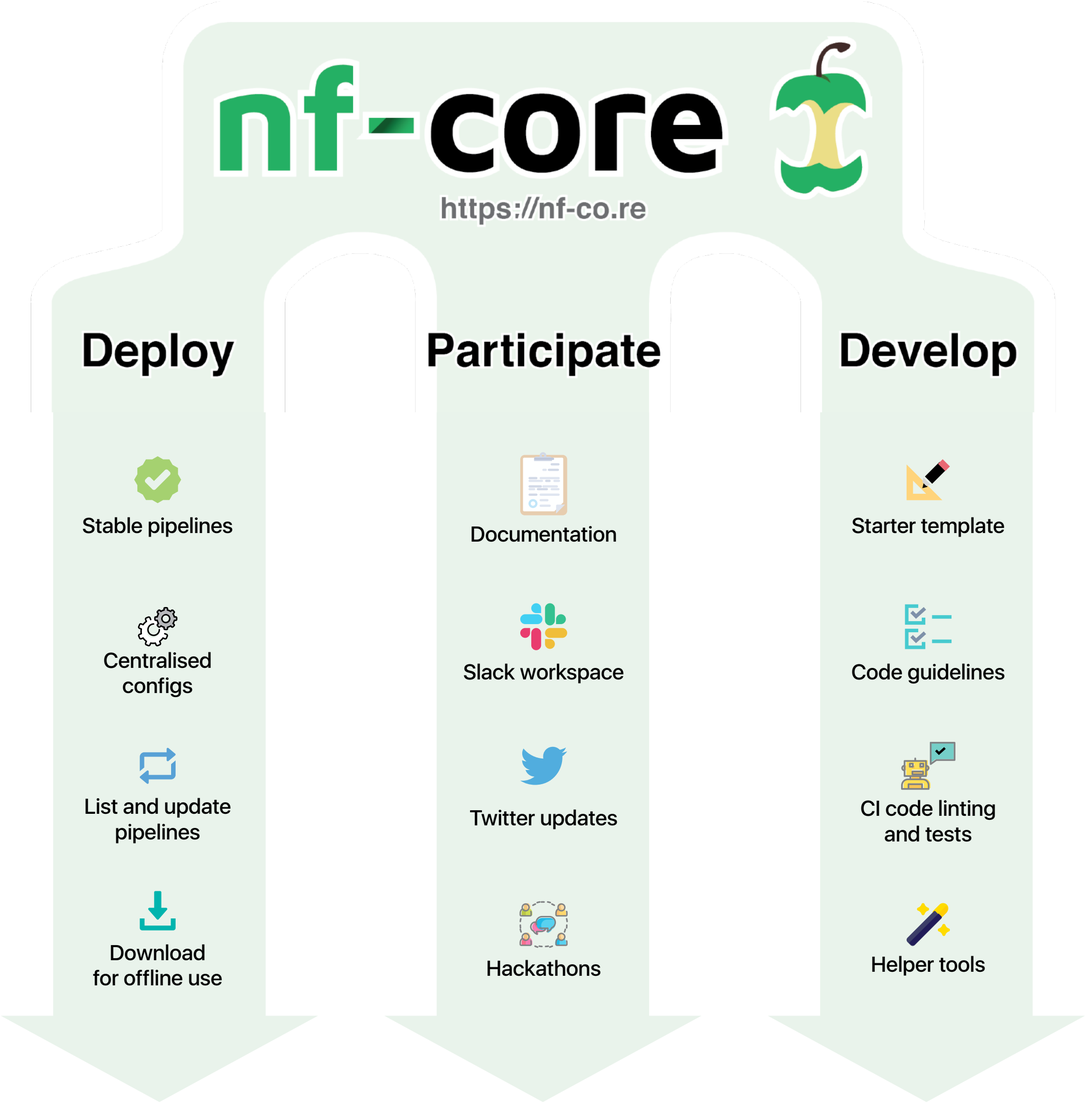
The nf-core framework for community-curated bioinformatics pipelines

Philip A. Ewels, Alexander Peltzer, Sven Fillinger, Harshil Patel, Johannes Alneberg, Andreas Wilm, Maxime Ulysse Garcia, Paolo Di Tommaso & Sven Nahnsen

