Bioinformatics session

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

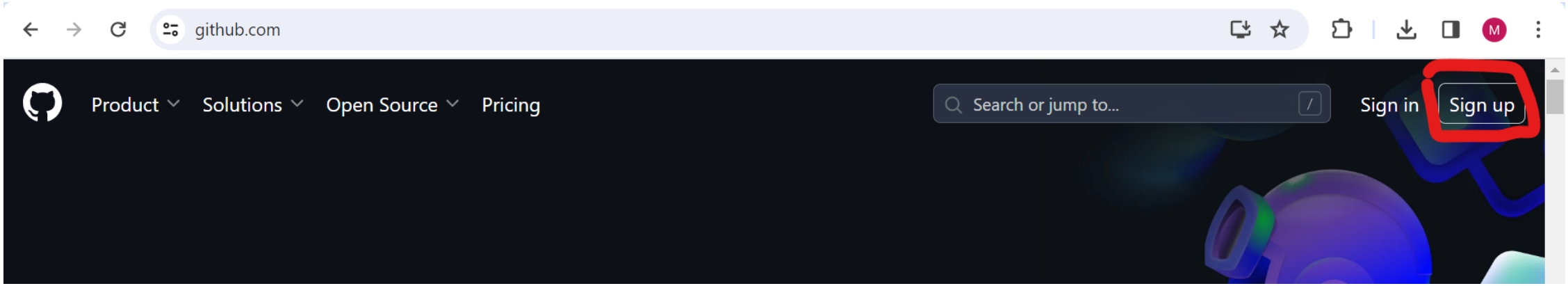
Overview

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

1. Setup

1.1. Create a GitHub account

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

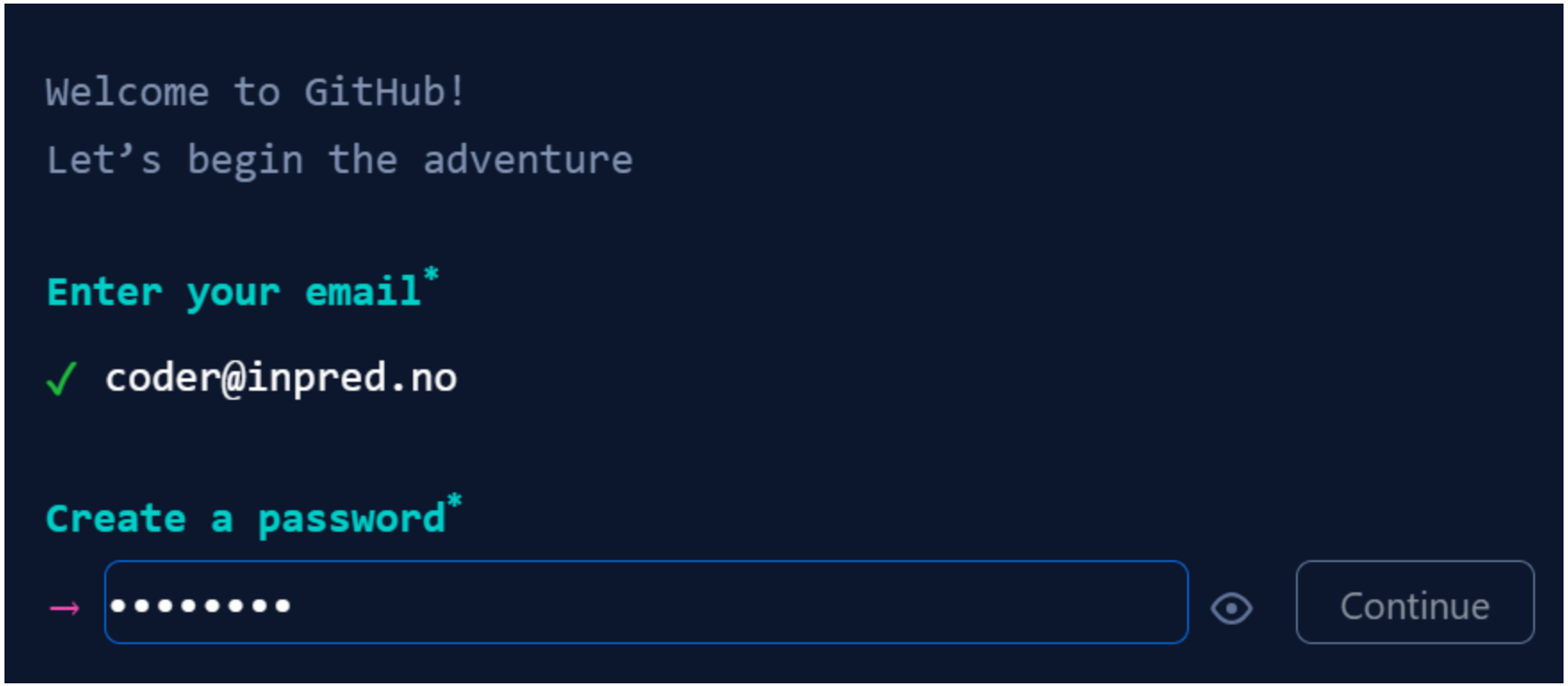


1.1. Create a GitHub account

- enter your email

1.1. Create a GitHub account

- set a password

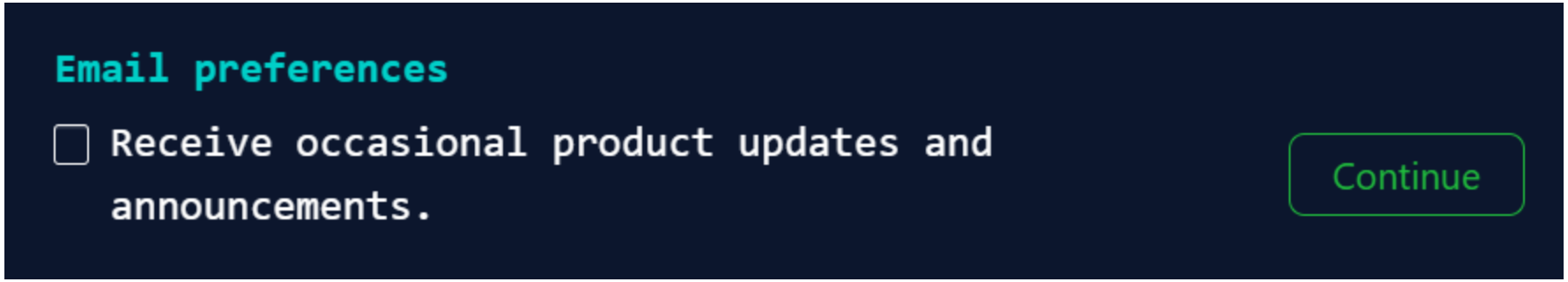


1.1 Create a GitHub account

- choose a username

1.1 Create a GitHub account

- choose email preferences

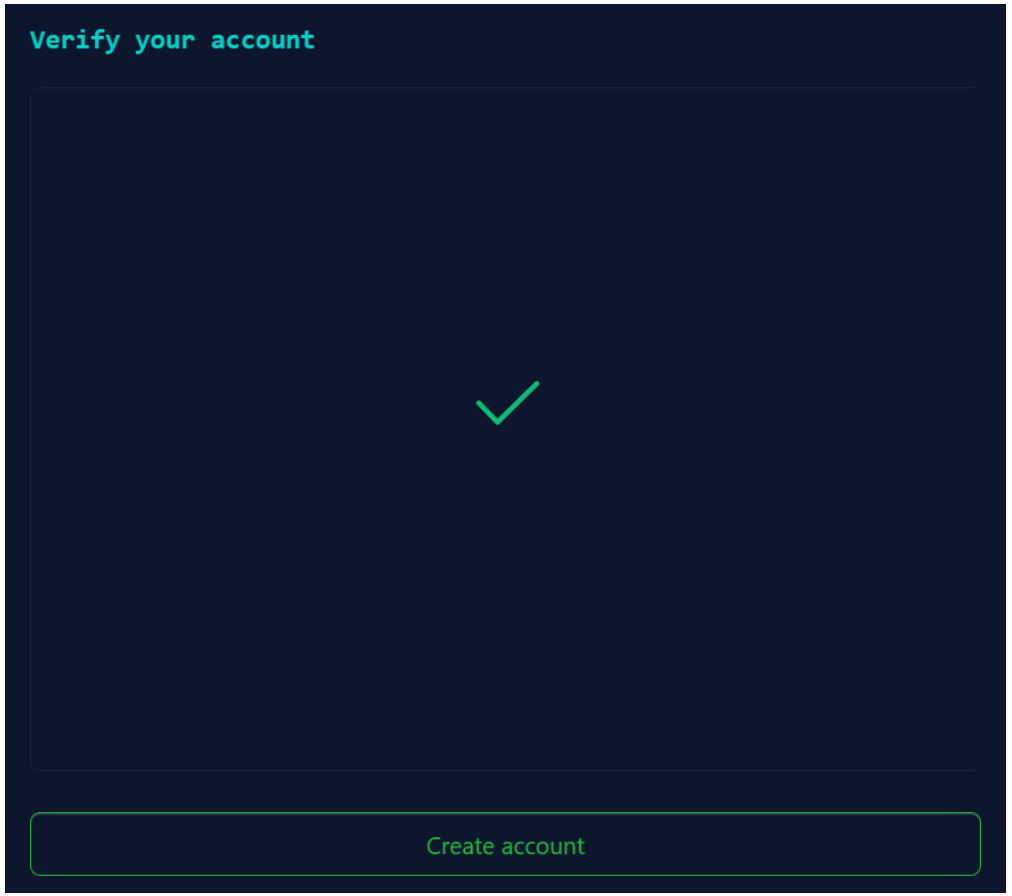


1.1 Create a GitHub account

- solve the puzzle

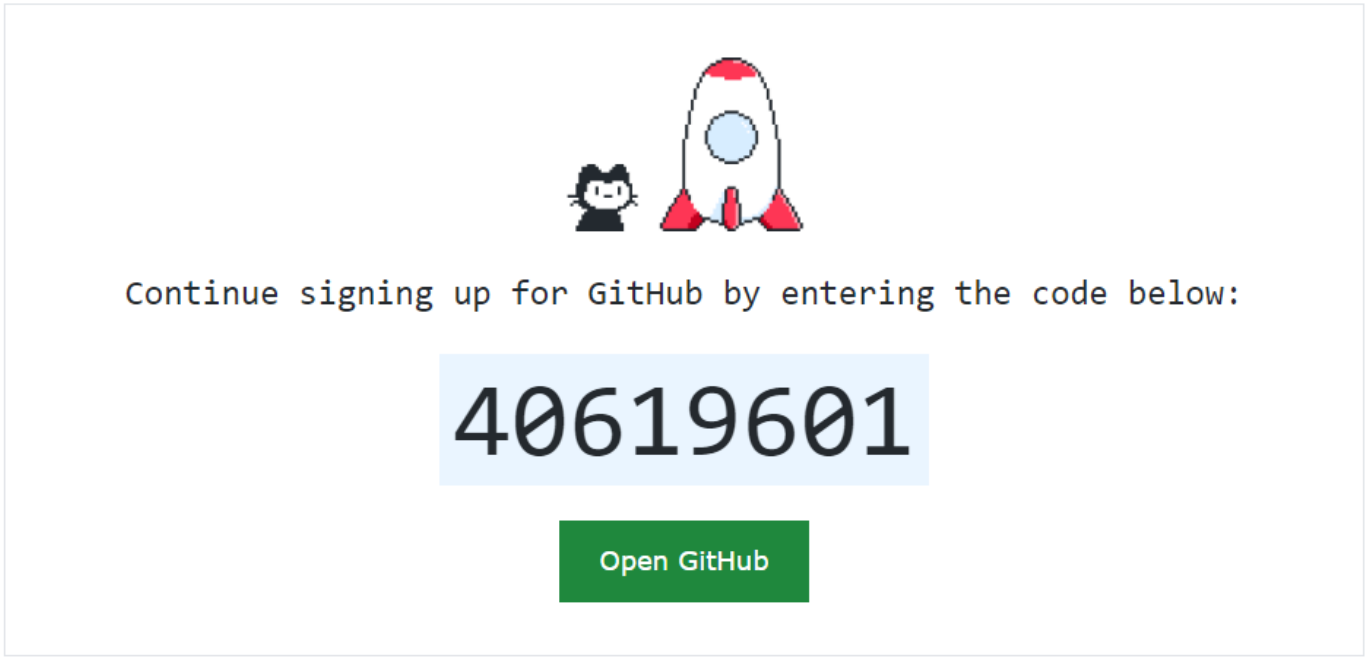
1.1 Create a GitHub account

- create your account



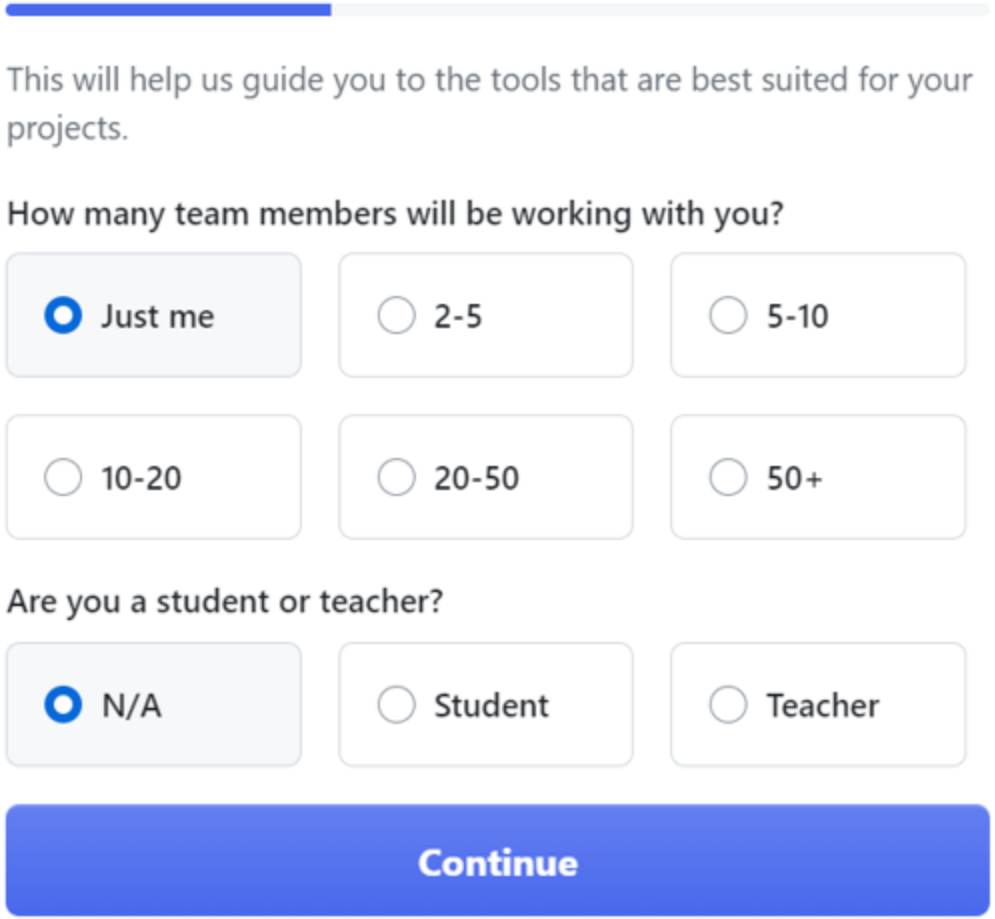
1.1 Create a GitHub account

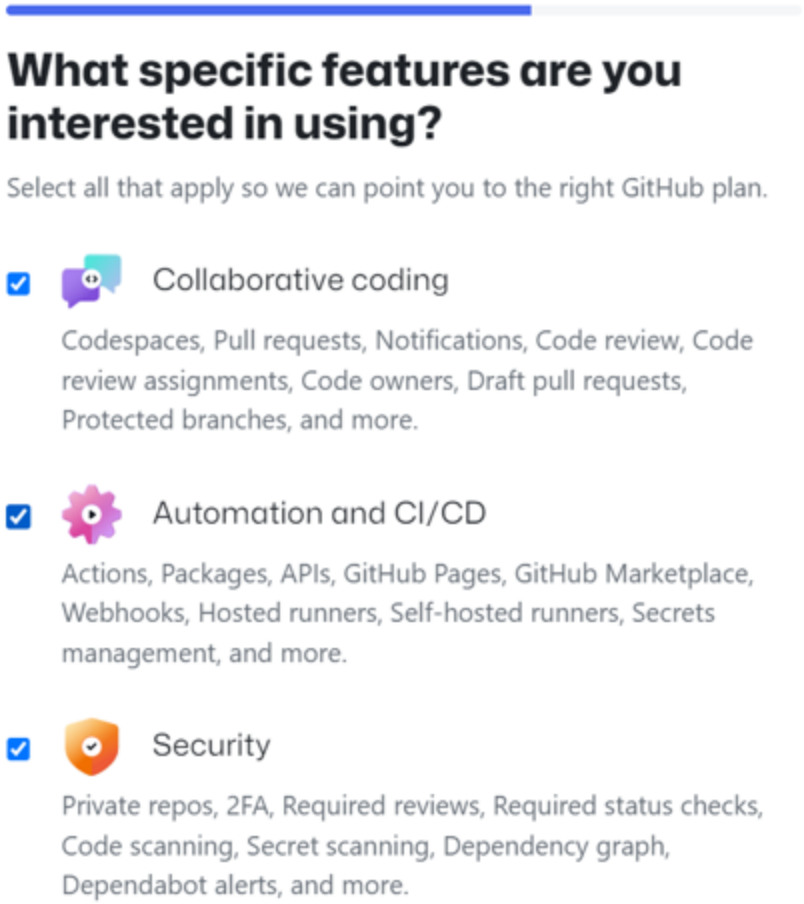
- find the activation code in the email you received



1.1 Create a GitHub account

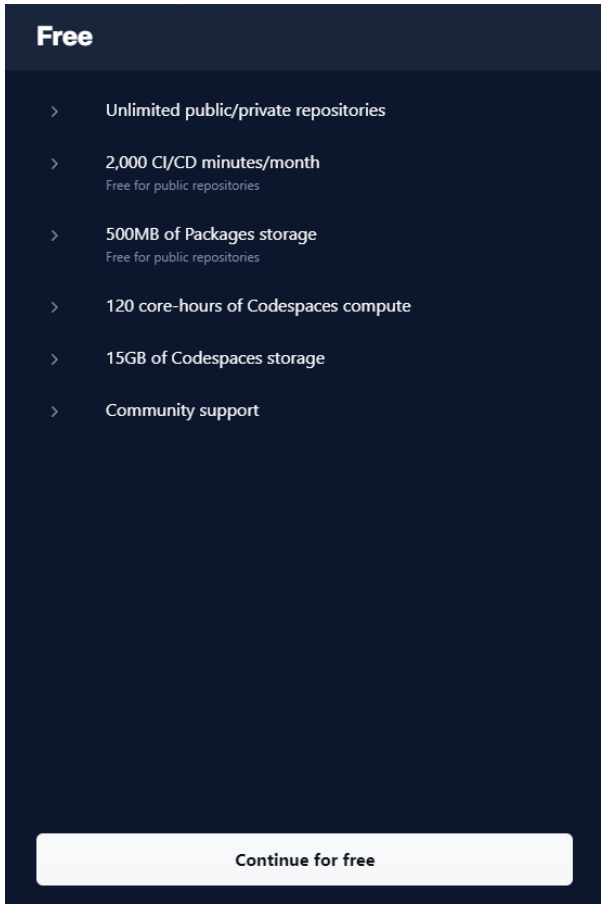
- select the desired options





1.1 Create a GitHub account

- choose the free plan



1.2. Be added to InPreD organisation at GitHub

1.3. Resources

- Getting started with your GitHub account

2. Development & Collaboration

2.1. Short `git` introduction

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

2.1.1 `git config`

```
git config --global user.name <your name>
git config --global user.email <your email>
```

2.1.2. 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

2.1.2.1. 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

2.1.2.1. 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

2.1.2. Basic `git` commands

`git status` : overview over untracked, modified and staged changes

`git branch` : show local branches

`git merge` : merge branches

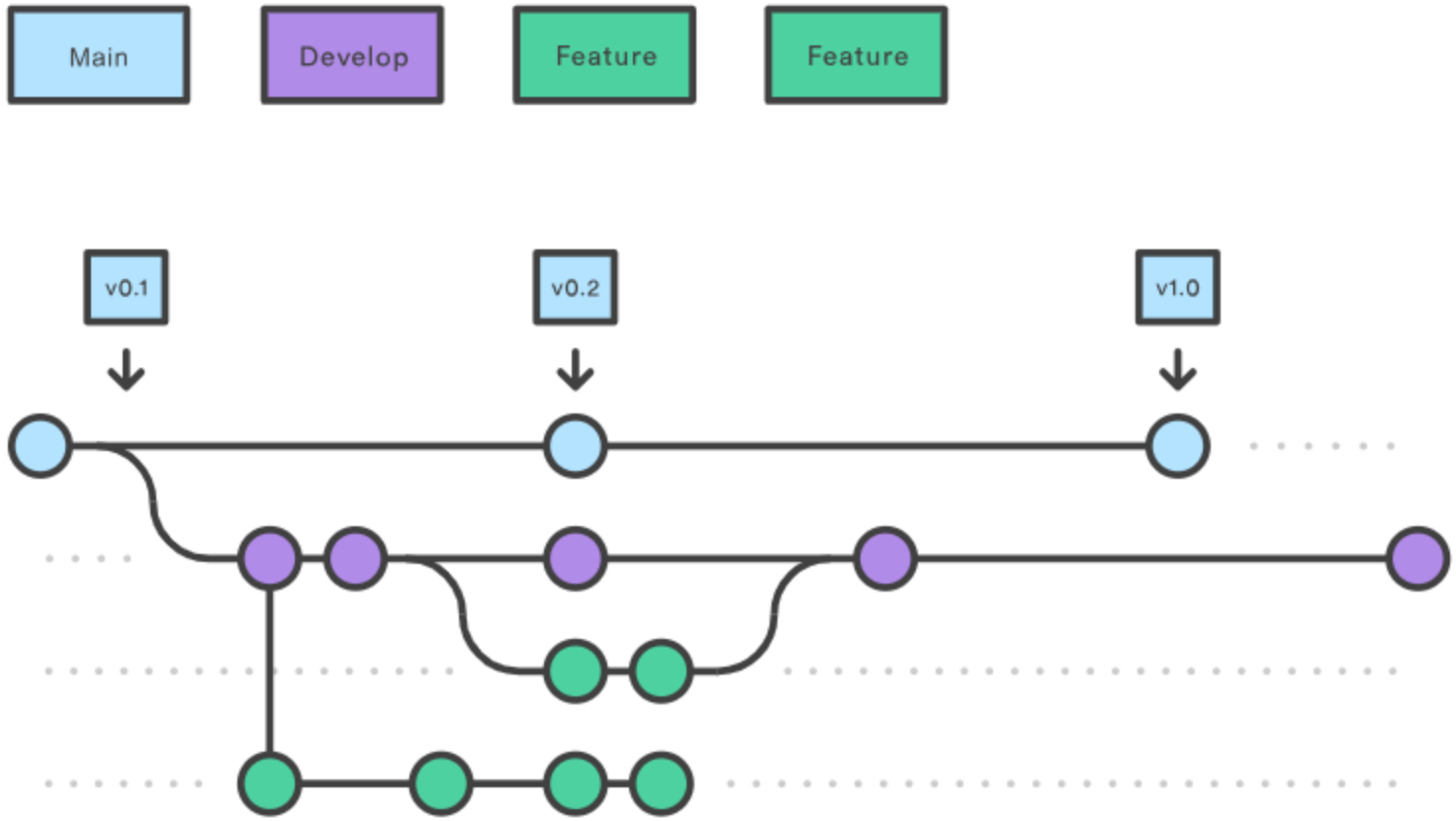
`git pull` : load changes from remote counterpart

`git push` : upload changes to remote counterpart

2.2. 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`

2.2. Branching model: simplied Gitflow workflow



2.3. GitHub Actions

- 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!"
```

2.3. GitHub Actions

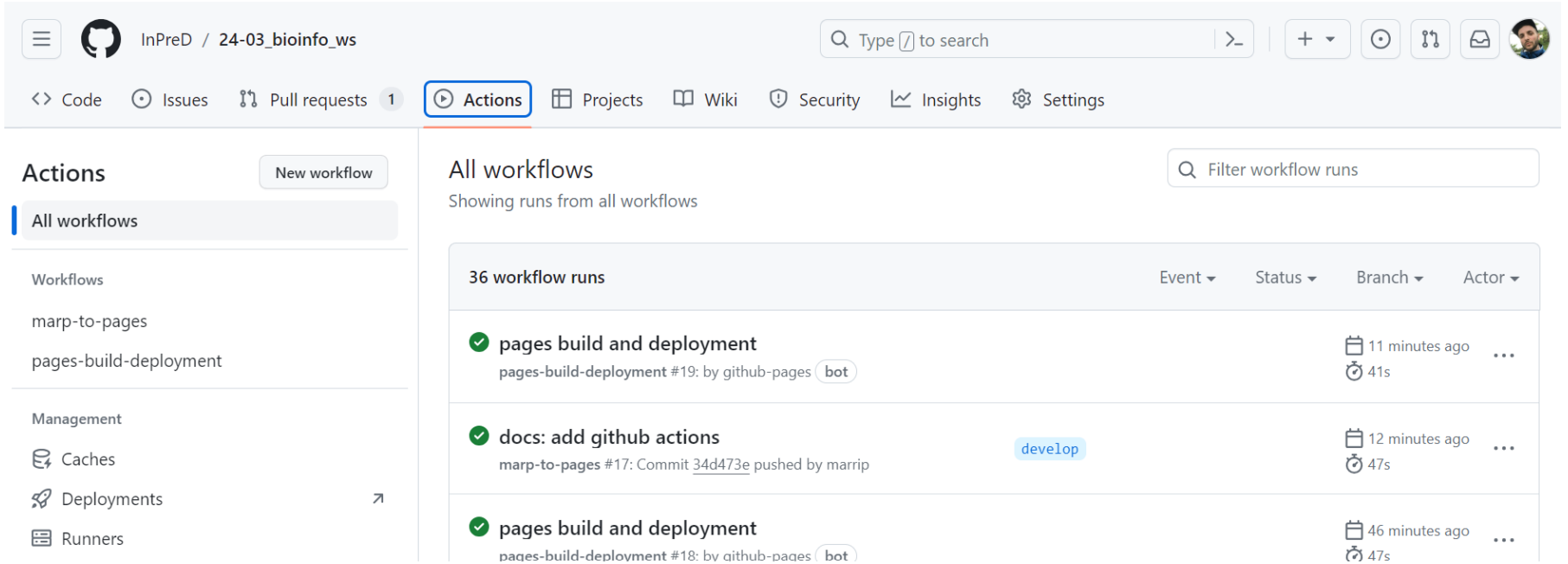
```yaml
name: Docker Build
on:
  push:
    branches:
      - main
      - develop
    tags:
      - '*.*.*'

