Bioinformatics session

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

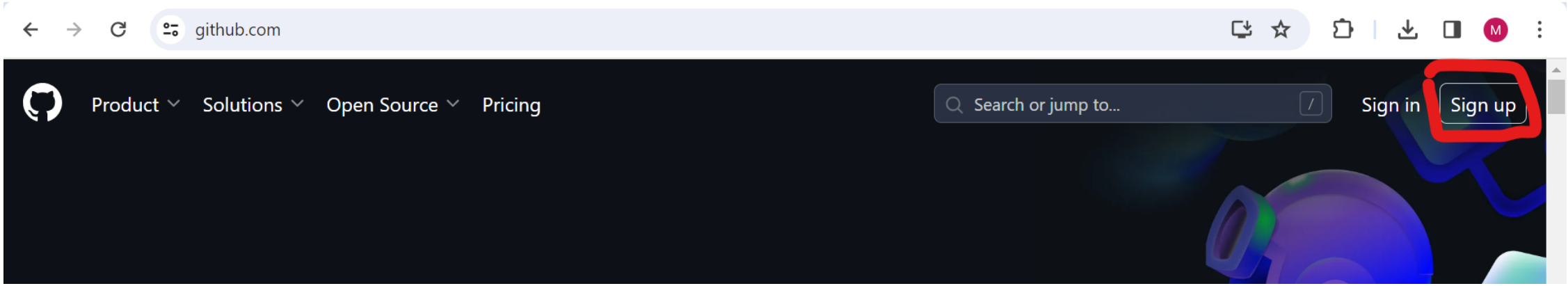
Overview

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

1. Setup

Create a GitHub account

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

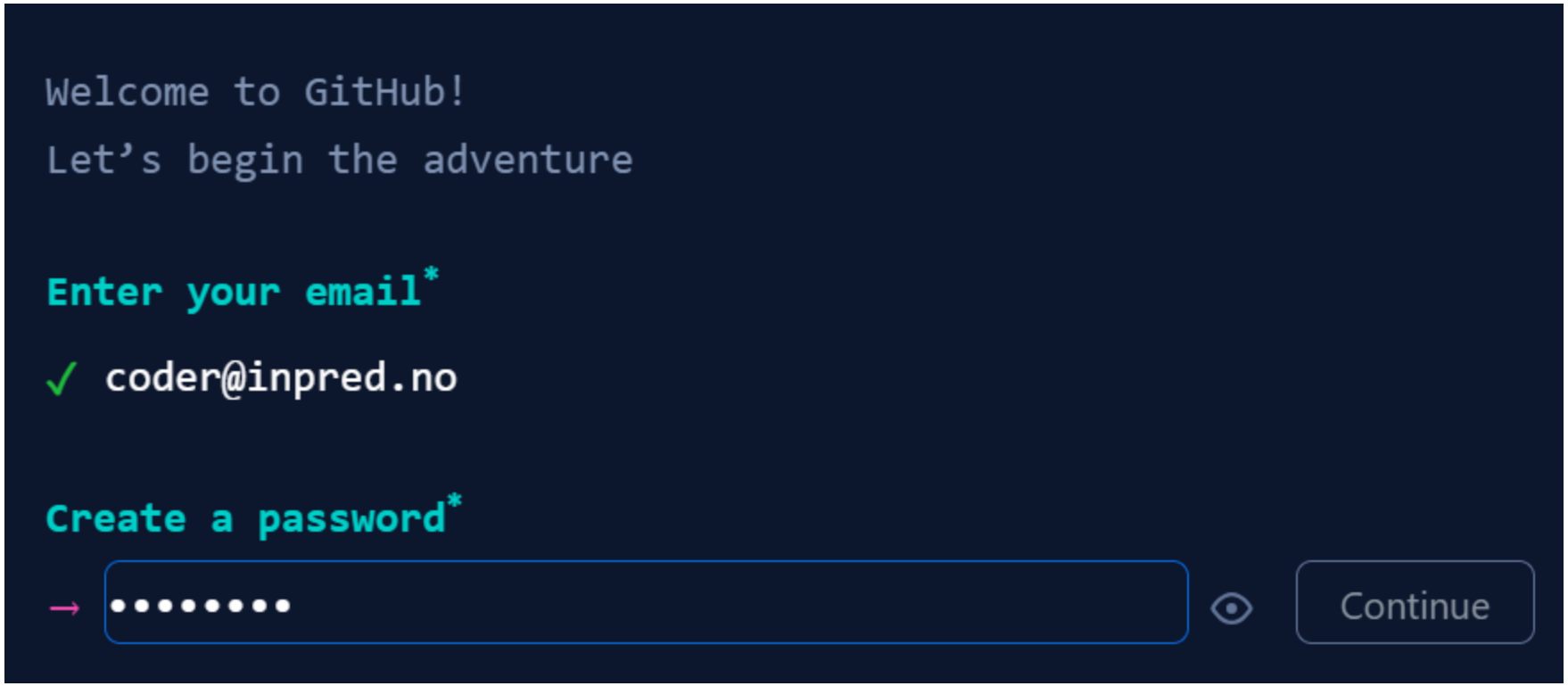


Create a GitHub account

- enter your email

Create a GitHub account