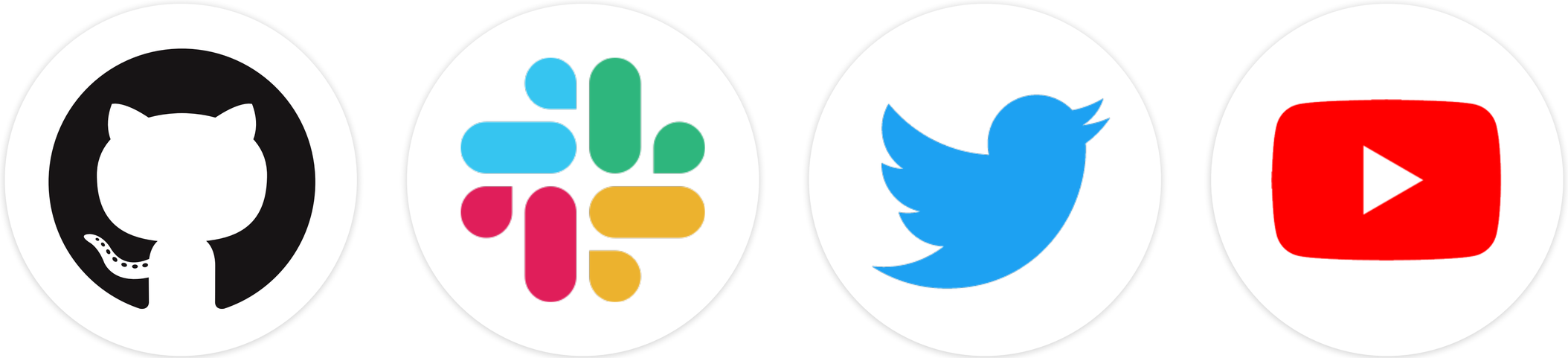
Nature Biotechnology **38**, 276–278(2020) | Cite this article

3253 Accesses | **3** Citations | **172** Altmetric | Metrics

To the Editor — The standardization, portability and reproducibility of analysis pipelines are key issues within the bioinformatics community. Most bioinformatics pipelines are designed for use on-premises; as a result, the associated software dependencies and execution logic are likely to be tightly coupled with proprietary computing environments. This can make it difficult or even impossible for others to reproduce the ensuing results, which is a fundamental requirement for the validation of scientific findings. Here, we introduce the nf-core framework as a means for the development of collaborative, peer-reviewed, best-practice analysis pipelines (Fig. 1). All nf-core pipelines are written in Nextflow and so inherit the ability to be executed on most computational infrastructures, as well as having native support for container technologies such as Docker and Singularity. The nf-core community (Supplementary Fig. 1) has developed a suite of tools that automate pipeline creation, testing, deployment and synchronization. Our goal is to provide a framework for high-quality bioinformatics pipelines that can be used across all institutions and research facilities.

