Bioinformatics session

A two-day workshop for bioinformaticians and molecular biologists with focus on the TSO500 pipeline in InPreD



Overview

- 1. Setup
- 2. Development & Collaboration
- 3. Nextflow
- 4. tso500_nxf_workflow
- 5. Python

1. Setup

• go to https://github.com/ and click on Sign up



• enter your email

```
Welcome to GitHub!

Let's begin the adventure

Enter your email*

→ coder@inpred.no

Continue
```

set a password

```
Welcome to GitHub!
Let's begin the adventure
Enter your email*

√ coder@inpred.no

Create a password*
                                                          Continue
```

• choose a username

```
Welcome to GitHub!
Let's begin the adventure
Enter your email*

√ coder@inpred.no

Create a password*
  •••••
Enter a username*
→ inpredder
                                                       Continue
```

• choose email preferences



• solve the puzzle





• create your account



find the activation code in the email you received



Here's your GitHub launch code, @inpredder!



select the desired options

This will help us guide you to the tools that are best suited for your projects. How many team members will be working with you? Just me O 2-5 5-10 0 10-20 20-50 50+ Are you a student or teacher? O N/A Student Teacher Continue

What specific features are you interested in using?

Select all that apply so we can point you to the right GitHub plan.

Collaborative coding

Codespaces, Pull requests, Notifications, Code review, Code review assignments, Code owners, Draft pull requests, Protected branches, and more.

Automation and CI/CD

Actions, Packages, APIs, GitHub Pages, GitHub Marketplace, Webhooks, Hosted runners, Self-hosted runners, Secrets management, and more.

Security

Private repos, 2FA, Required reviews, Required status checks, Code scanning, Secret scanning, Dependency graph, Dependabot alerts, and more.

• choose the free plan



1. Setup

Be added to InPreD organisation at GitHub

1. Resources

• Getting started with your GitHub account

2. Development & Collaboration

Short git introduction

- distributed version control system
- tracks history of changes committed by different contributors
- every developer has full copy of project and its history

Short git introduction

Basic git commands

```
git init : initialises new git repository
git clone <repository url> : creates local copy of remote repository
git add <file/s> : stage new or changed files (anything that should be committed to the repository)
```

git commit -m "feat: my new feature" : commit changes to the repository

Basic git commands

commit message conventions

```
<type>[optional scope]: <description>
```

- feat : new feature
- fix: patching bug
- refactor : code change that neither is neither feat nor fix
- build : build system related changes
- perf: improving performance

commit message conventions

```
<type>[optional scope]: <description>
```

- chore : code unrelated changes, e.g. dependencies
- style : code change that does not change meaning
- test : changes to tests
- docs : adding/updating documentation
- ci : continuous integration, e.g. github actions

Basic git commands

git status: overview over untracked, modified and staged changes

git branch: show local branches

git merge: merge branches

git pull: load changes from remote counterpart

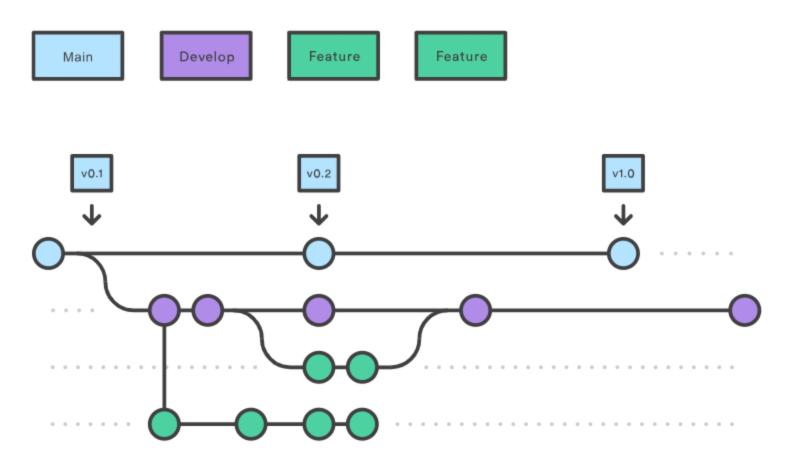
git push: upload changes to remote counterpart

2. Development & Collaboration

Branching model: simplied Gitflow workflow

- start with two branches to record project history: main and develop
- each new feature resides in its own branch (feature branch)
- feature branch is generally created off latest develop commit
- upon feature completion, feature branch is merged into develop