- set a password

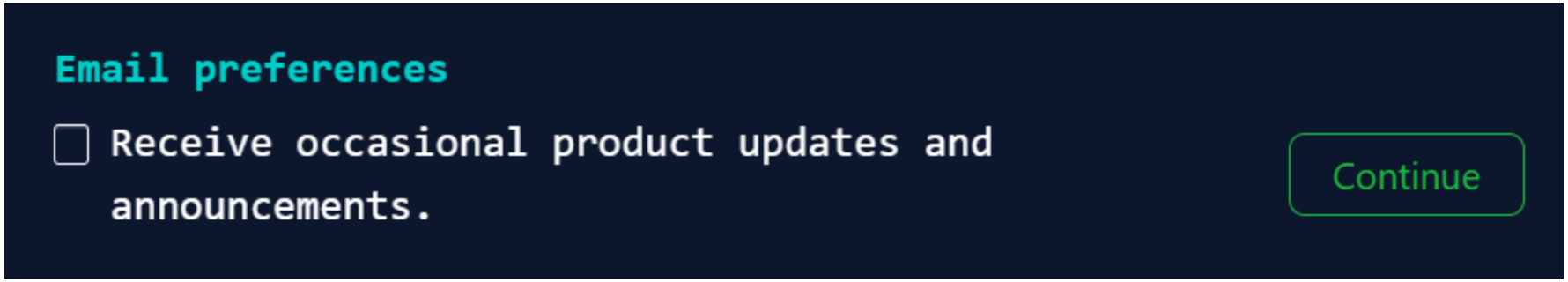


Create a GitHub account

- choose a username

Create a GitHub account

- choose email preferences

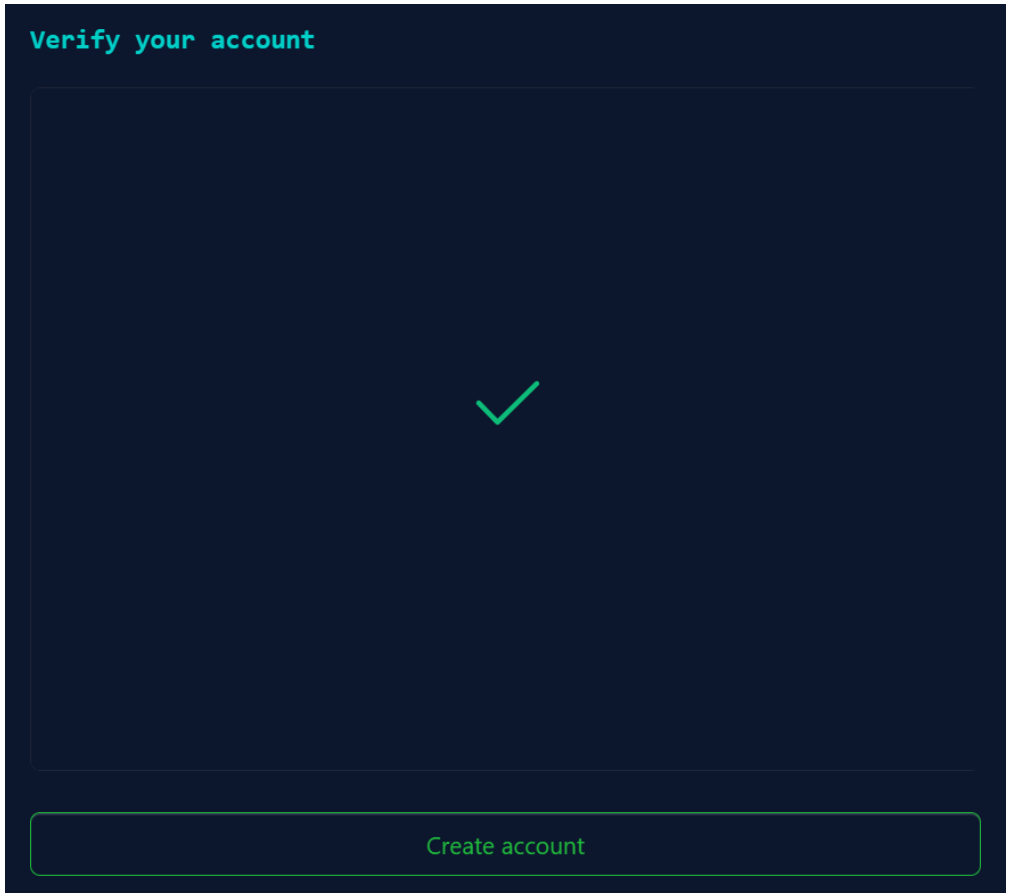


Create a GitHub account

- solve the puzzle

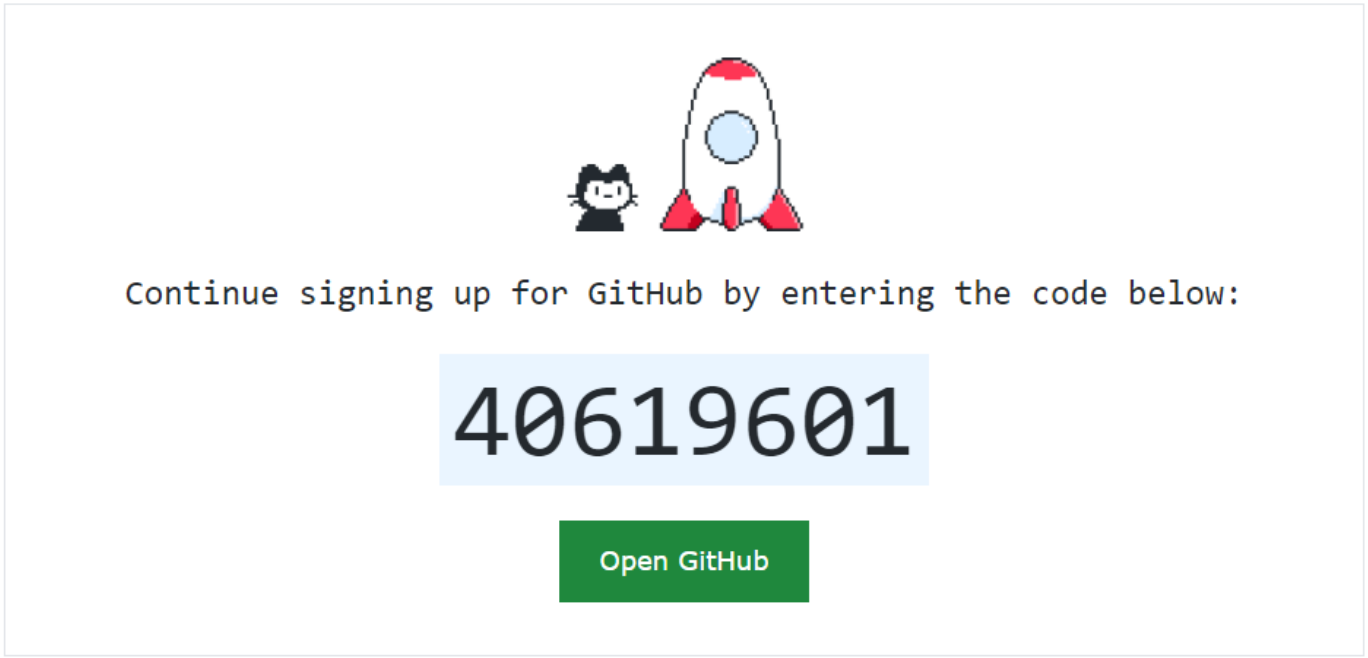
Create a GitHub account

- create your account



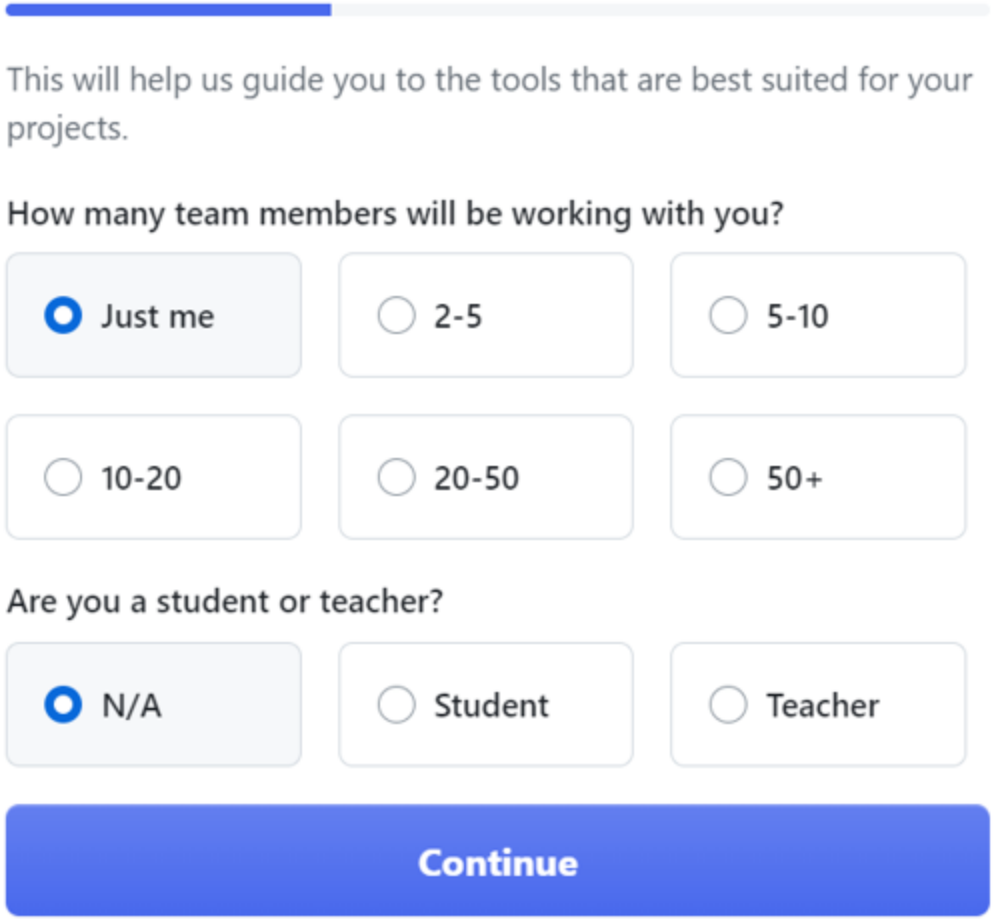
