

June, 2023

# Nextflow best practices

Leveraging nf-core tooling and standards within your organization

# **Overview**

### **01** Introduction

Phil - 20 mins

### 02 Live demo

Harshil - 20 mins

### **03** Conclusion

Phil - 5 mins

### **04** Q&A

15 mins



# **01**Introduction

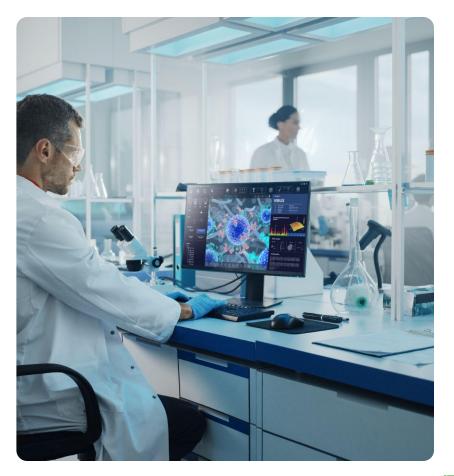
Segera, Nextflow, nf-core and Tower.



# Seqera at a glance

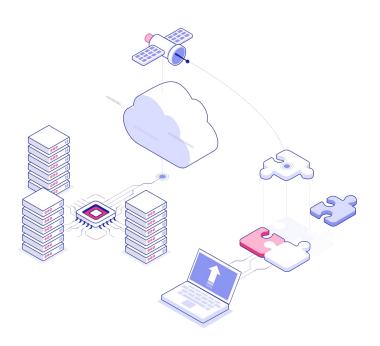
Key Highlights

- Founded in 2018 by Evan Floden and Paolo di Tommaso. HQ in Barcelona and Toronto
- Trusted by over 8,000 researchers and over
   150 leading pharma and biotech companies
- Raised over €27M and recipient of several grants from the Chan Zuckerberg Foundation
- Creators of Nextflow, the global standard for workflow orchestration
- Championing open science, acting as a steward of over 70 open-source data pipelines available to its wider community of 10,000 researchers





# **The Seqera Stack**



### **Nextflow**

Scientific workflow management

### **Tower**

Platform for collaborative scientific data analysis

### **MultiQC**

Bioinformatics reporting

### **Fusion**

File-system for cloud-native data pipelines

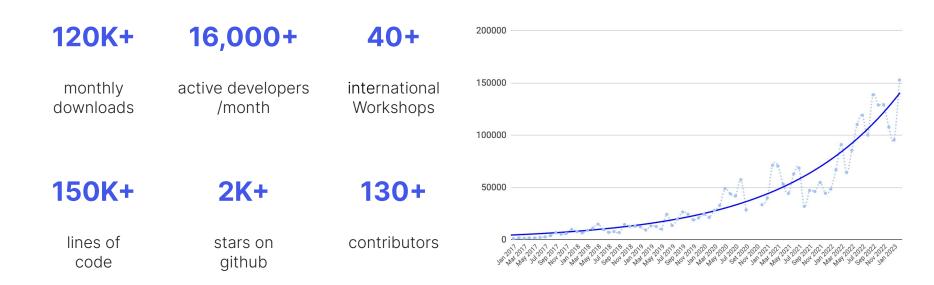
#### Wave

Container provisioning



### **Nextflow**

Nextflow has a vast open source community actively using it on their day-to-day, supporting its development and contributing to new pipelines





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# Reproducible

Integration with code management tools, with versioned releases.



### **Portable**

Docker, Singularity,
Conda, works with most
compute environments.



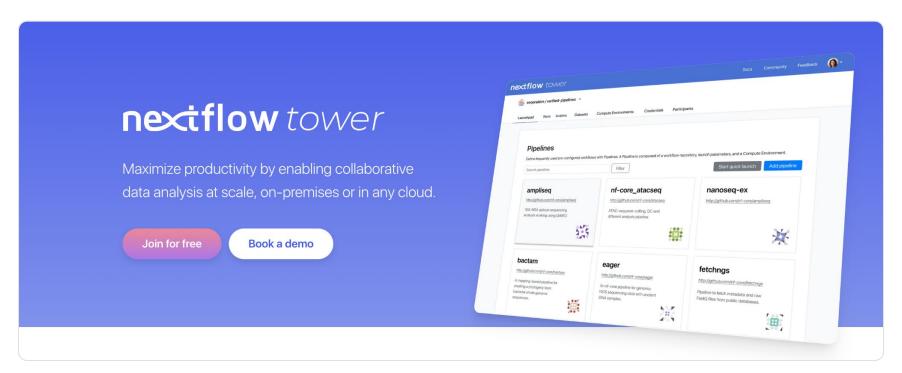
### Scalable

5 samples on your laptop, 5k on an HPC or 5 million in the cloud.