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
  ...
```

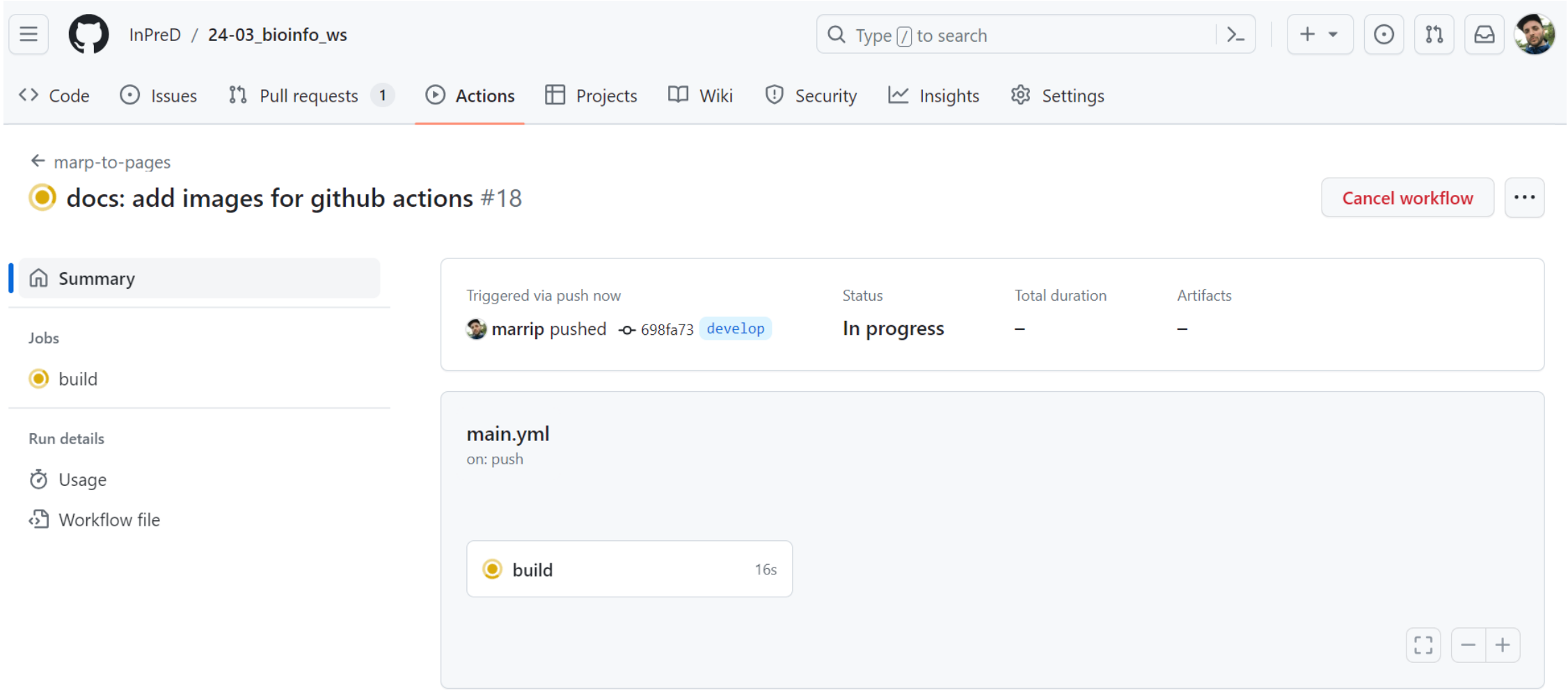
2.3. GitHub Actions