Create a GitHub account

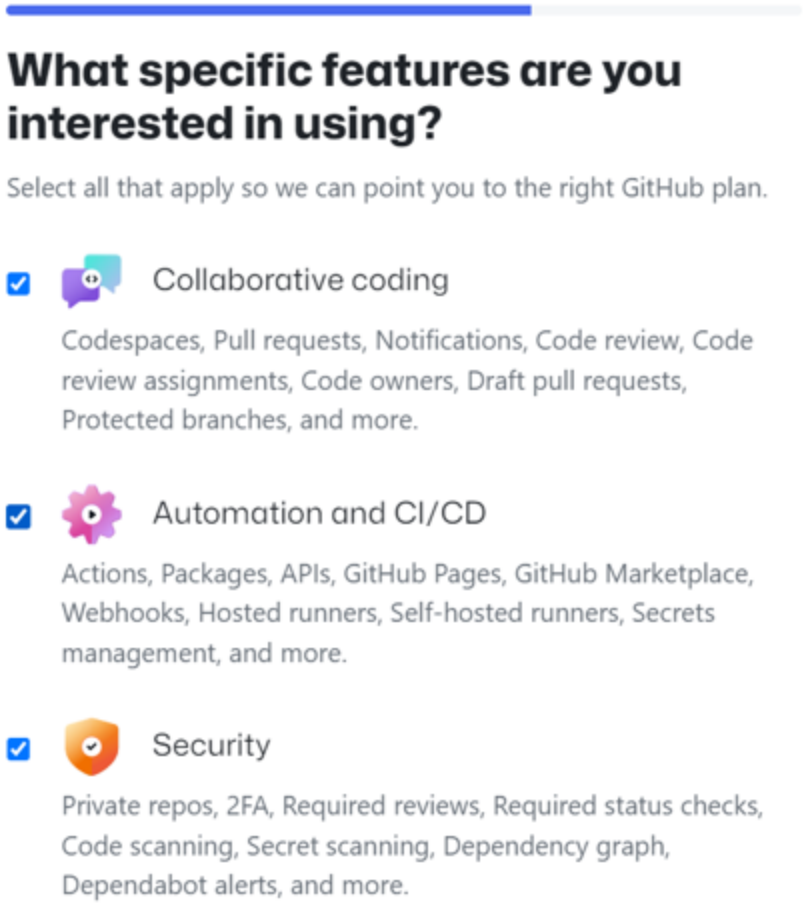
- find the activation code in the email you received



Create a GitHub account

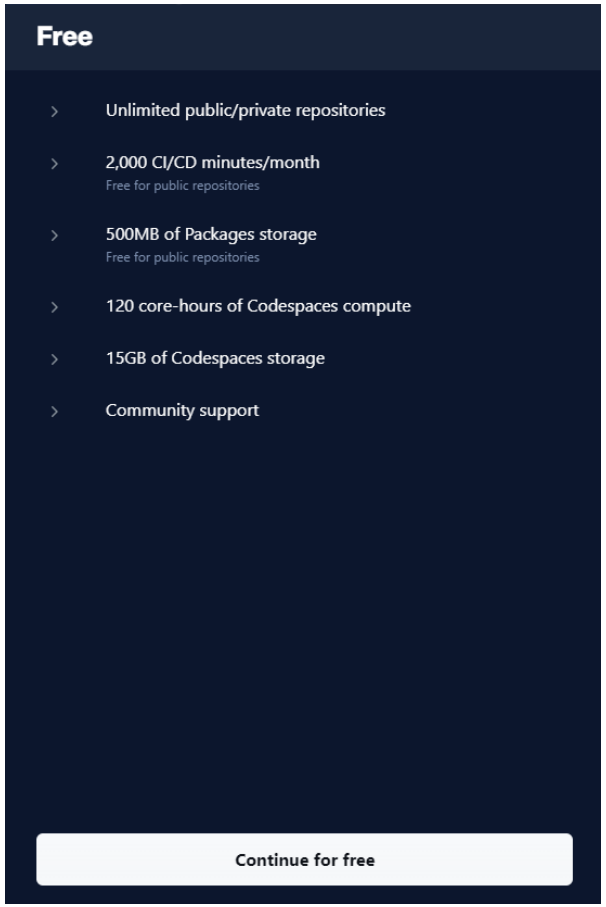
- select the desired options





Create a GitHub account

- 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 commited 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