### **Tower**

A central command post for managing data analysis pipelines at scale





### **Tower**

A central command post for managing data analysis pipelines at scale

Web interface

Command line interface

**nextflow** tower

Compute infrastructure

Configuration

Sharing

nextflow

Pipeline logic

Software containers

Executor support



### **Tower**

A central command post for managing data analysis pipelines at scale



### **Reduce cloud expenses**

Instance selection, control & monitoring, automated resource optimization



### **Ensure reproducibility**

Data provenance, auditability and compliance with versioned flows, containers & datasets



### **Automate manual tasks**

Boost efficiency and avoid errors with Tower API and sequencer platform integrations



### Flexible provisioning

Run locally, on HPC clusters, or auto-provision resources on your choice of cloud



### **Secure collaboration**

Share pipelines, compute environments, and data with fine-grained access controls



# **Boost productivity**

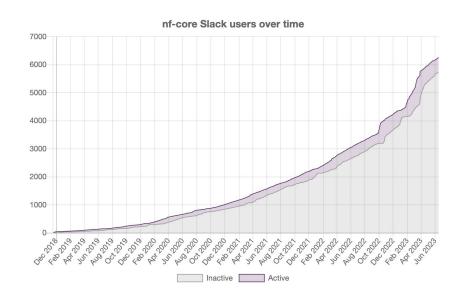
Access in-house or production-proven pipelines through an intuitive web UI



# nf-core

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

6k+	2k+	100+
Slack	GitHub	GitHub
members	contributors	repositories
46K+	15K+	6.7k+
GitHub	Pull	GitHub
commits	requests	issues