```
...
  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 }}
```

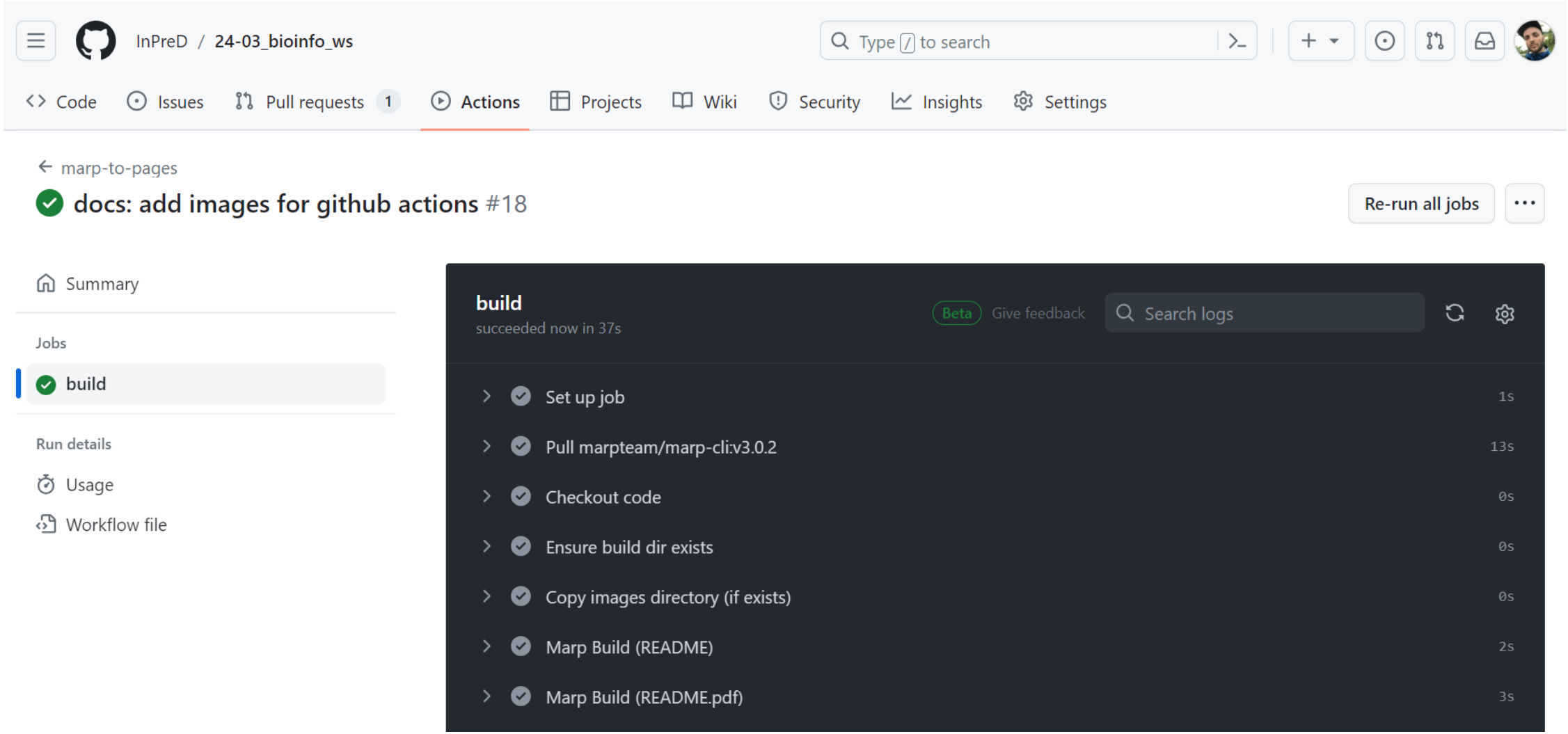
2.3. GitHub Actions



2.3. GitHub Actions

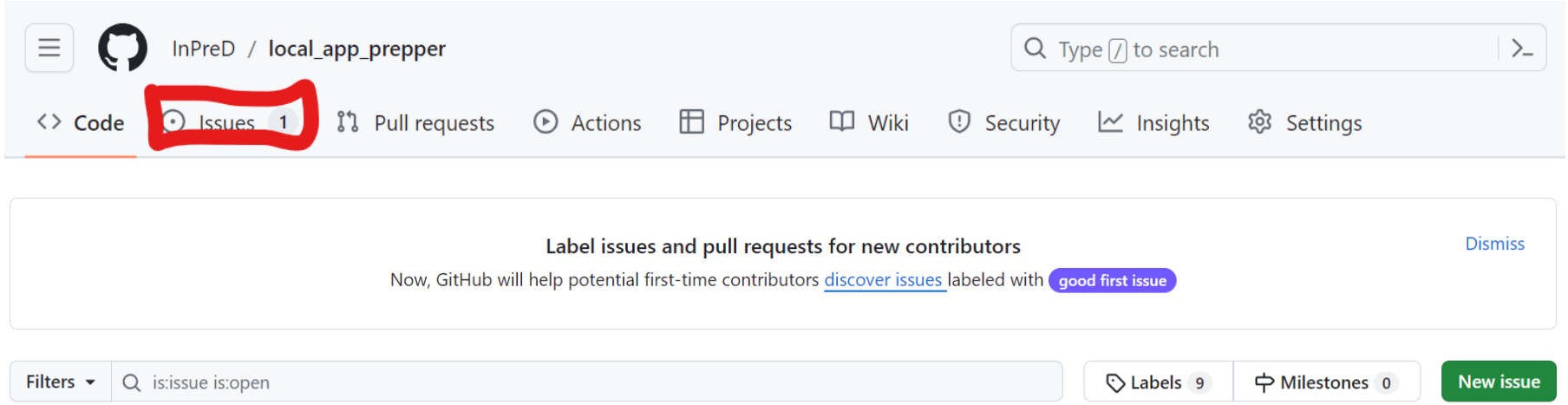


2.3. GitHub Actions



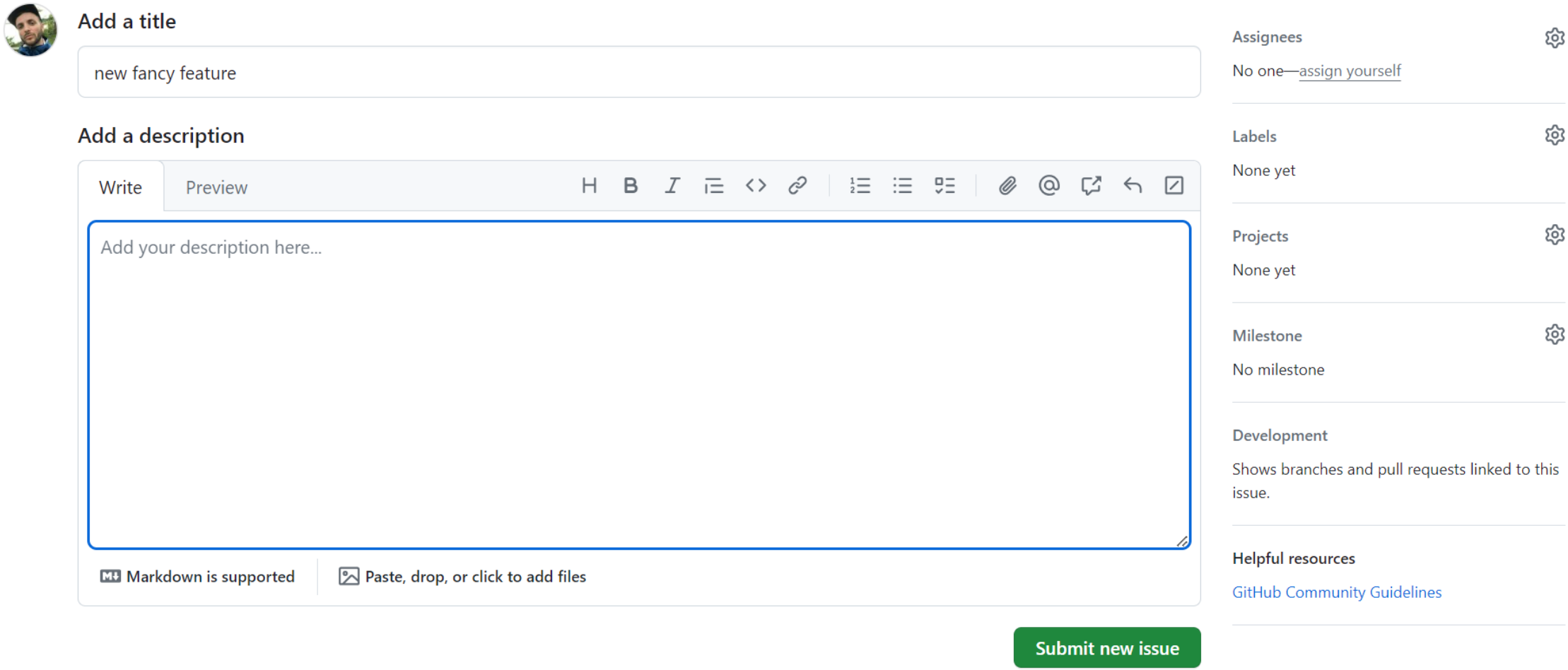
2.4. GitHub workflow

- go to issues and create a `New issue`



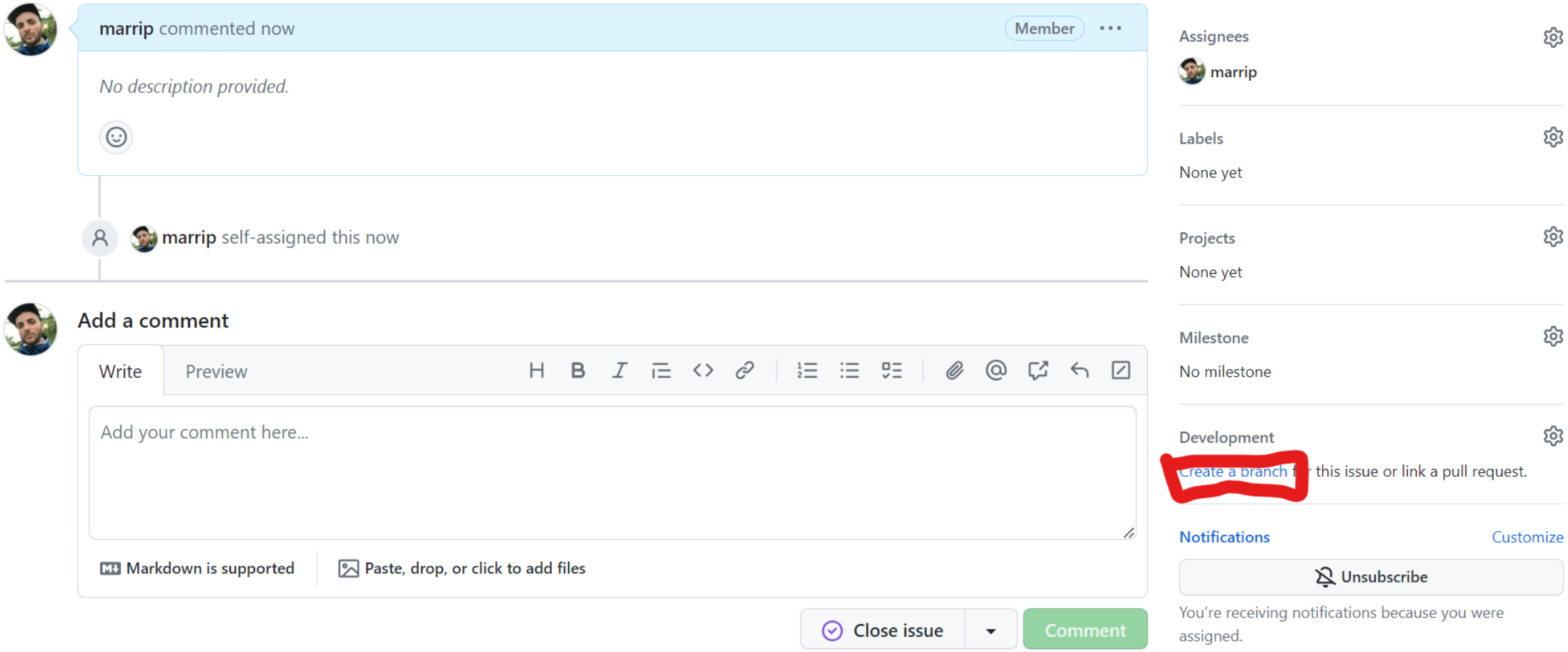
2.4. GitHub workflow

- give the issue a descriptive title and a description and `Submit new issue`



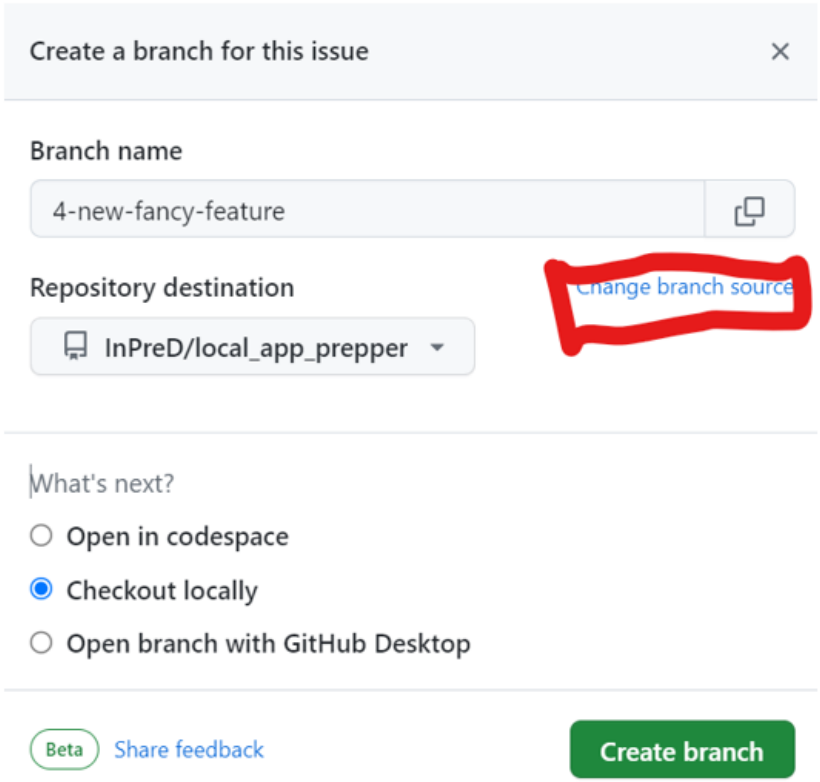
2.4. GitHub workflow

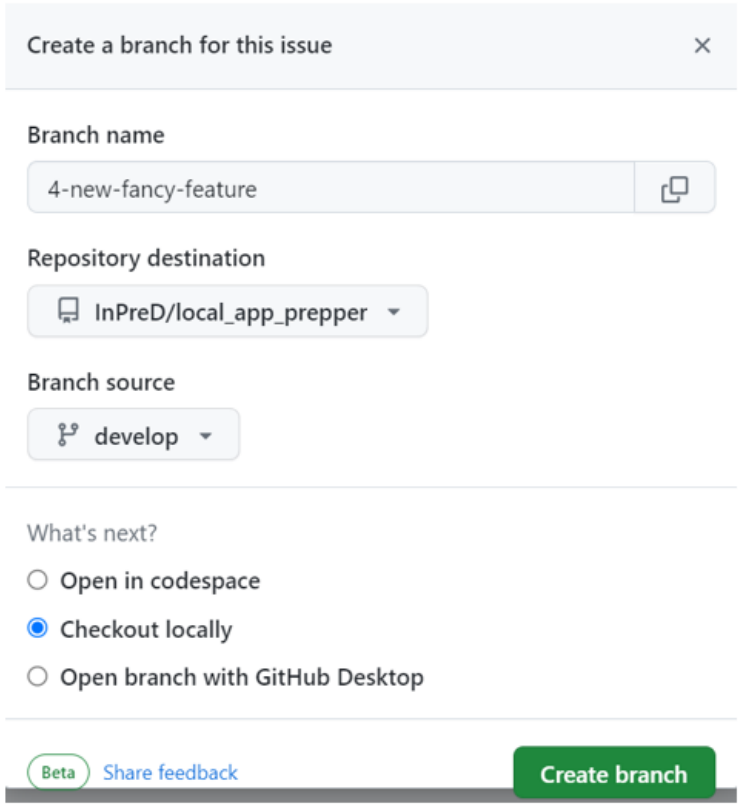
- if you decide to work on the issue (own repository), `Create a branch` via the issue



2.4. GitHub workflow

- `Change branch source` to `develop` and `Create branch`





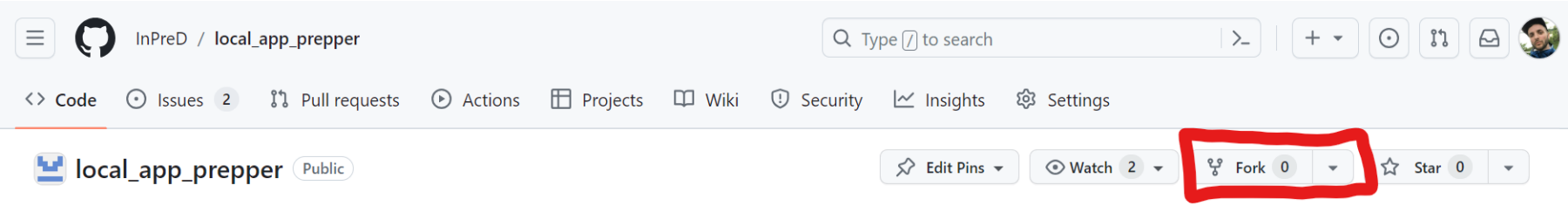
2.4. GitHub workflow

- load the new branch to your local repository, check it out and start working
- push your changes back to the remote

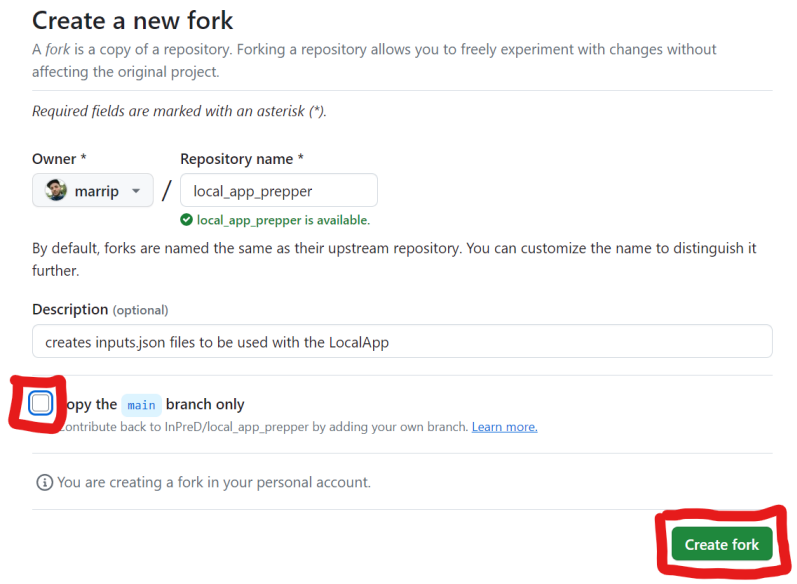
```
$ git pull
$ git checkout 4-new-fancy-feature
$ git add README.md
$ git commit -m "docs: updating docs"
$ git push
```

2.4. GitHub workflow

- for repositories you don't have access to, create a fork



2.4. GitHub workflow

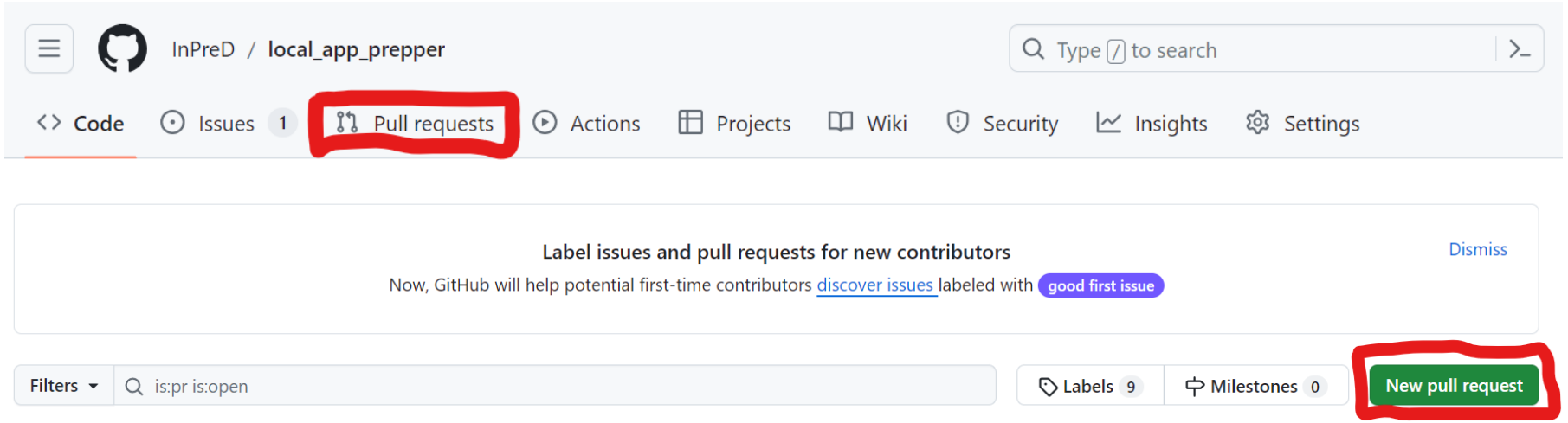


2.4. GitHub workflow

- once you have a fork, `git clone` your forked repository
