Practical Course Computational Workflows - 2025 -

Mark Polster and Julian Flesch

Introduction to Computational Workflows

Prof. Sven Nahnsen

Course Information

Attendance

Attendance is mandatory!

We start at 09:15 every morning (lunch-break between 11:45 and 12:45)

There might be interfering meetings, that require our room. We will adapt our breaks to match that, where possible

Friday 03.10. is public holiday: No course day

Structure of the course

Week 1: Analyzing data using nf-core pipelines / Intro to Nextflow

Week 2: Pipeline project

Contact

In person during the course

via Mail:

julian.flesch@uni-tuebingen.de mark.polster@uni-tuebingen.de

always to both of us, please!

Missing a course date

If you are sick, inform us before the course starts in the morning

A doctor's note **must** always be handed in **via mail to Prof. Sven Nahnsen**sven.nahnsen@uni-tuebingen.de

Unexcused absence will lead to failing the course!

Grading

Attendance is mandatory to get credits

All hand-ins are done via Github as a Release.

Any work committed after the deadlines will not count!

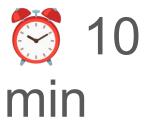
Each student is required to hand-in their own week 1 assignments

You will hand-in your course project in teams of two including:

- 1) A reproducible nextflow/nf-core workflow for RNA-sequencing analysis
- 2) A scientific report of roughly 5 pages

Git Basics: Using your favorite LLM ...

- ... What is **git** and what are repositories?
- ... What is a **fork** on Github?
- ... What is the difference between origin and upstream?







Gemini

Your typical Day in the Computational Workflows Course

- You pull today's updates from our upstream
- 2. Work on the assignments
- 3. Frequently commit and push to your own fork
- 4. Ask questions, if you have problems



Let's get started!

Demo

Let's get started!

1. Fork the assignment repository on github:



github.com/qbic-pipelines/computational-workflows-2025

Let's get started!

- 1. Fork the assignment repository
- 2. Set up ssh-key for Github
- 3. Clone your personal fork to your local machine
- 4. Set the assignment repository as upstream
- 5. Add us to your fork
- Start working on today's jupyter notebook
- 7. Commit and push your work frequently!

```
$ mkdir -p ~/.ssh && cd ~/.ssh
$ ssh-keygen -t rsa
$ nano config
$ cd <your-workspace>
$ git clone git@<your-fork>
$ git remote add upstream < gbic>
$ git add <file1> <file2>
$ git commit -m "adds files"
$ git push origin main
```

Practical Course Computational Workflows

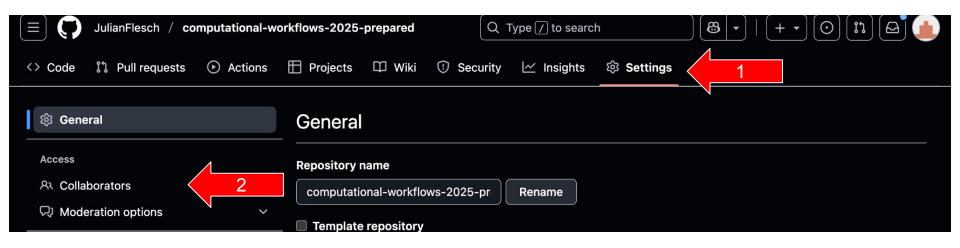
Day 2

Mark Polster and Julian Flesch

Upfront Information

Please add us to your forks on Github!

@JulianFlesch @mapo9

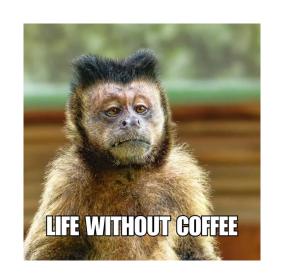


Upfront Information

Help yourself to coffee, if you want (list at our desk)

Push your work to Github regularly

Lunch break today from 12:00 to 13:00



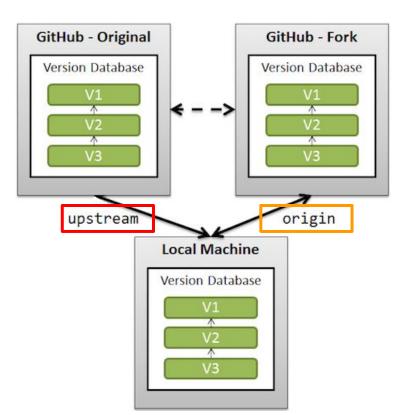


Quick recap: Github Fork and Upstream

We update only the upstream

You work on your fork, keeping local and remote in sync and pulling in updates

(if we do not change files you worked on, there should be no *merge conflicts*)



Getting your Material for today

Step 1: Save your work to your fork

Step 2: Get today's notebook from upstream

```
$ git add <file1> <file2>
$ git commit -m "adds files"
$ git push
```

```
# pull from upstream
$ git pull upstream main
# To leave vi:
# ":" -> "q" -> "w" -> "enter"
```