# **nf-core: Principles**

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



Develop with the community



# > Standards

Use a common template



# Collaboration

No duplicate pipelines within nf-core



Tools built for everyone



# Compatibility

Tools work for any Nextflow pipeline



# Components

Collaborate on component-level



### nf-core

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

### 82 Pipelines

Ready to use, covering most techniques in NGS



### **Helper tools**

Running pipelines, writing pipelines, testing & automation

### 951 Modules

Tool process wrappers, with software and CI testing

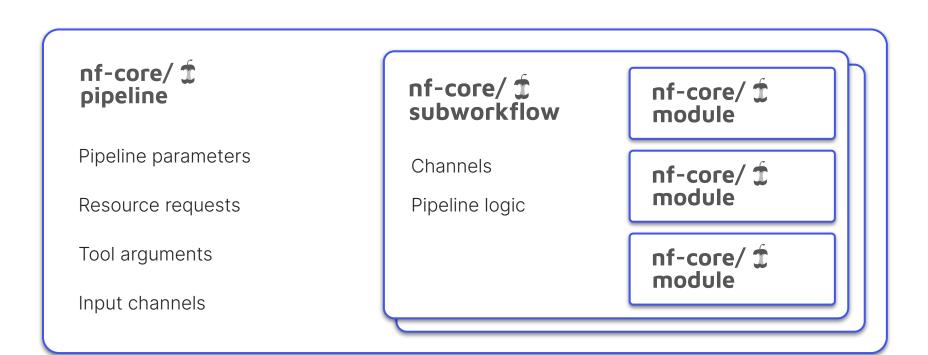


Shared subworkflows for common analysis pathways



# nf-core: Anatomy of a pipeline

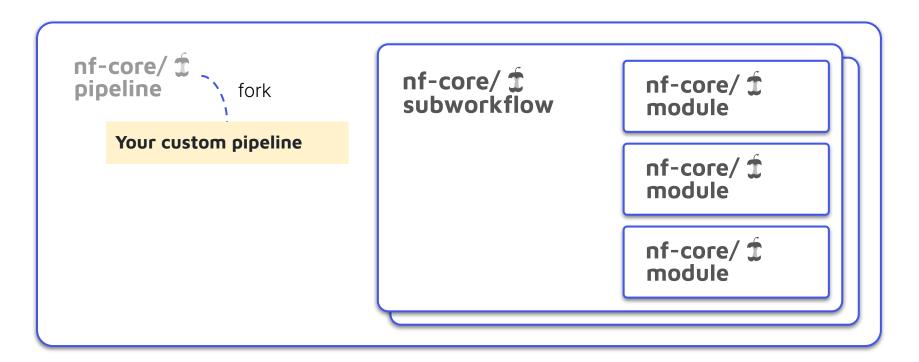
Building pipelines with units of reusability.





# nf-core: Smörgåsbord

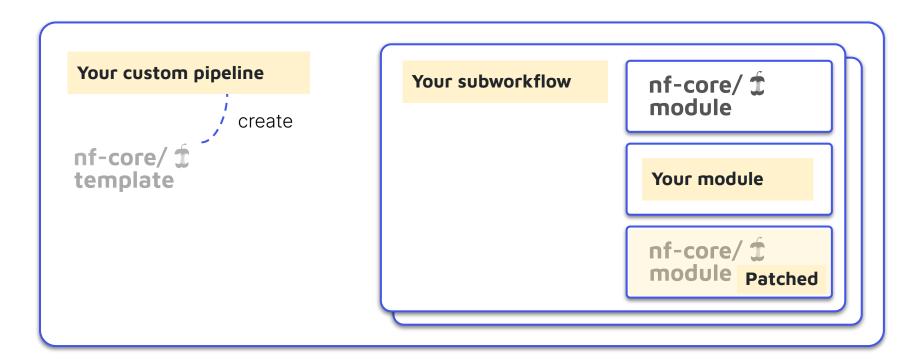
Pick and choose which smörgåsar you need





# nf-core: Smörgåsbord

Pick and choose which smörgåsar you need





# nf-core: Anatomy of a pipeline

Building pipelines with units of reusability.



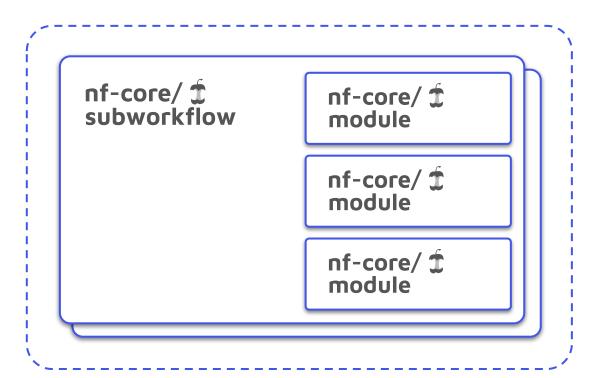
Local to pipeline



nf-core/modules



Your custom repository





# nf-core/tools

Command line package to help you build your pipeline with ease





# **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.



### nf-validation

Nextflow plugin to natively handle schema files





# Parameter validation

Functions to validate pipeline parameters and print CLI help text.



# Sample sheet validation

Validate input sample sheets - formatting and contents.



# Sample sheet channels

fromSamplesheet() channel factory, including meta maps.



nextflow-io/nf-validation



https://nextflow-io.github.io/nf-validation/



# nf-core: Smörgåsbord

Pick and choose which smörgåsar you need



## **Pipelines / template**

82 pipelines and a base template



### Linting

Choose conventions to test for



### Subworkflows

44 subworkflows



#### **Schema**

Validation, channels and user interface



### Modules

951 modules



### Tooling

Development and deployment



Battle tested examples out in the wild



**Pipelines / template** 



**Subworkflows** 



**Modules** 



**Schema** 



Linting



**Tooling** 



**Custom modules repository** 

**ATLASSIAN** 





Battle tested examples out in the wild



**Pipelines / template** 



Subworkflows



**Modules** 



**Schema** 



Linting



**Tooling** 





Pushes modules back to central nf-core repository



Battle tested examples out in the wild



**Pipelines / template** 



Subworkflows



Modules



**Schema** 



Linting



**Tooling** 









Battle tested examples out in the wild



Pipelines / template



**Subworkflows** 



**Modules** 



**Schema** 



Linting



**Tooling** 













Who is using the template anyway?