- create a new branch and work on that
- `git push` your changes back to the forked remote

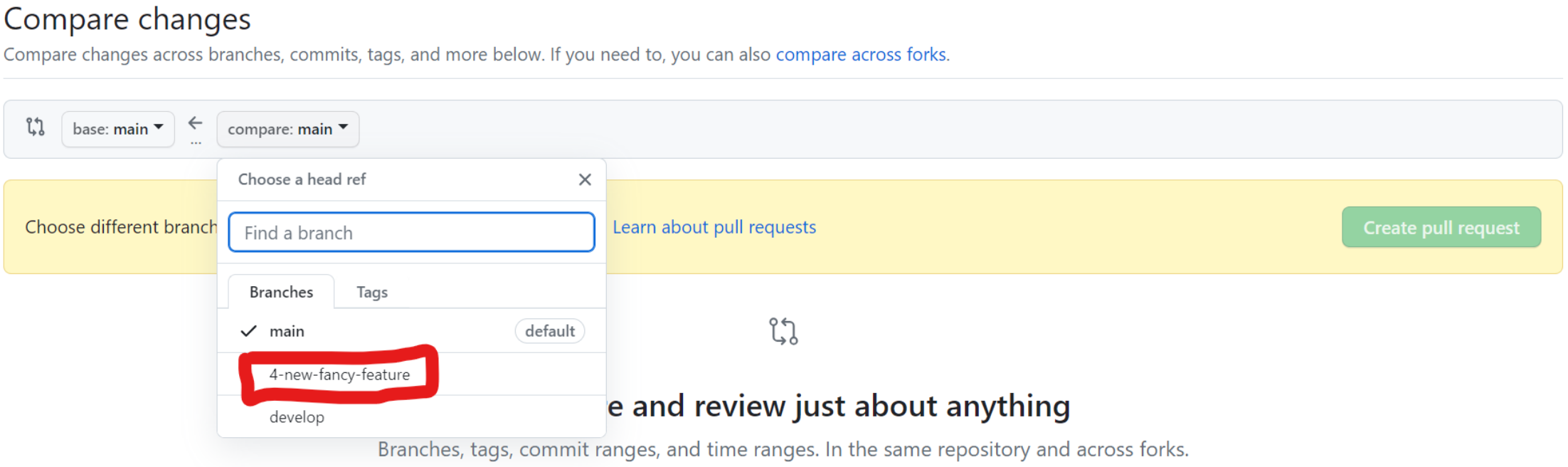
2.4. GitHub workflow

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



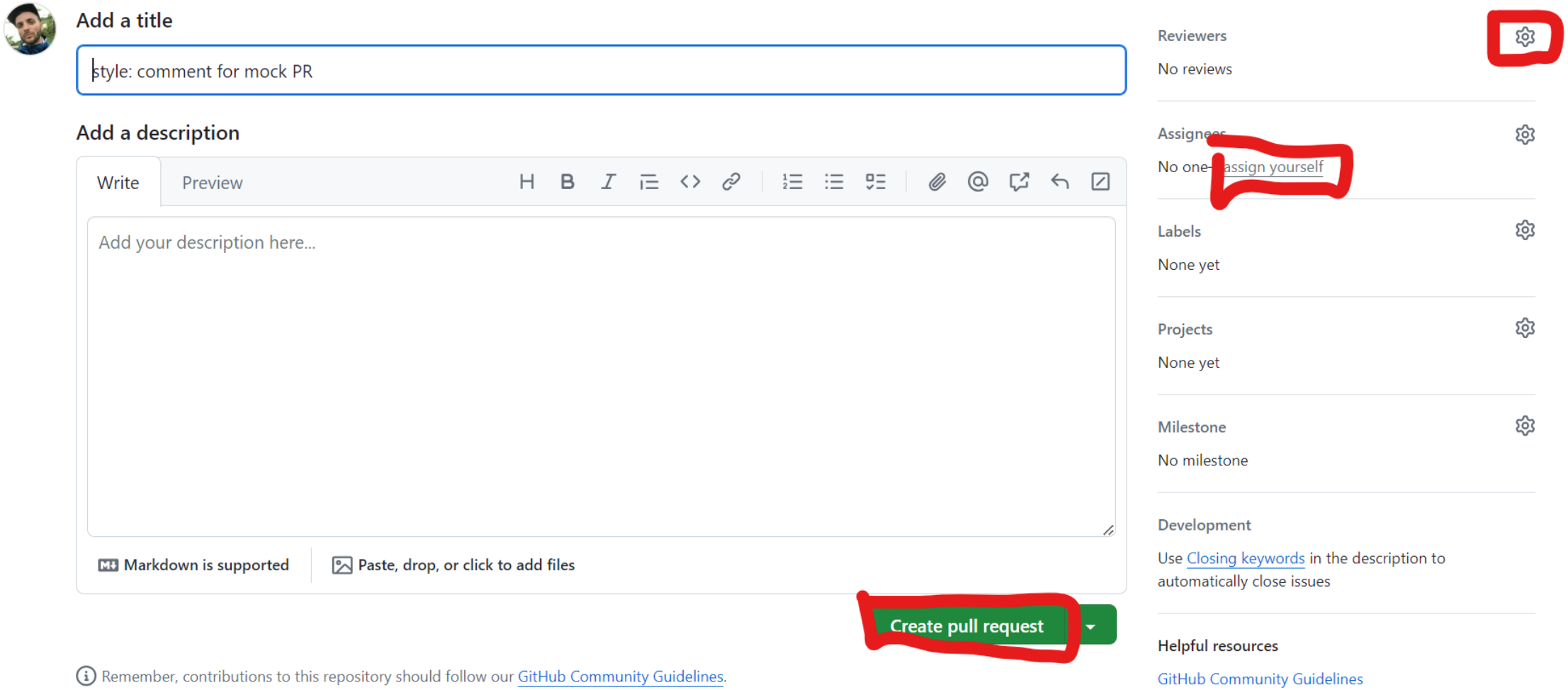
2.4. GitHub workflow

- choose `develop` as `base` and your new feature branch (same repo or forked) for `compare`



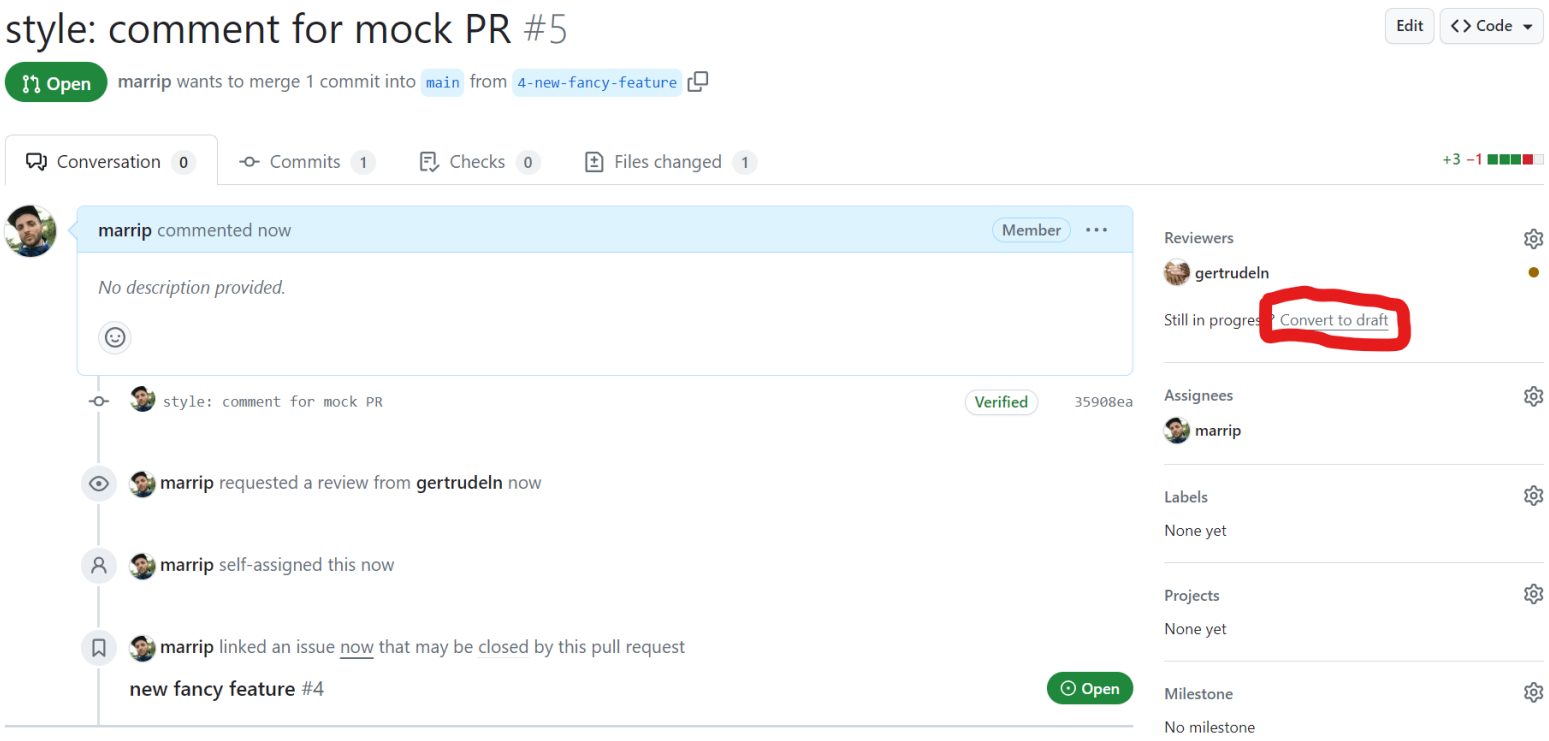
2.4. GitHub workflow

- `assign yourself`, add at least one reviewer (cog icon), provide some context and `Create pull request`



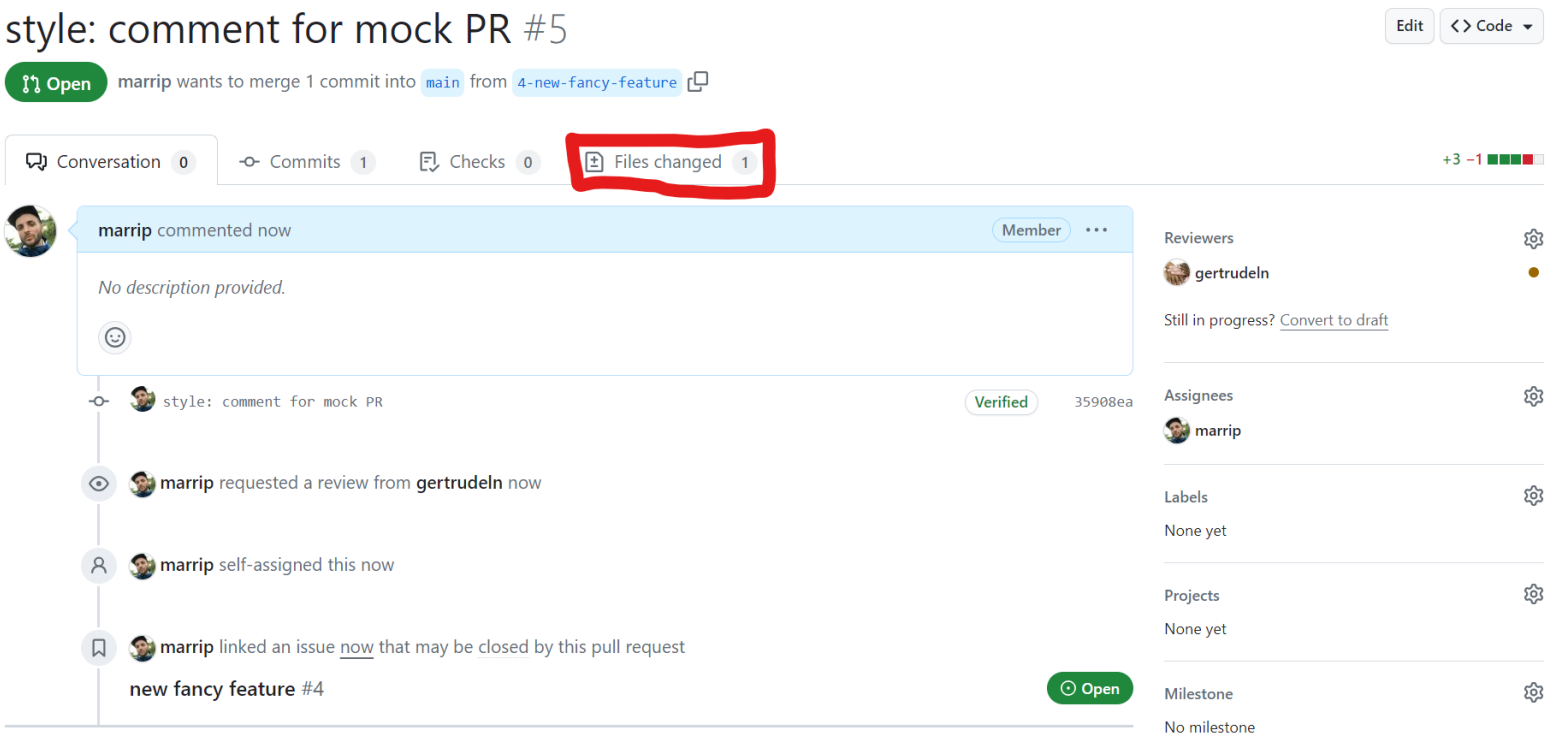
2.4. GitHub workflow

- if you still want to work on the pull request, you can `Convert to draft` to let the reviewers know that it is not done yet
- otherwise you can just wait for them to review your changes



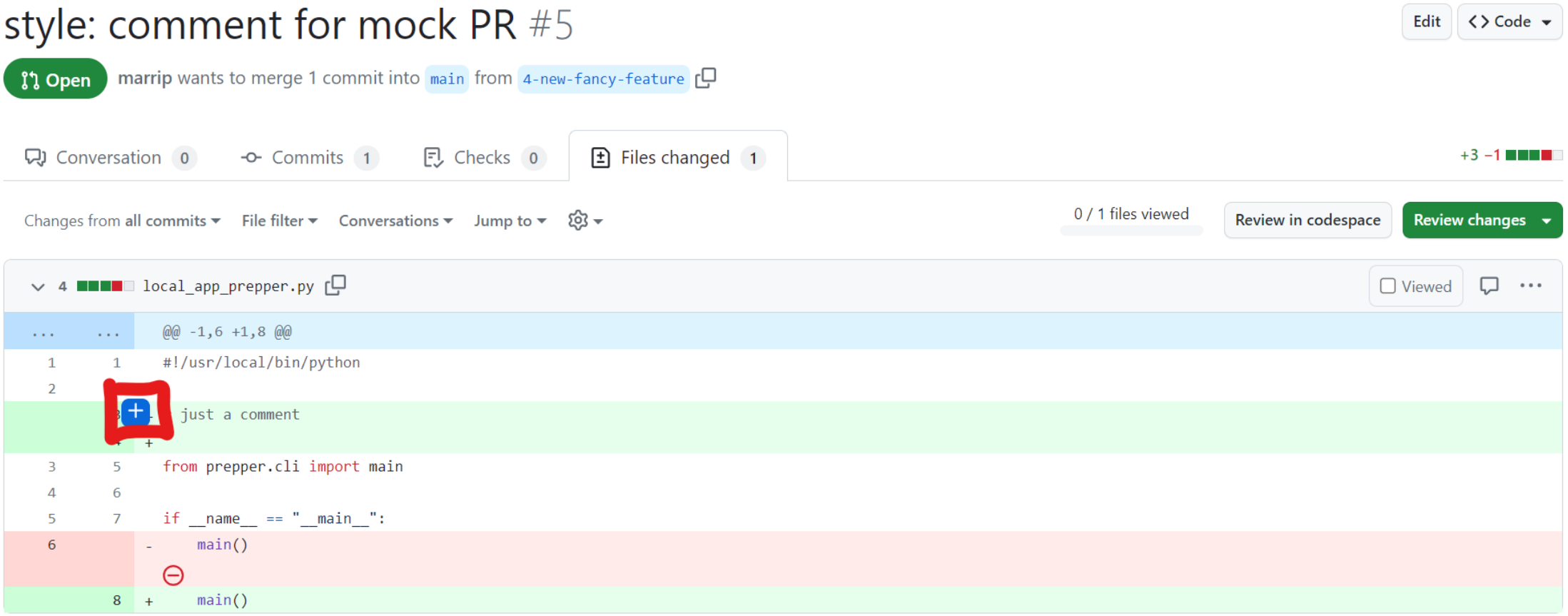
2.4. GitHub workflow

- as a reviewer, make your you check your email notifications to see if there is pull requests waiting for you
- open the pull request and start the review in the `Files changed` tab



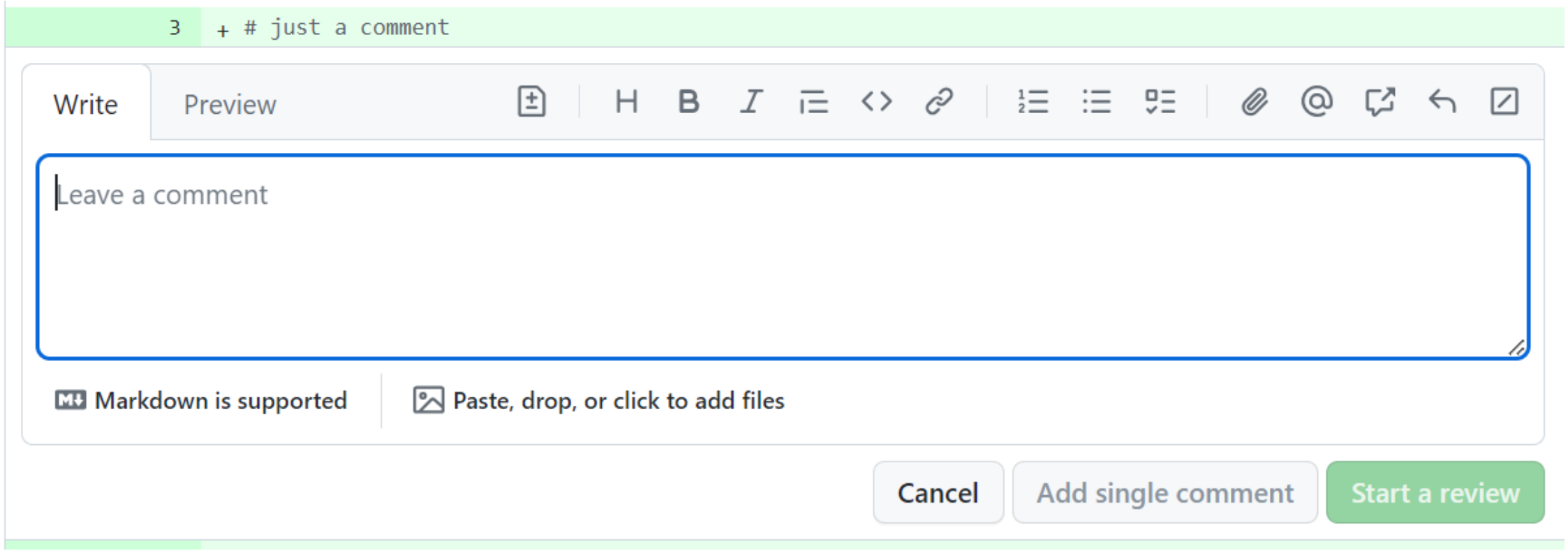
2.4. GitHub workflow

- you can leave comments and suggestions in the code by hovering over the line with the changes and clicking on `+`



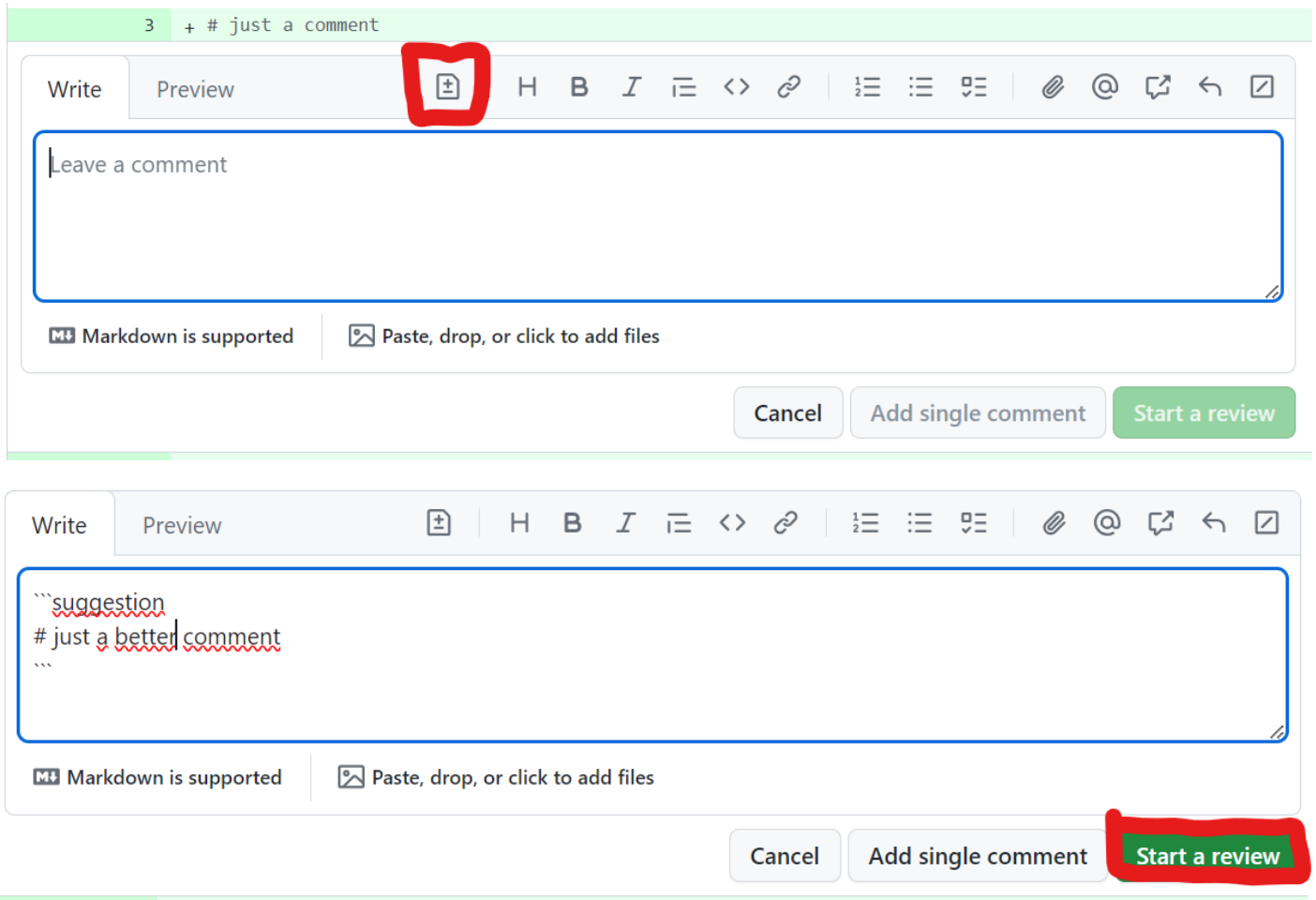
2.4. GitHub workflow

- you can type your comment



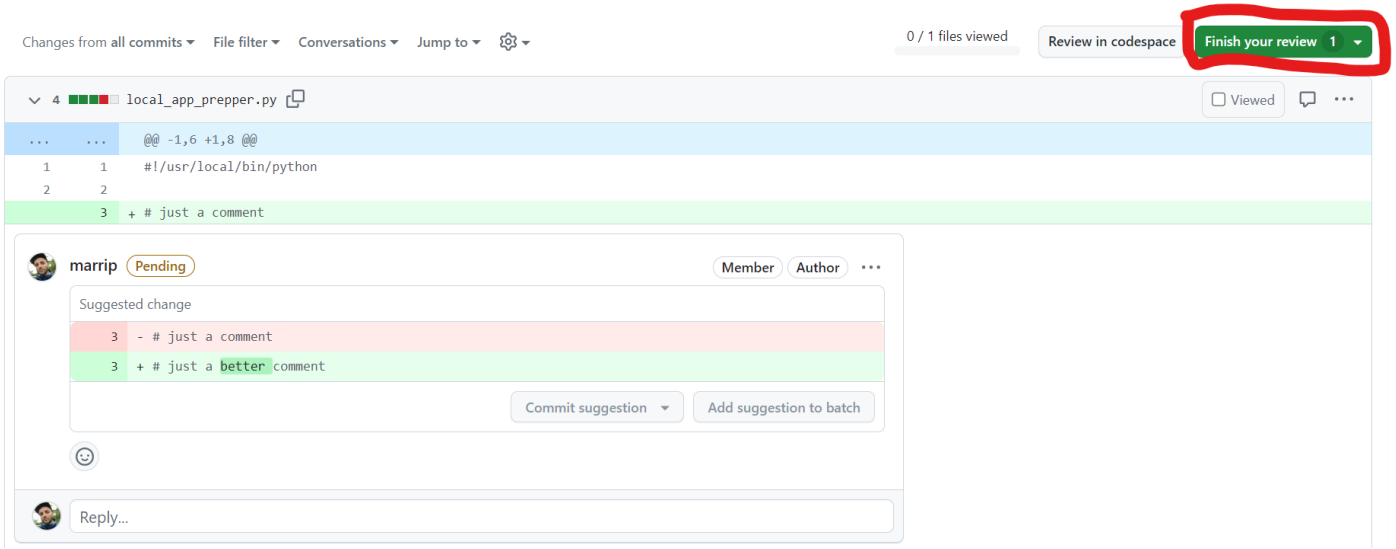