Branching model: simplied Gitflow workflow



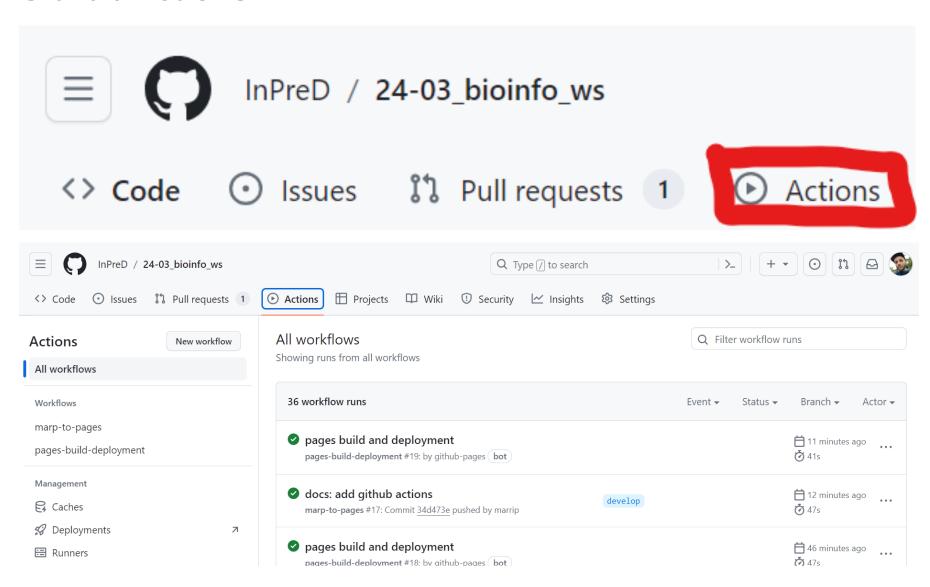
2. Development & Collaboration

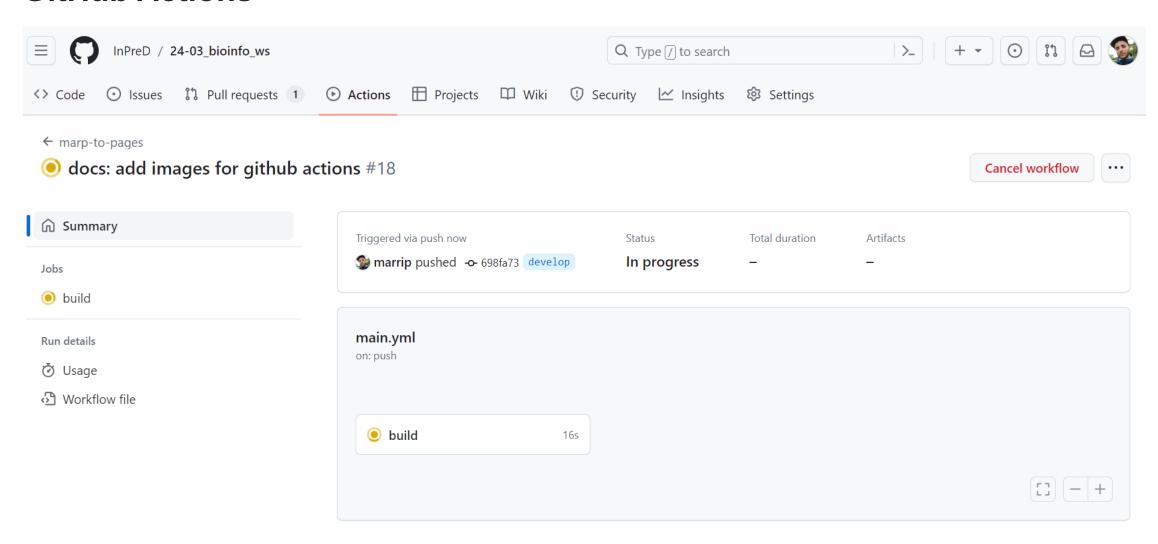
- continuous integration (CI) and continuous deployment (CD)
- building, testing and deploying directly from GitHub
- set up by adding yaml instructions to .github/workflows