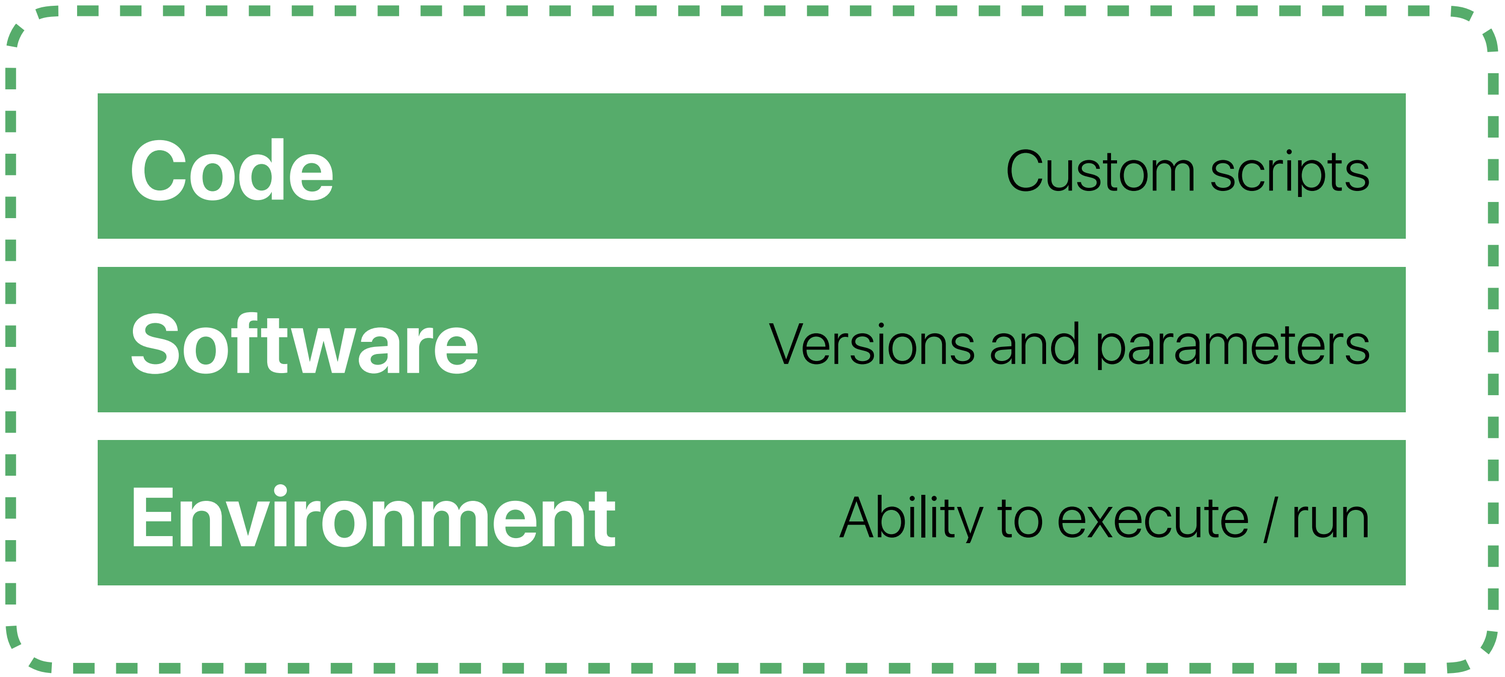


Join the community



https://nf-co.re/join

Reproducible bioinformatics



Workflow

Reproducible bioinformatics for everyone

nextflow

Code	Custom scripts
Software	Versions and parameters
Environment	Ability to execute / run