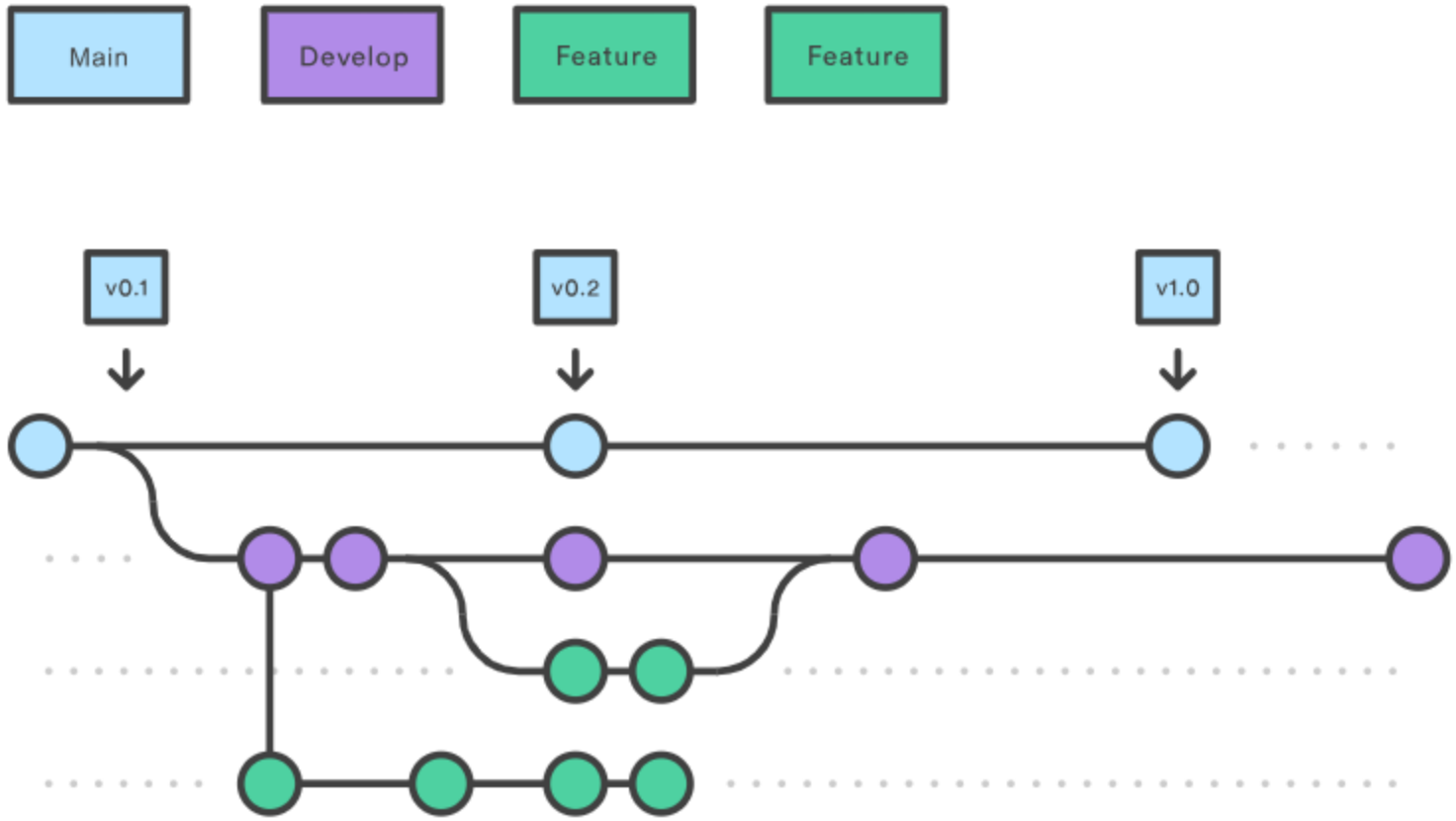
`git push` : upload changes to remote counterpart

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

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`

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

GitHub Actions

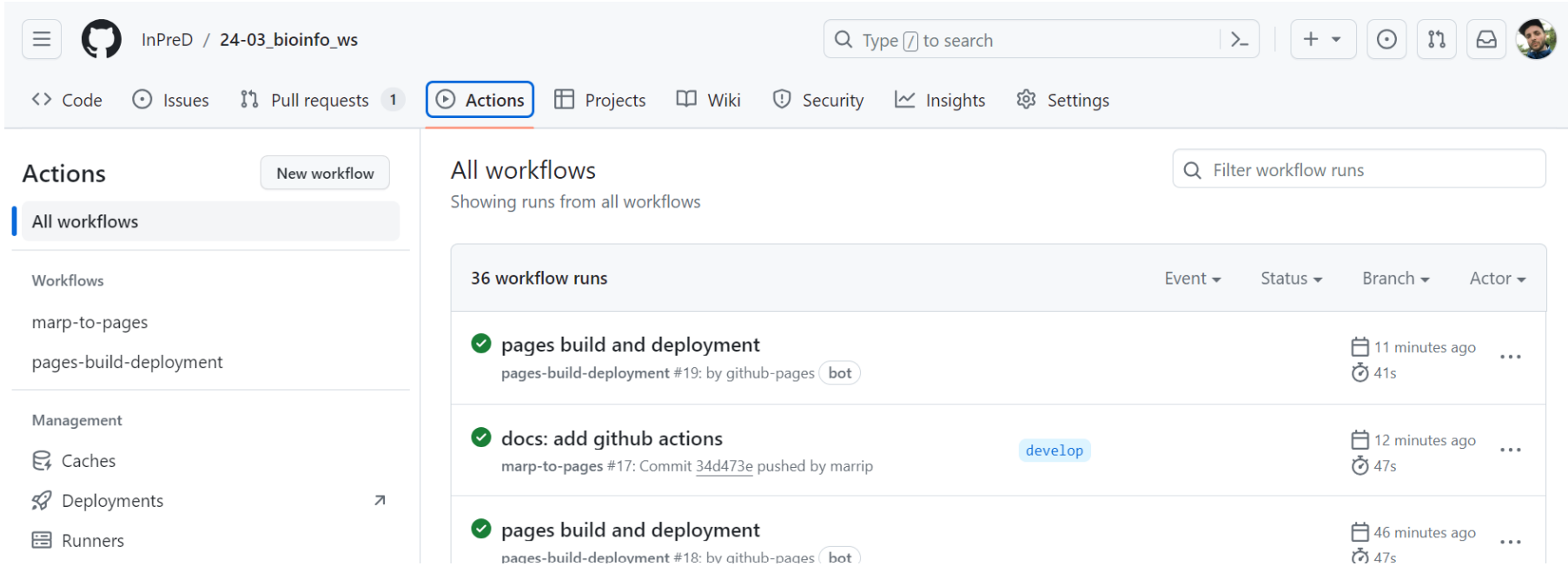
```yaml
name: Docker Build
on:
  push:
    branches:
      - main
      - develop
    tags:
      - '*.*.*'

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
  ...
```