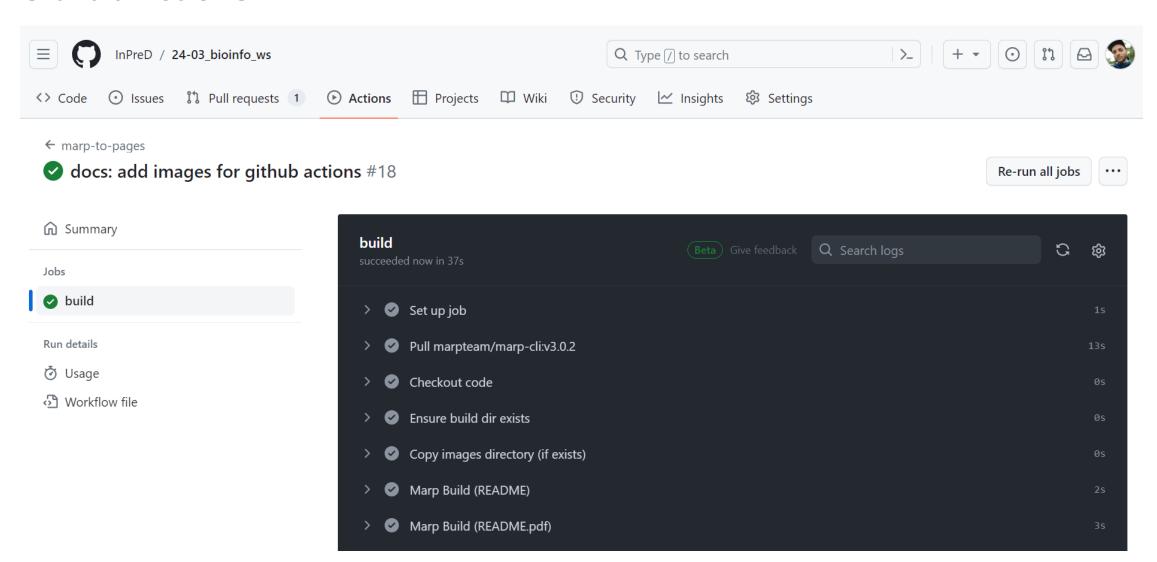
```
name: GitHub Actions Demo
on: [push]
jobs:
    Explore-GitHub-Actions:
    runs-on: ubuntu-latest
    steps:
    - run: echo "Hello world!"
```

```
name: Docker Build
on:
  push:
    branches:
      - main
      develop
    tags:
      _ '* * * * !
jobs:
  test:
    name: Run unit tests
    runs-on: ubuntu-latest
    steps:
        name: Check out the repo
        uses: actions/checkout@v4
        name: Unit testing
        uses: fylein/python-pytest-github-action@v2
        with:
          args: pip3 install -r requirements.txt && pytest
  . . .
```

```
build:
 name: Build Image
  runs-on: ubuntu-latest
  needs: test
  steps:
     name: Check out the repo
      uses: actions/checkout@v4
     name: Lint Dockerfile
      uses: hadolint/hadolint-action@v3.1.0
      name: Docker Meta
      id: meta
      uses: docker/metadata-action@v5
      with:
       images: |
          inpred/local_app_prepper
        tags: |
          latest
          type=semver, pattern={{version}}
          type=semver,pattern={{major}}.{{minor}}
          type=semver, pattern={{major}}
      name: Login to Dockerhub
      uses: docker/login-action@v3
      with:
        username: ${{ secrets.DOCKERHUB_USERNAME }}
        password: ${{ secrets.DOCKERHUB_TOKEN }}
      name: Build and push image to Docker Hub
      uses: docker/build-push-action@v5
      with:
        push: true
        tags: ${{ steps.meta.outputs.tags }}
        labels: ${{ steps.meta.outputs.labels }}
```