~ 1000

Pipelines built with the nf-core template in public GitHub repositories



# 02 Live demo

Build and run a pipeline in 20 minutes



# 03 Conclusion

Future directions



### nf-core: Future directions

Improving the developer experience



### Flexible template

Fine-grained control over what's included, improved support for GitLab, BitBucket.



### **New website**

Rebuilt from the ground up, better navigation and content.



# Sample sheet schema

Tooling to help create sample sheets and manage their schema.



# **Better testing**

Moving to nf-test Release testing with Azure AWS runners for CI tests



### **Nextflow: Future directions**

Coming soon to a runtime near you\*



# **Clean intermediates**

Delete intermediate files during pipeline execution



# **Better error messages**

Tell you what went wrong and where (precisely)



# **Fusion for HPC**

Lightning fast file I/O available on both Cloud and HPC



# Spack / multi-arch

Nextflow + Spack, containers on the fly via Wave, multi-arch pipeline deployments.





# **Seqera Platform**

Streamlining the scientific data analysis life cycle

### **Data Developer**

Tools & workflows
IDEs - VSCode
CI/CD
Containers

### **Data Explorer**

Instruments
Cloud storage
File systems
LIMS
Public resources

#### **Nextflow**

Scientific workflow management

#### **MultiQC**

Bioinformatics reporting

#### **Fusion**

File-system for cloud-native data pipelines

#### Wave

Container provisioning

### **Data Pipelines**

Batch Compute Orchestration Performant Storage

### **Data Analytics**

Reporting Metrics Provenance Compliance

#### **Data Studio**

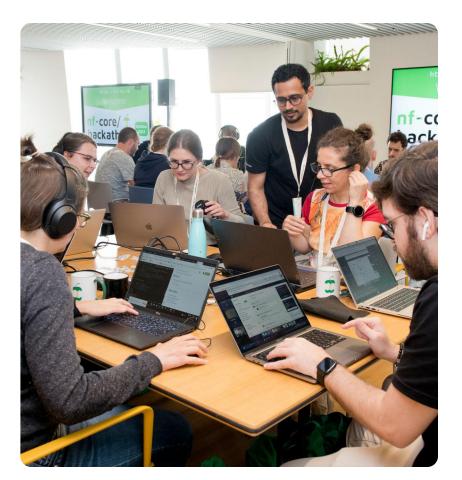
Interactive Notebooks RStudio RShiny Applications Genome Browsers



# **Take-home message**

You can build *with* nf-core, even if you're not building *for* nf-core

We can do great things together!





# **Hackathon and Summit 2023**

Join us at the next nf-core hackathons!



October 16-20, 2023



November 28-30, 2023

https://summit.nextflow.io/





# Thanks: the nf-core community

Taking the phrase "team effort" to a whole new level





# Schedule your demo today





# Schedule a personalized demo

Experience how you can streamline your research workflows and accelerate scientific discover.

https://seqera.io/demo/



### Resources

Links to find out more information

#### Websites

- nf-core: <a href="https://nf-co.re/">https://nf-co.re/</a>
- o nf-validation: <a href="https://nextflow-io.github.io/nf-validation/">https://nextflow-io.github.io/nf-validation/</a>
- o nf-core on GitHub: <a href="https://github.com/nf-core">https://github.com/nf-core</a>
- Seqera: <a href="https://seqera.io/">https://seqera.io/</a>
- Nextflow: <a href="https://nextflow.io/">https://nextflow.io/</a>
- Nextflow Tower: <a href="https://tower.io/">https://tower.io/</a>

#### Content

- Blog: <u>Best Practices for Deploying Pipelines with Nextflow Tower</u>
- Podcast: <u>Infrastructure team: nf-validation and nf-core components</u>
- Nextflow training: <a href="https://training.nextflow.io/">https://training.nextflow.io/</a>
- o nf-core documentation: <a href="https://nf-co.re/docs">https://nf-co.re/docs</a>







# Thank you



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