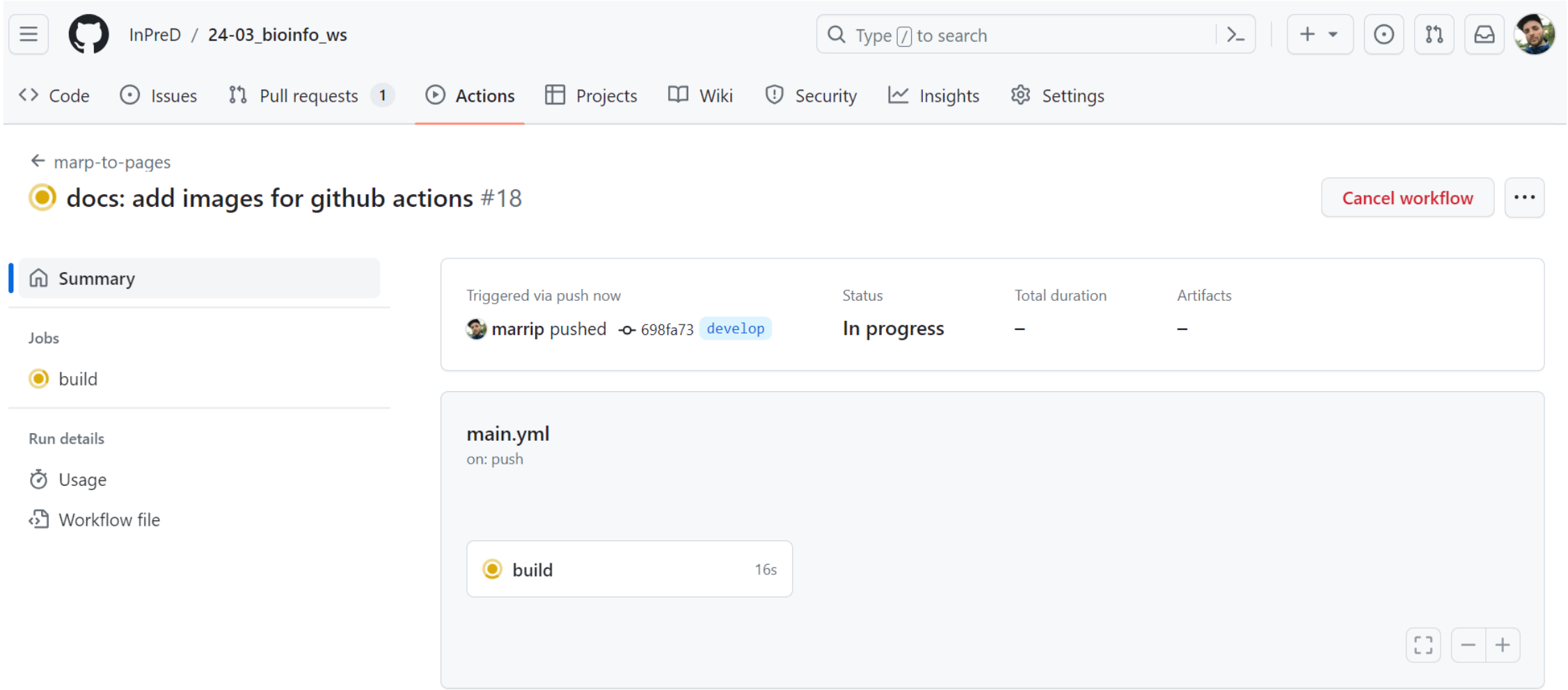
GitHub Actions

```
...
  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 }}
```