2.4. GitHub workflow

- or you leave a suggestion, ideally you click `Start a review` to initialise the reviewing process



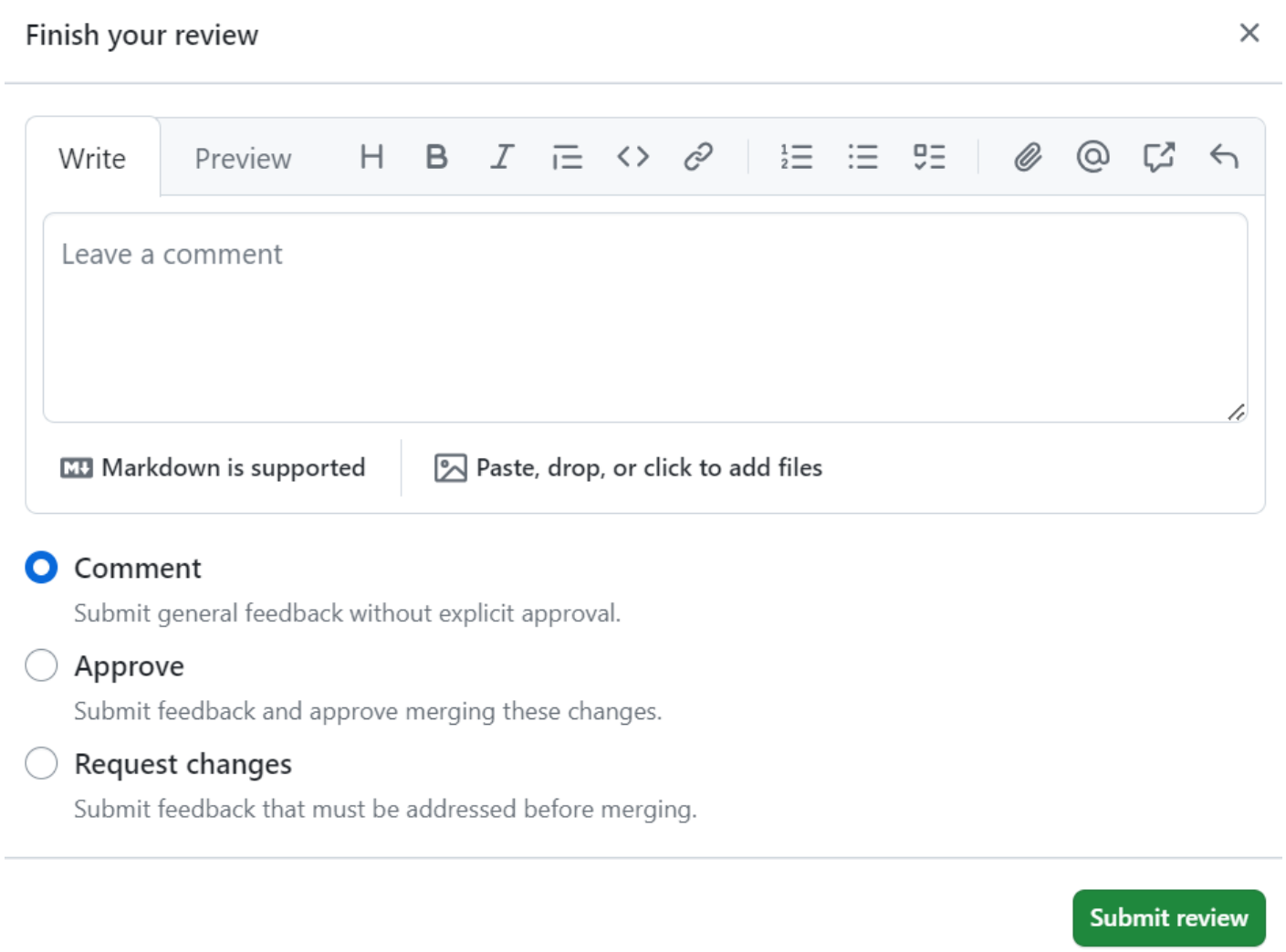
2.4. GitHub workflow

- when you are done with reviewing, `Finish your review`



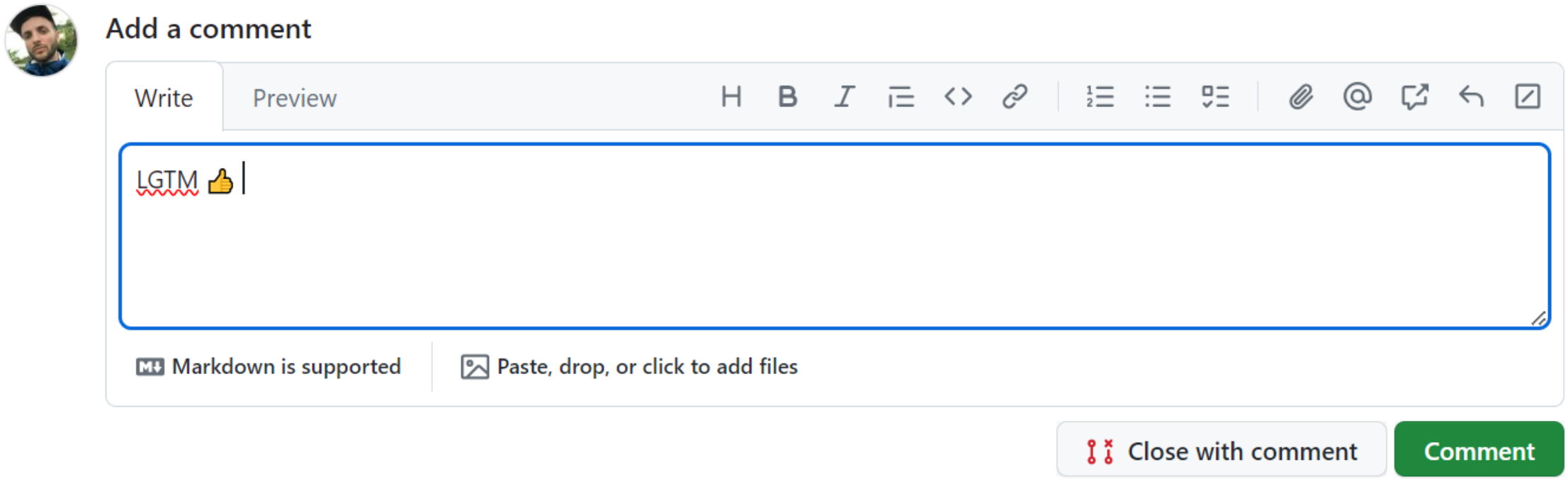
2.4. GitHub workflow

- again, leave a comment if you like, and choose if you just want to `Comment`, `Approve` or `Request changes`



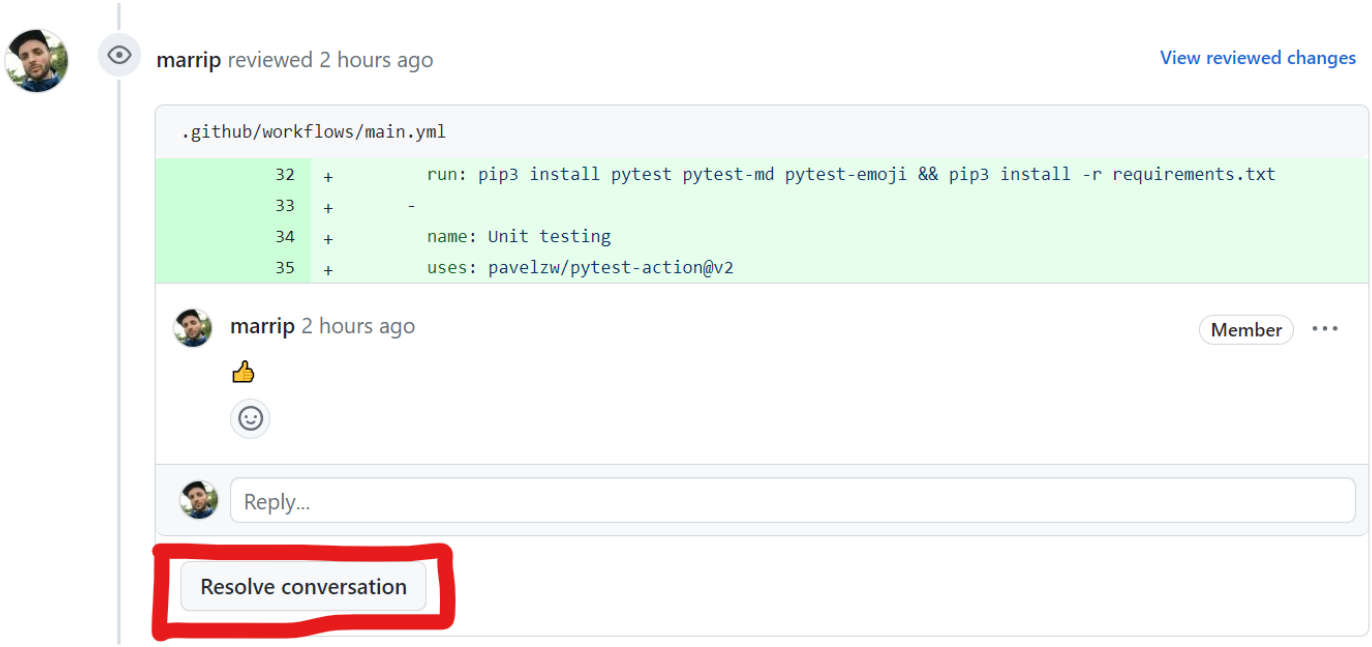
2.4. GitHub workflow

- you can add a general comment to the pull request under `Conversation`



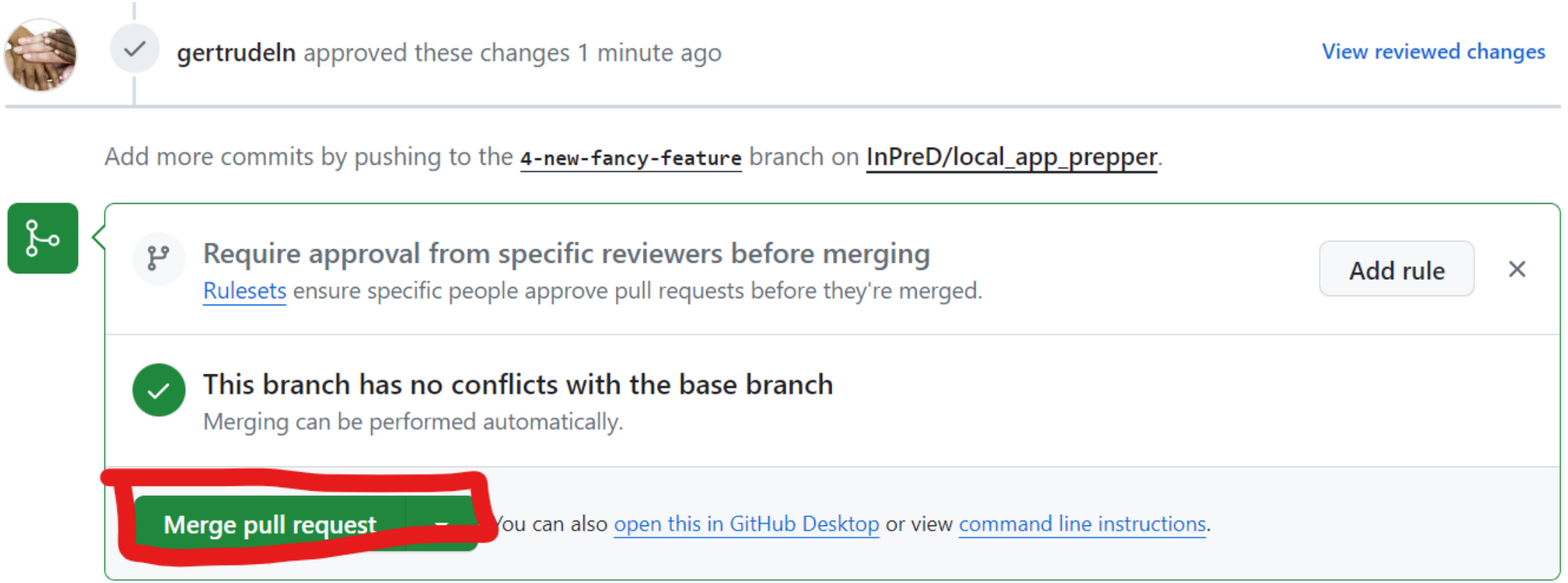
2.4. GitHub workflow

- after the reviewer left their comments and suggestions, you can address them one by one by replying or applying the suggested changes
- whenever a certain comment/suggestion is handled (discussion comes to conclusion, suggestion was applied), you can resolve it



2.4. GitHub workflow

- as soon as the reviewers gave you an approval, you can finally `Merge pull request`



2.4.1 Hands-on pull request

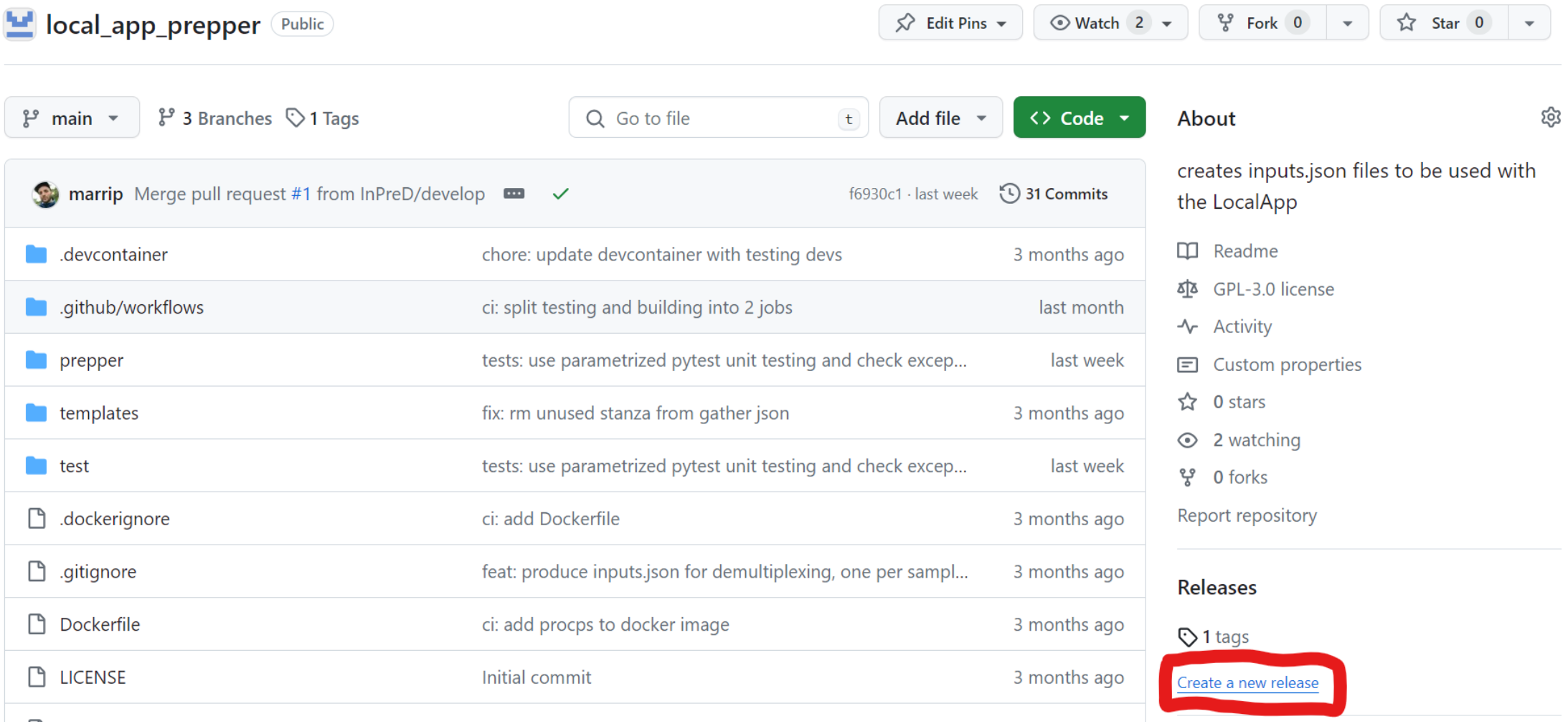
- go to https://github.com/InPreD/24-03_bioinfo_ws/
- create fork to your own account
- open an issue "test pull request" or similar and create a branch
- go to the branch and add a markdown file with your first name and favorite emoji to the `participants` folder, ideally the file is named `<your first name>.md`