nextflow *tower*

Compute infrastructure

Configuration

Sharing results

https://tower.nf

nextflow *tower*

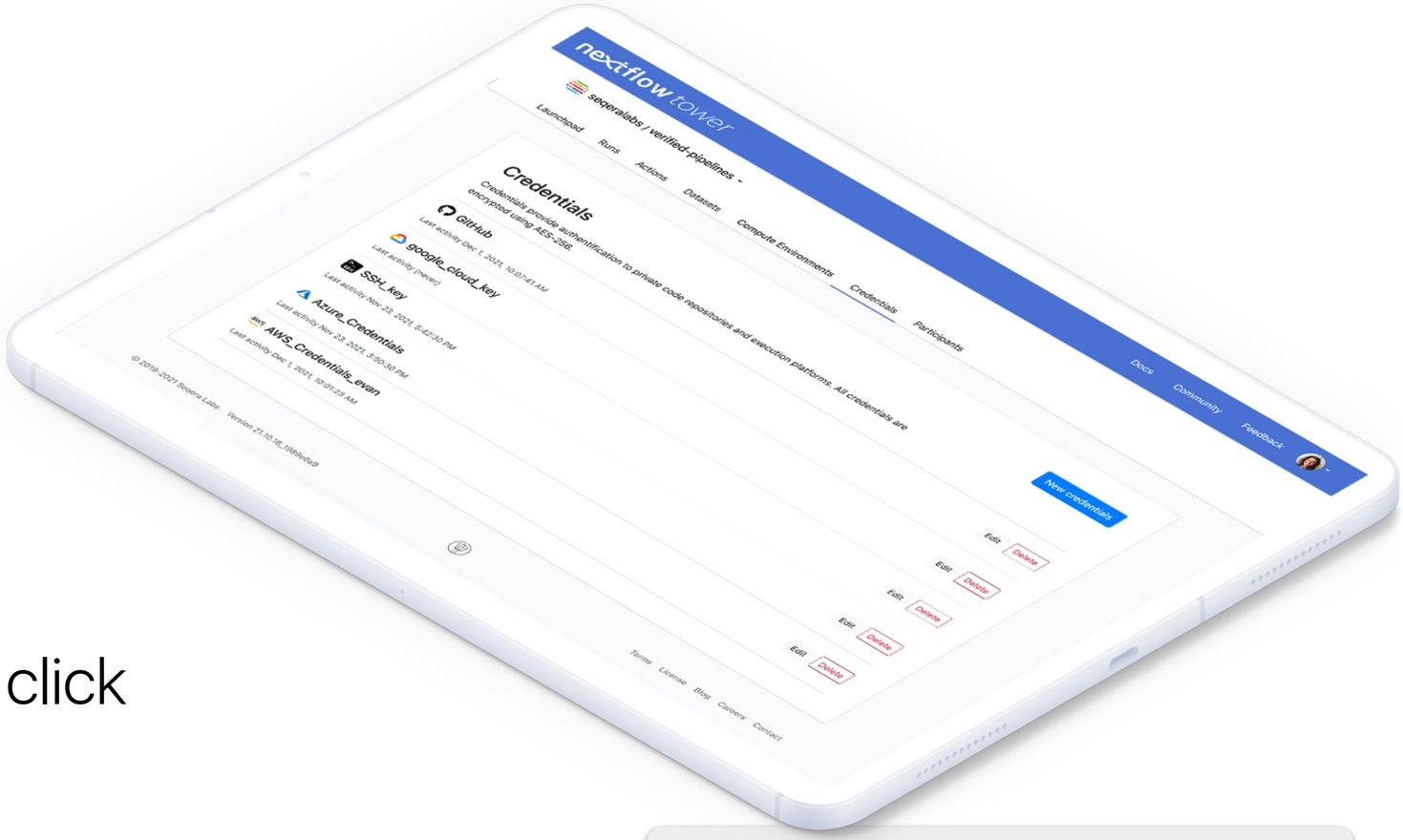
seqeralabs

Intuitive launchpad interface

Launch, manage, and monitor

Share runs and work in teams

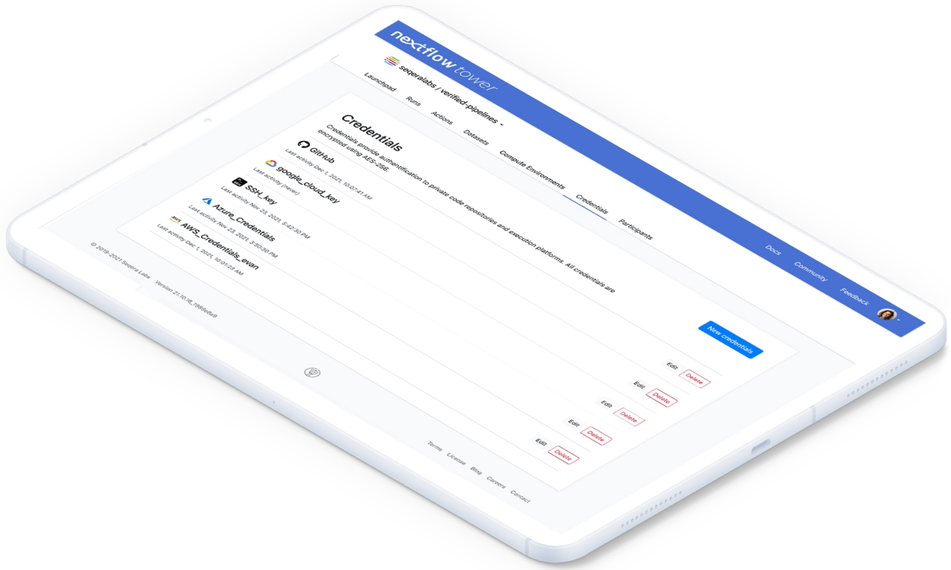
Create cloud infrastructure with a click



https://tower.nf

nextflow tower

seqeralabs



Cloud Free: (for ever)

Cloud Pro: Unlimited

Enterprise: Install yourself

`https://tower.nf`

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https://seqera.io

Chan Zuckerberg Initiative

Basic training

Free to watch online

`youtube.com/@nf-core`

nextflow
SUMMIT 2023

https://summit.nextflow.io

Advanced training

27-28 September 2023

Barcelona Summit 2023

16-20 October 2023

`https://nf-co.re`

`https://nextflow.io`