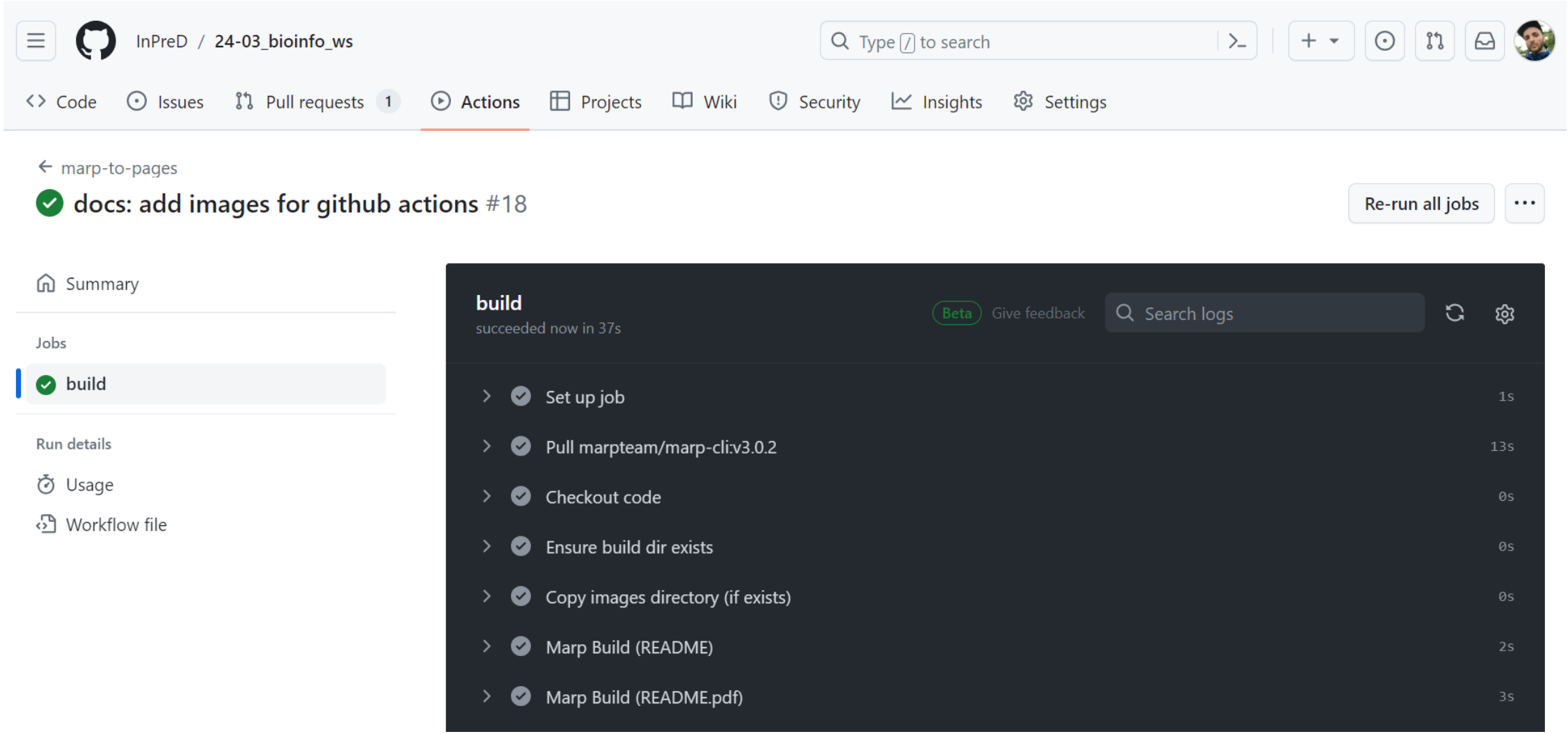
GitHub Actions



GitHub Actions



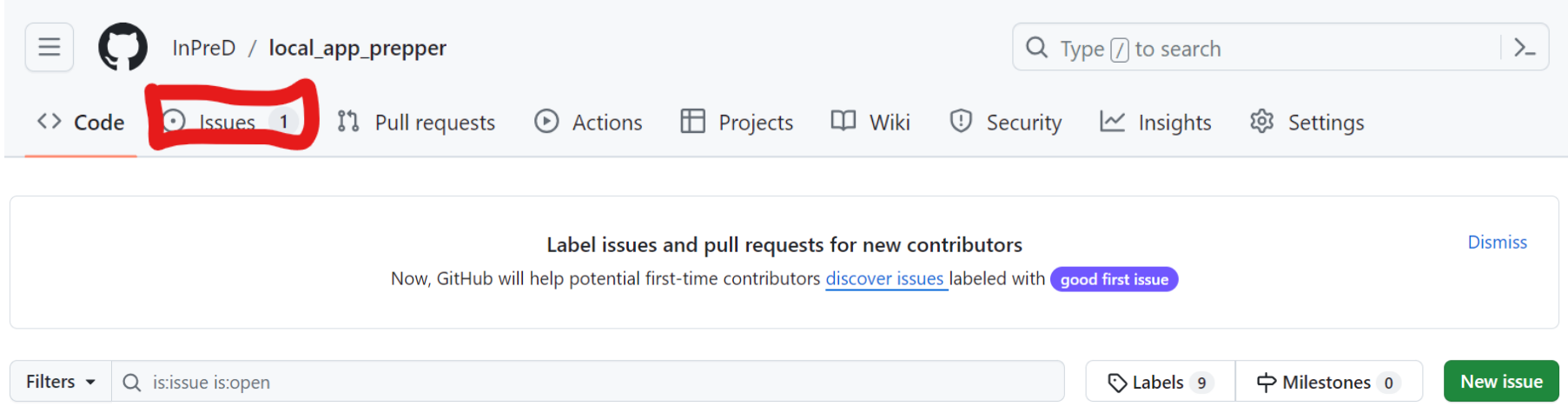
GitHub Actions



2. Development & Collaboration

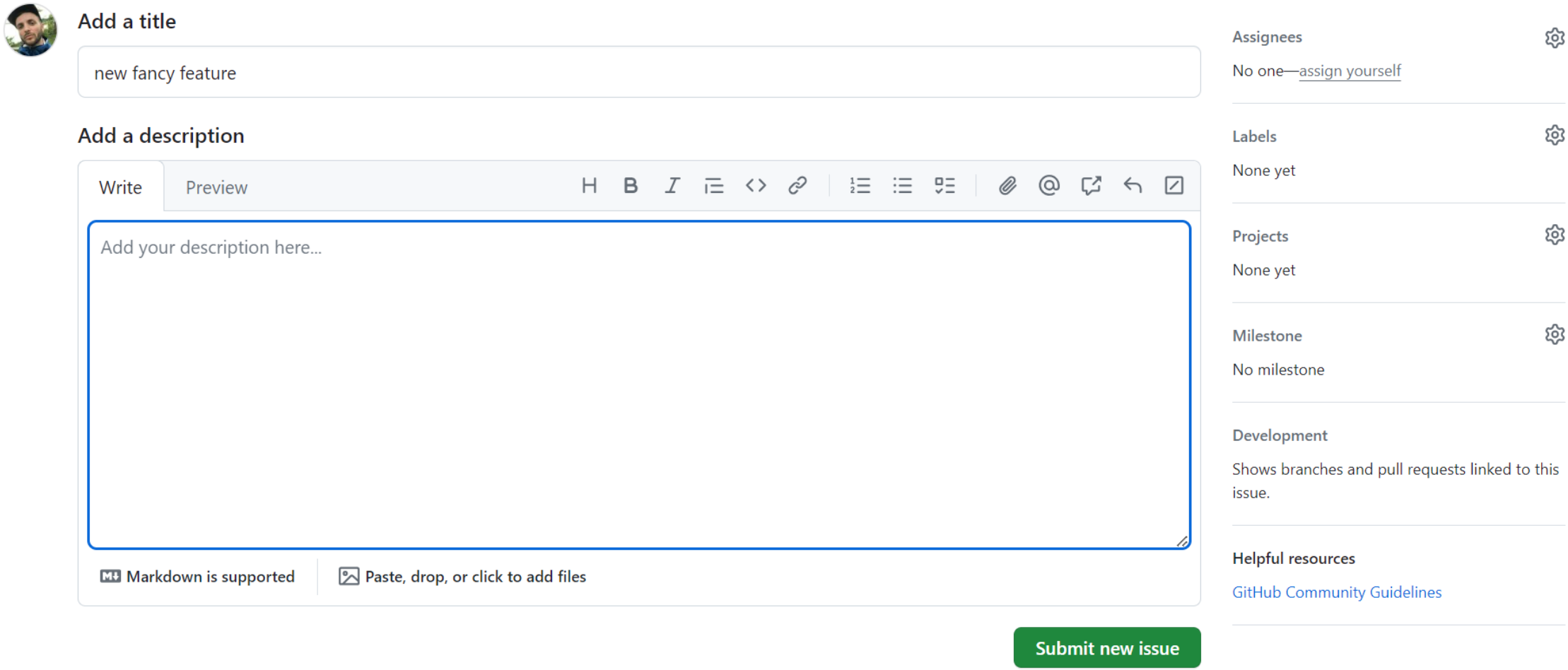
GitHub workflow

- go to issues and create a `New issue`