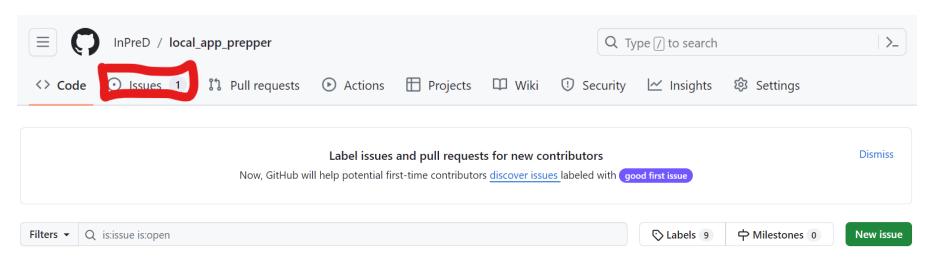




2. Development & Collaboration

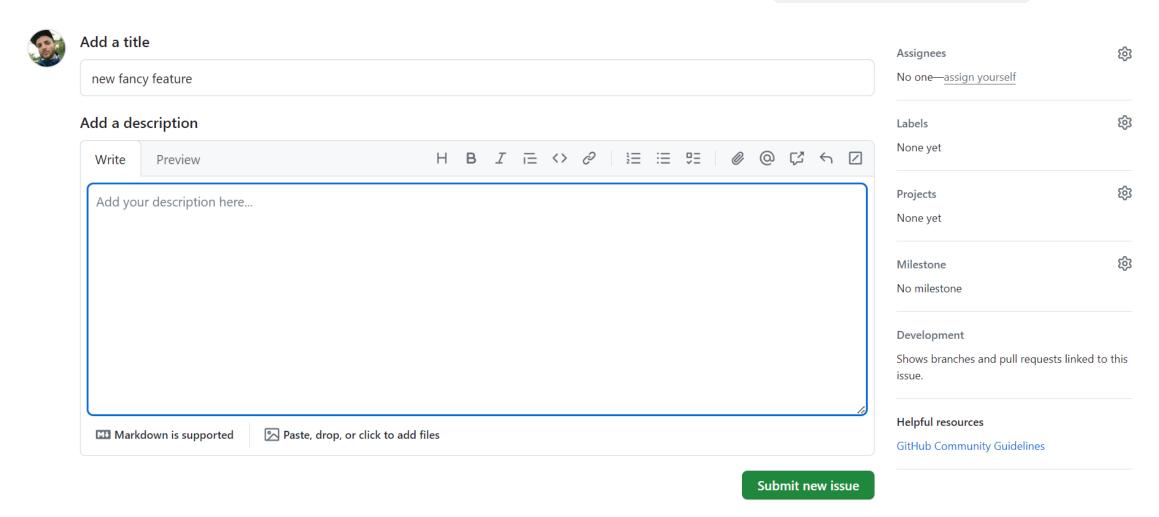
GitHub workflow

• go to issues and create a New issue



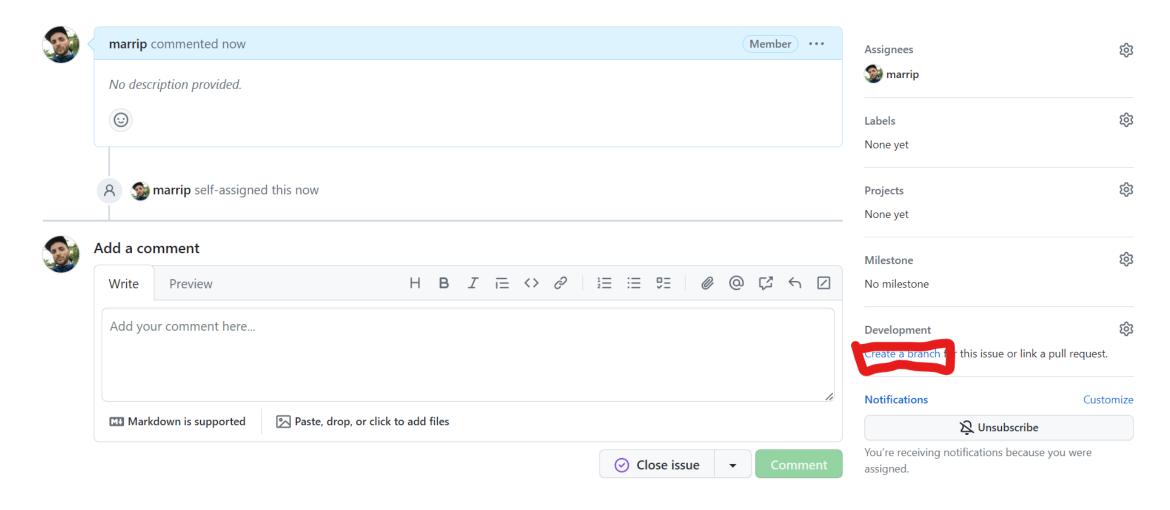
GitHub workflow

• give the issue a descriptive title and a description and Submit new issue

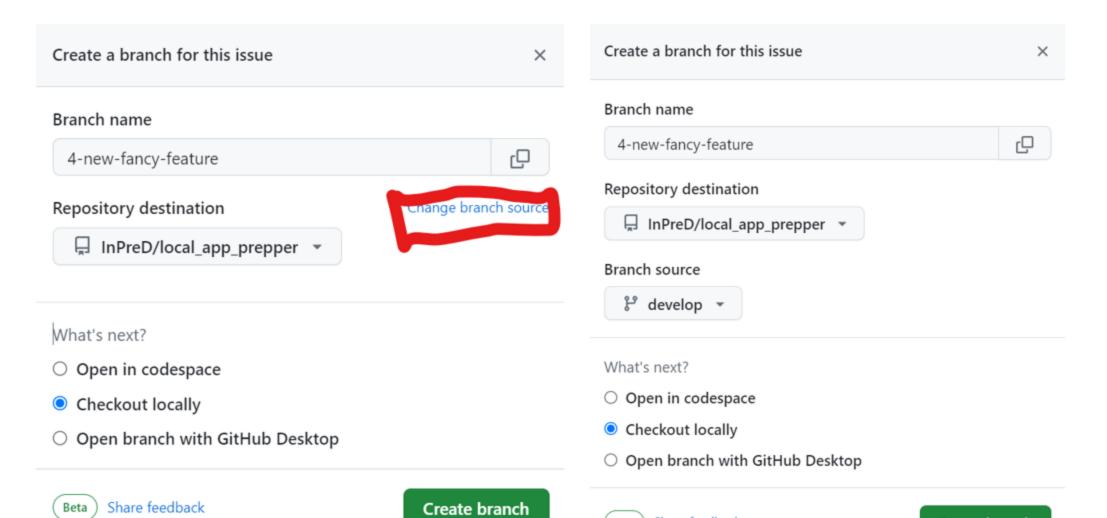


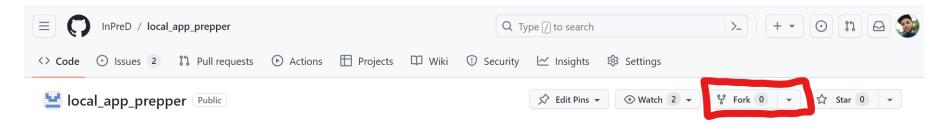
GitHub workflow

• if you decide to work on the issue (own repository), Create a branch via the issue



- Change branch source to develop and Create branch
- get the new branch locally using git pull and git checkout 4-new-fancy-feature
- start making changes and push them to the remote repository





Create a new fork

A *fork* is a copy of a repository. Forking a repository allows you to freely experiment with changes without affecting the original project.

Required fields are marked with an asterisk (*).