- open a pull request in the original repository and add someone else in the group to review your pull request
- review someone else's pull request, give feedback and approve if correct

2.5. Release

- releases should be from `main` branch
- good practice is to open a pull request for `develop` into `main` when you are done with the desired features

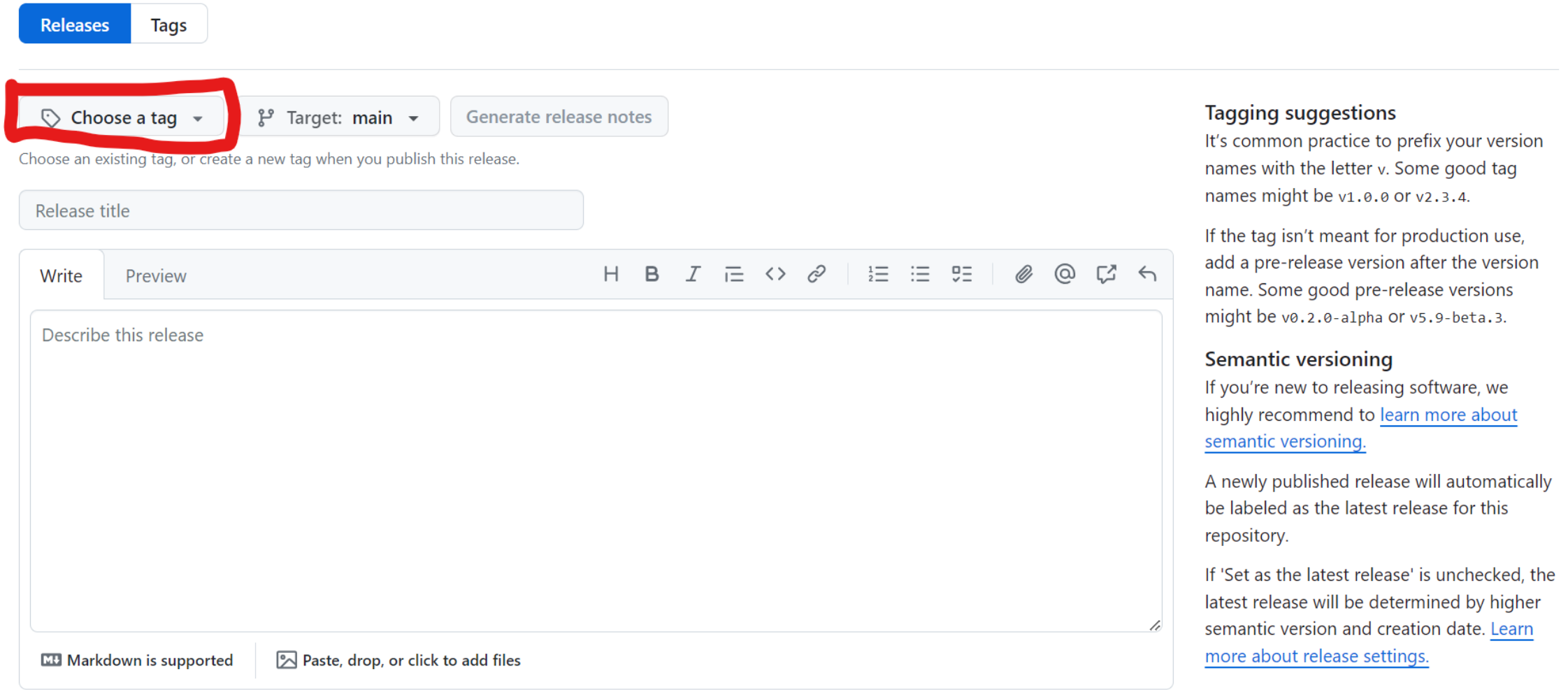
2.5. Release

- whenever you are ready for a new release, `create a new release`



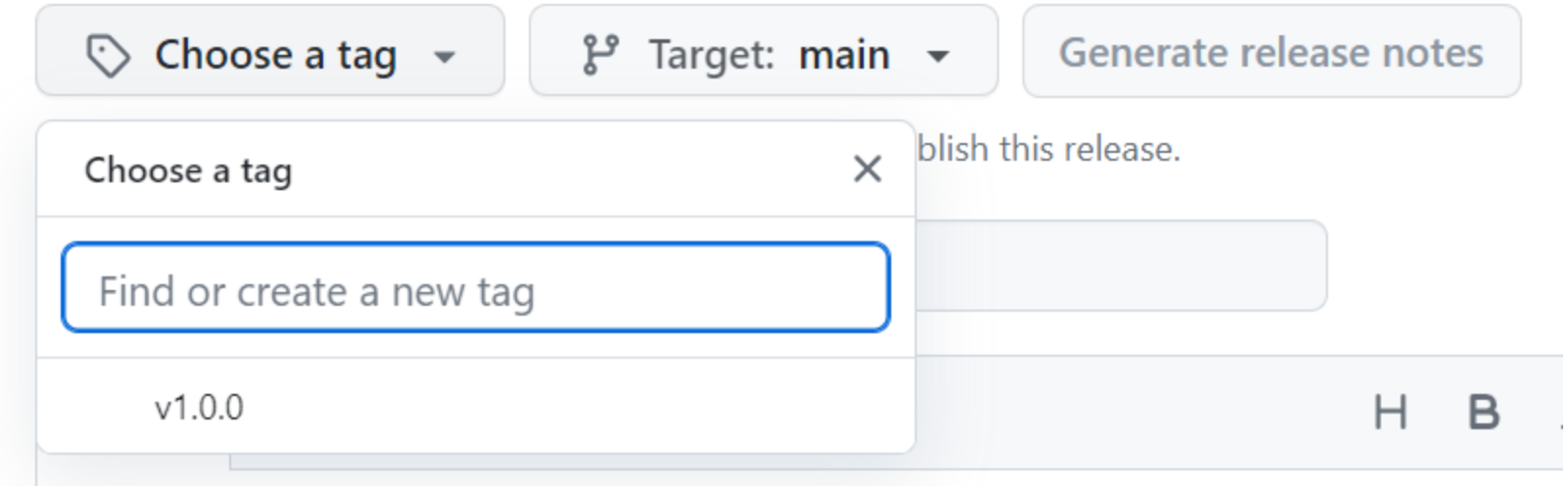
2.5. Release

- add a title and a description for your release and `Choose a tag`



2.5. Release

- ideally, you choose a tag according to semantic versioning

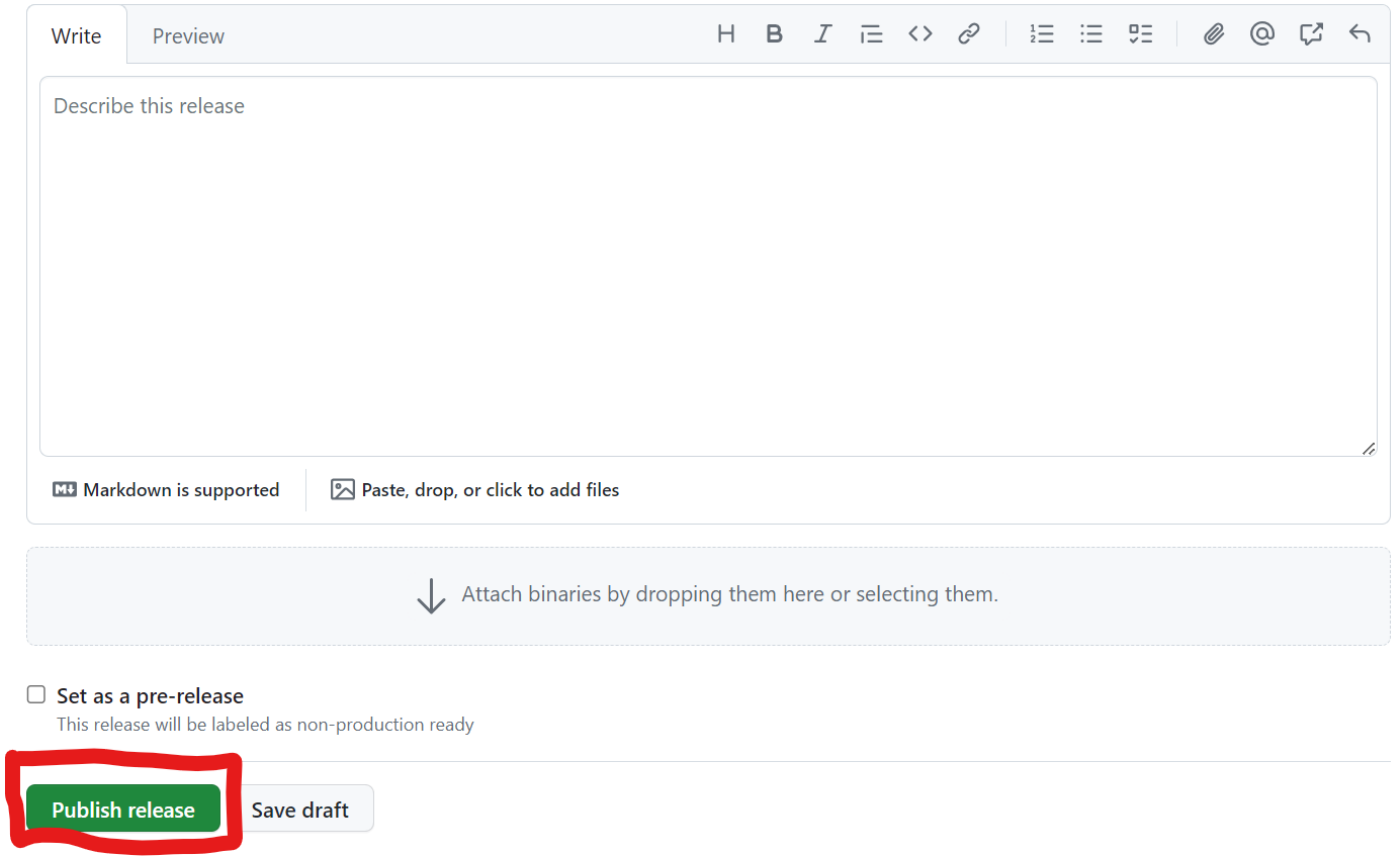


2.5.1. Semantic versioning

- version tag should be **MAJOR.MINOR.PATCH**
- you increment one of the three depending on the change
    - **MAJOR**: version when you make incompatible API changes
    - **MINOR**: version when you add functionality in a backward compatible manner
    - **PATCH**: version when you make backward compatible bug fixes

2.5. Release

- when you are satisfied with your release, `Publish release`



2.6. Licensing

- let's discuss

I need to work in a community.

Use the **license preferred by the community** you're contributing to or depending on. Your project will fit right in.

If you have a dependency that doesn't have a license, ask its maintainers to **add a license**.

I want it simple and permissive.

The **MIT License** is short and to the point. It lets people do almost anything they want with your project, like making and distributing closed source versions.

Babel, **.NET**, and **Rails** use the MIT License.

I care about sharing improvements.

The **GNU GPLv3** also lets people do almost anything they want with your project, *except* distributing closed source versions.

Ansible, **Bash**, and **GIMP** use the GNU GPLv3.

2.7. Resources

- About Git
- Gitflow workflow
- GitHub Actions
- Semantic versioning
- Licensing

3. Nextflow

3.1. Short introduction

- workflow manager that enables scalable and reproducible scientific workflows using software containers
- an extension of groovy which is object-oriented programming language for the Java platform
- can be used with an array of executors, such as SLURM, k8s, AWS, Azure, Google Cloud and many more
- **nf-core**: project/community that develops framework for nextflow including guidelines, tools, modules, subworkflows, pipelines and test data

3.2. Requirements

- POSIX compatible system (e.g. Linux, Os X)
- Bash
- Java ≥ 11 / ≤ 21
- Docker/Singularity

3.3. Installation