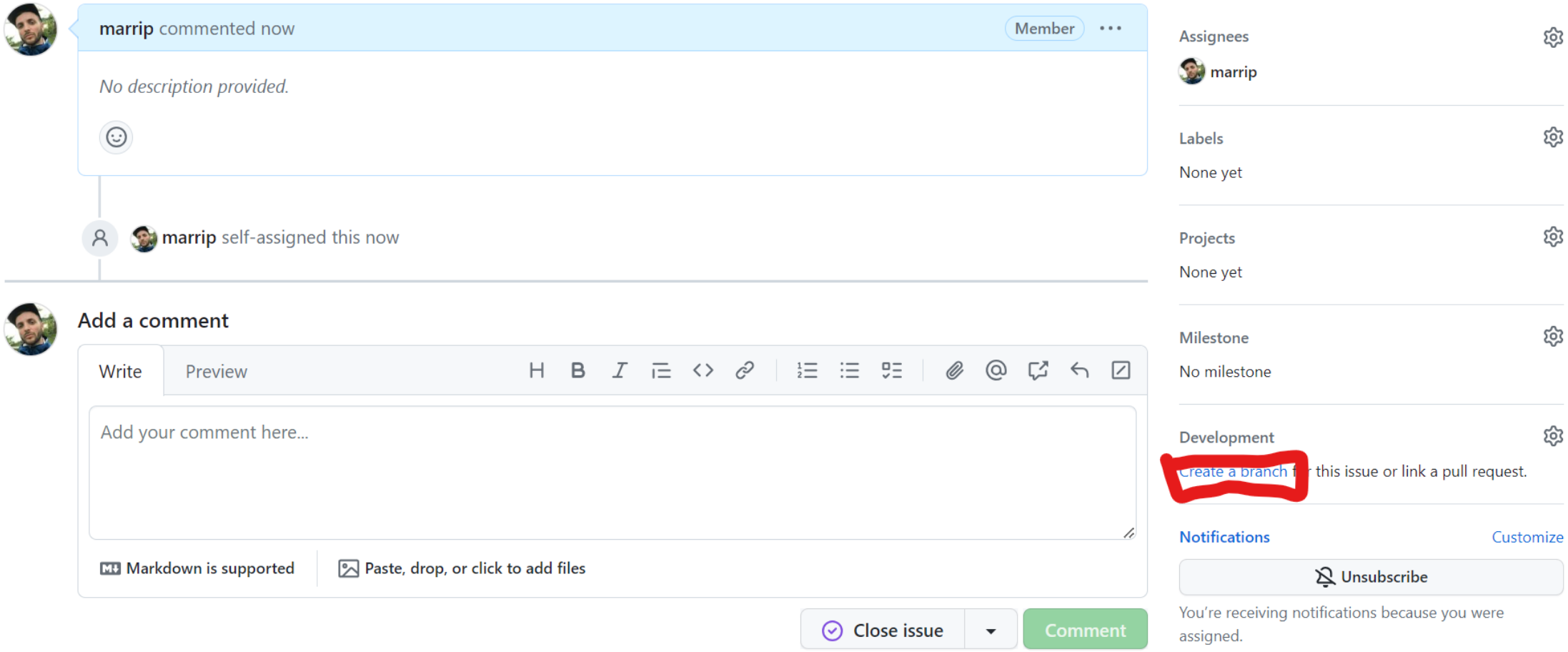
GitHub workflow

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



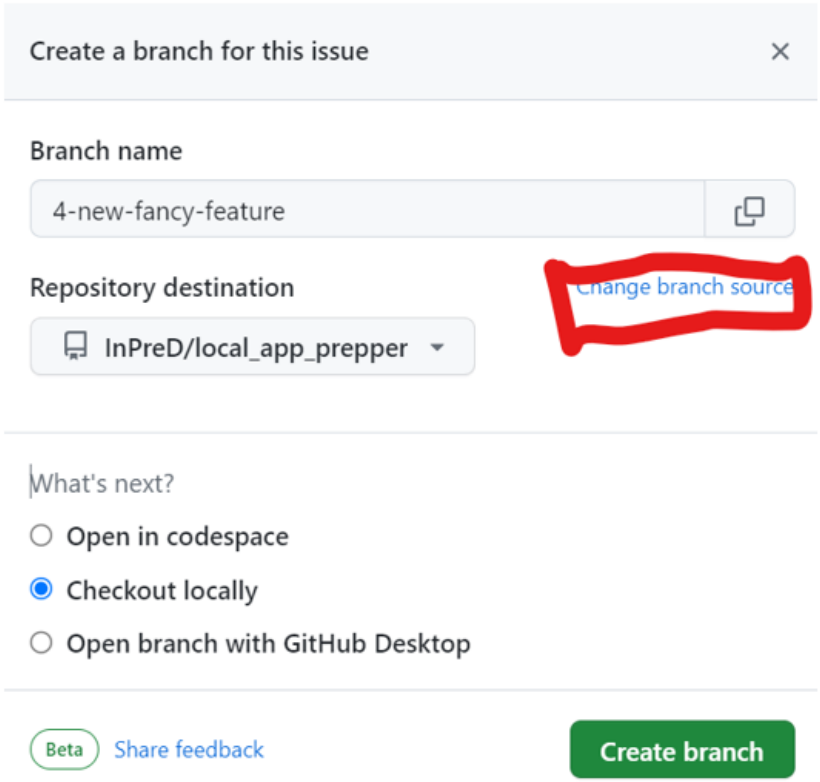
GitHub workflow

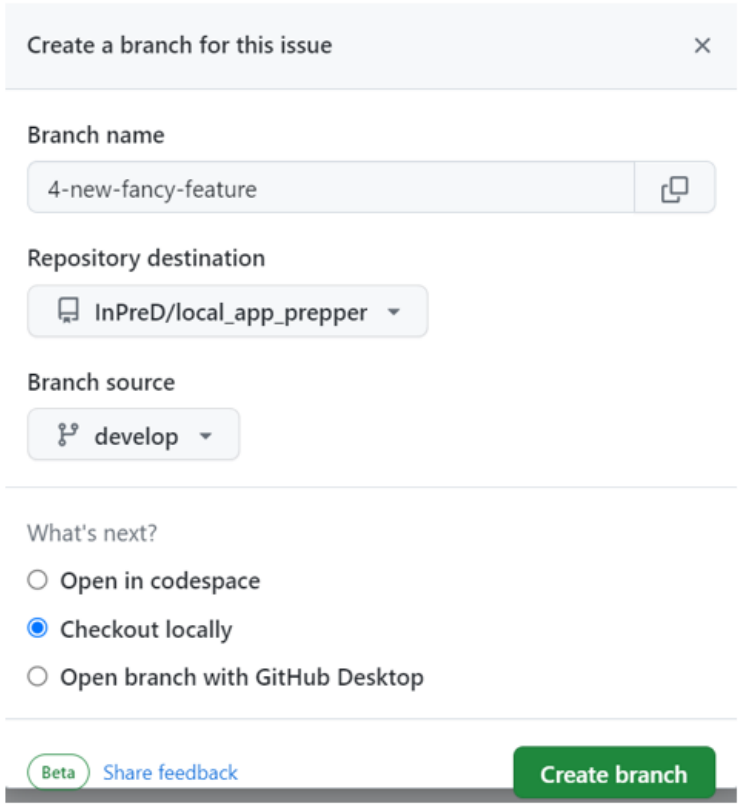
- if you decide to work on the issue (own repository), `Create a branch` via the issue