By default, forks are named the same as their upstream repository. You can customize the name to distinguish it further.

Description (optional)

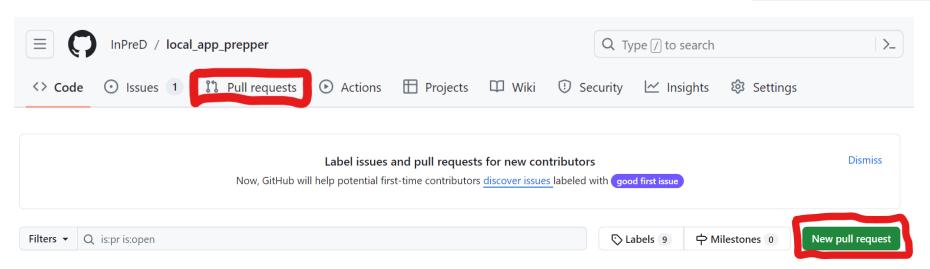
creates inputs.json files to be used with the LocalApp



You are creating a fork in your personal account.

GitHub workflow

• when you are done, go to pull requests and create a New pull request

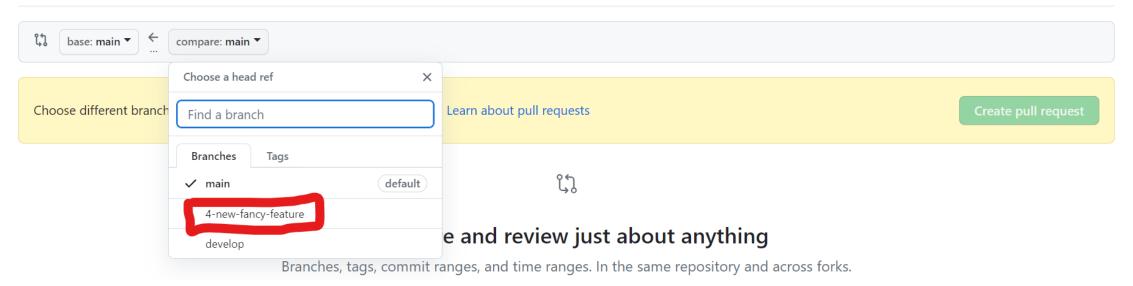


GitHub workflow

• choose develop as base and your new feature branch for compare

Compare changes

Compare changes across branches, commits, tags, and more below. If you need to, you can also compare across forks.



- release and semantic versioning
- licensing

2. Resources

- About Git
- Gitflow workflow
- GitHub Actions

3. Nextflow

- general (install, best practice)
- nf-core template
- stubbing

4. tso500_nxf_workflow

- status
- demonstration

5. Python

- general (best practice, cli)
- unit testing (pytest)

Resources

- github actions
- nf-core
- pytest unittesting
- semantic versioning