```
$ curl -s https://get.nextflow.io | bash
$ chmod +x nextflow
```

or

```
$ wget -O nextflow https://github.com/nextflow-io/nextflow/releases/download/v23.10.1/nextflow-23.10.1-all
```

or via browser at https://github.com/nextflow-io/nextflow/releases

3.4. Best pratice: nf-core template

```
workflow_repo
├── LICENSE
├── README.md
├── assets
│   ├── mock.genome.fasta
│   ├── samplesheet.csv
│   └── schema_input.json
├── bin
│   └── script.py
├── conf
│   ├── base.config
│   ├── modules.config
│   └── test_stub.config
├── lib
│   ├── NfcoreSchema.groovy
│   ├── NfcoreTemplate.groovy
│   ├── WorkflowMain.groovy
│   └── nfcore_external_java_deps.jar
├── main.nf
├── modules
│   ├── local
│   │   ├── module_1.nf
│   │   └── module_2.nf
│   └── nf-core
│       ├── module_1
│       │   └── arg_1
│       │       ├── main.nf
│       │       └── meta.yml
│       └── custom
│           └── dumpsoftwareversions
│               ├── main.nf
│               ├── meta.yml
│               └── templates
│                   └── dumpsoftwareversions.py
├── modules.json
├── nextflow.config
├── nextflow_schema.json
└── workflows
    └── main.nf
```

3.6 Resources

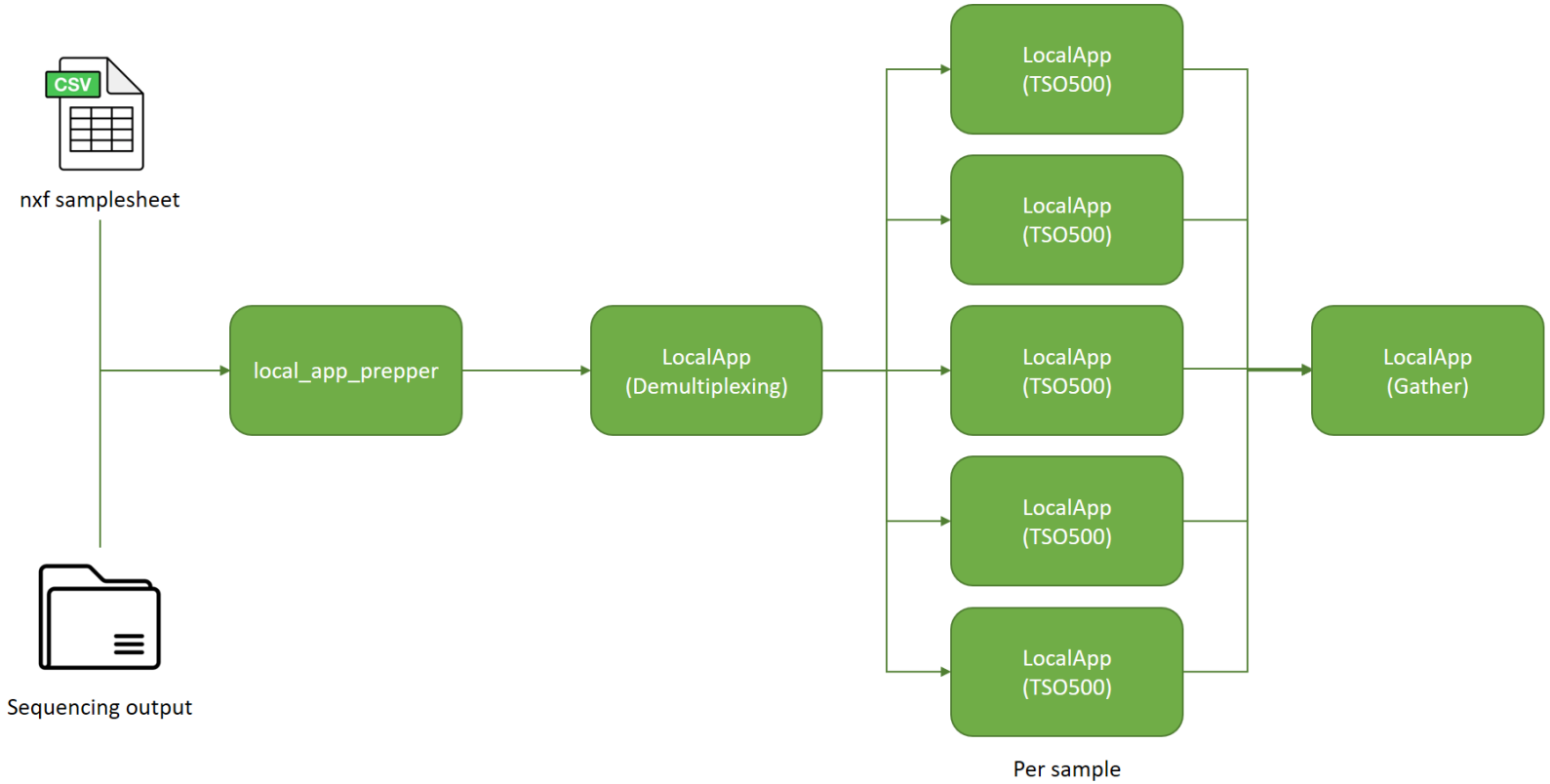
- nextflow.io
- nf-co.re
- nf-core github

4. `tso500_nxf_workflow`

4.1. Status update

- modified nf-core template (removed unnecessary functionality, config and metadata files)
- added devcontainer to have controlled environment (dind and sind available)
- stubbing data available
- containing three modules so far (`localapp_prepper` , `LocalApp` , `dumpsoftwareversions`)
- using nf-validation plugin

4.2. Overview


CSV
nxf samplesheet
Sequencing output
local_app_prepper
LocalApp
(Demultiplexing)
LocalApp
(TSO500)
LocalApp
(TSO500)
LocalApp
(TSO500)
LocalApp
(TSO500)
LocalApp
(TSO500)
Per sample
LocalApp
(Gather)

4.3. Demonstration

4.4. Outlook

- `samplesheet_generator`
- `tsoppi` (requires some restructuring)
- `PRONTO`
- include configuration files for each node
- Documentation

4.5. Resources

- repository
- local_app_prepper
- samplesheet_generator

5. Python project

5.1. Repository structure

- consistency/standard
- keep main script short and sweet - functionality in modules

```
#!/usr/local/bin/python

from my_module import main

if __name__ == "__main__":
    main()
```

5.1. Repository structure

- module folder should contain `__init__.py`
- keep functions short and try to refactor big functions
- leave descriptive comments in code
- use libraries to make your life easier
    - `pandas`: csv/tsv files
    - `click` or `argparse`: define cli input flags
- introduce proper exception handling
- logging with log levels

5.1.1. Unit testing

- `pytest` for testing
- include unit tests for functions, preferable table-driven

```
def addition(x, y):
  return x+y
```

```
import pytest

@pytest.mark.parametrize("x, y, z", [(1, 1, 2), (1, -1, 0)])
def test_eval(x, y, z):
    assert addition(x, y) == z
```

```
$ pytest
```

5.1. Repository structure

- include test data for unit testing if necessary
- create container image from project, preferably docker
- include all necessary dependencies in `requirements.txt` (locked versions)
- add GitHub actions for testing, linting, building, etc.
- preferable include a devcontainer definition
- `README.md` and other `docs`

5.1. Repository structure

```
/repo
|-- .devcontainer
|   `-- devcontainer.json
|-- .github
|   `-- workflows
|       `-- main.yml
|-- .gitignore
|-- Dockerfile
|-- docs
|-- LICENSE
|-- README.md
|-- my_tool.py
|-- my_module
|   |-- __init__.py
|   |-- my_module.py
|   `-- tests
|       |-- __init__.py
|       `-- my_module_test.py
|-- requirements.txt
`-- test
```

5.2. Resources

- pandas
- click
- argparse
- exception handling
- logging
- pytest unittesting
- inpred dockerhub
- devcontainers