GitHub workflow

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





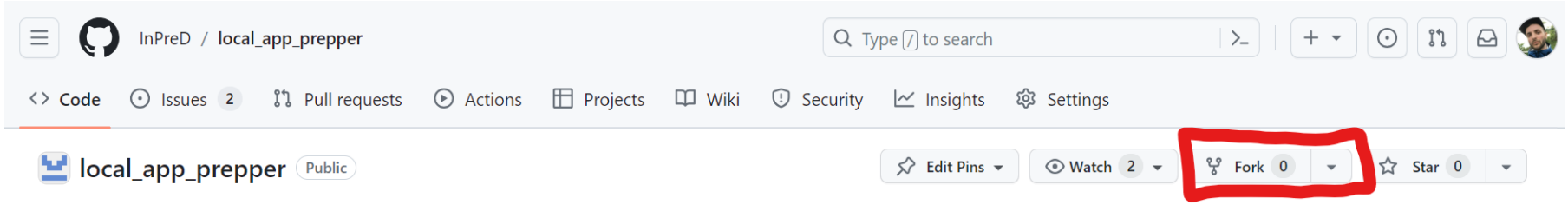
GitHub workflow

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

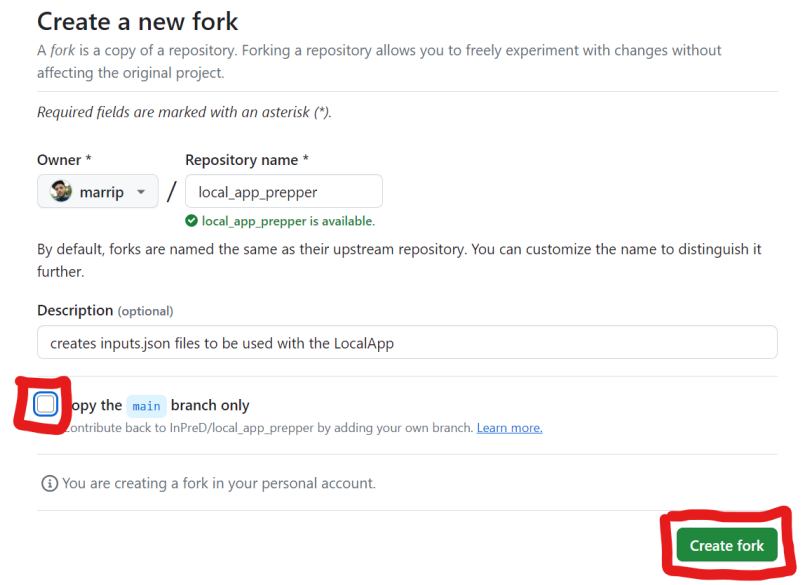
```
$ git pull
$ git checkout 4-new-fancy-feature
$ git add README.md
$ git commit -m "docs: updating docs"
$ git push
```

GitHub workflow

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



GitHub workflow

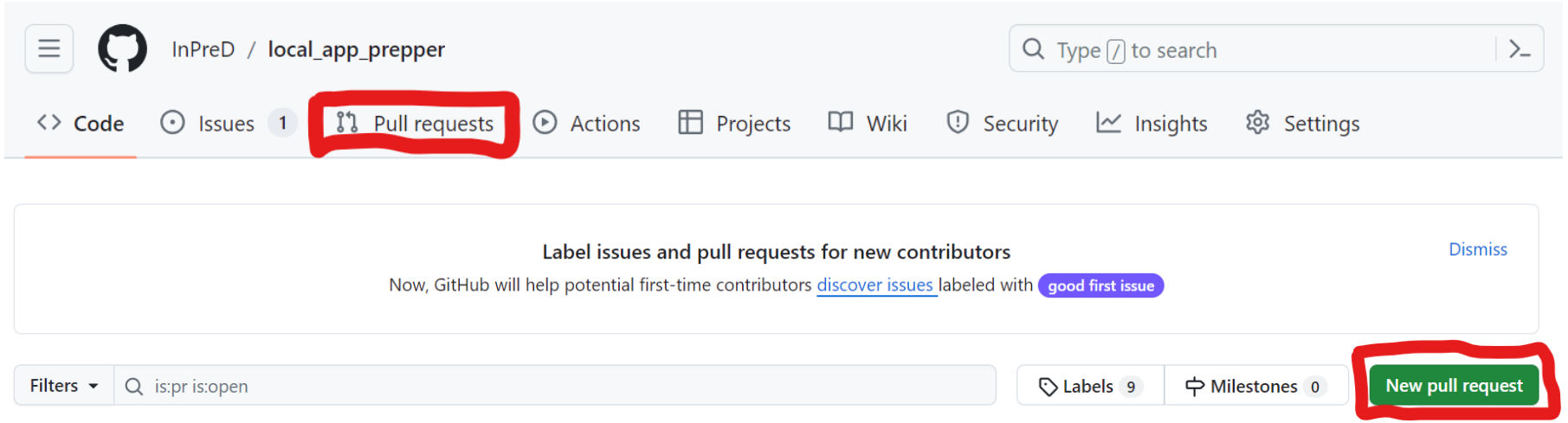


GitHub workflow

- 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

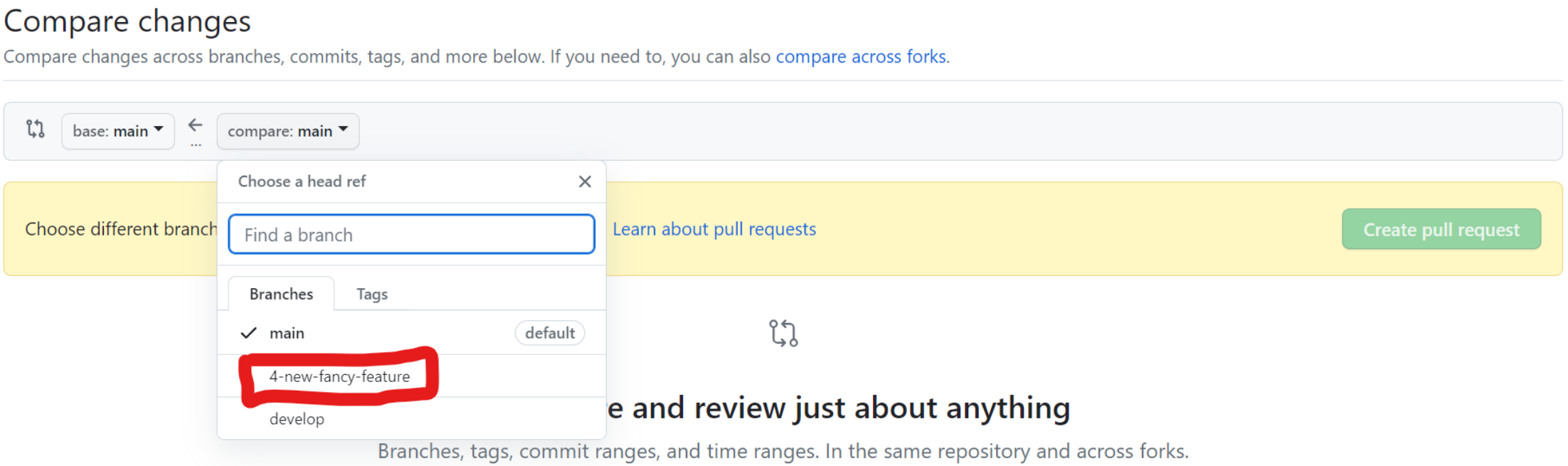
GitHub workflow

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



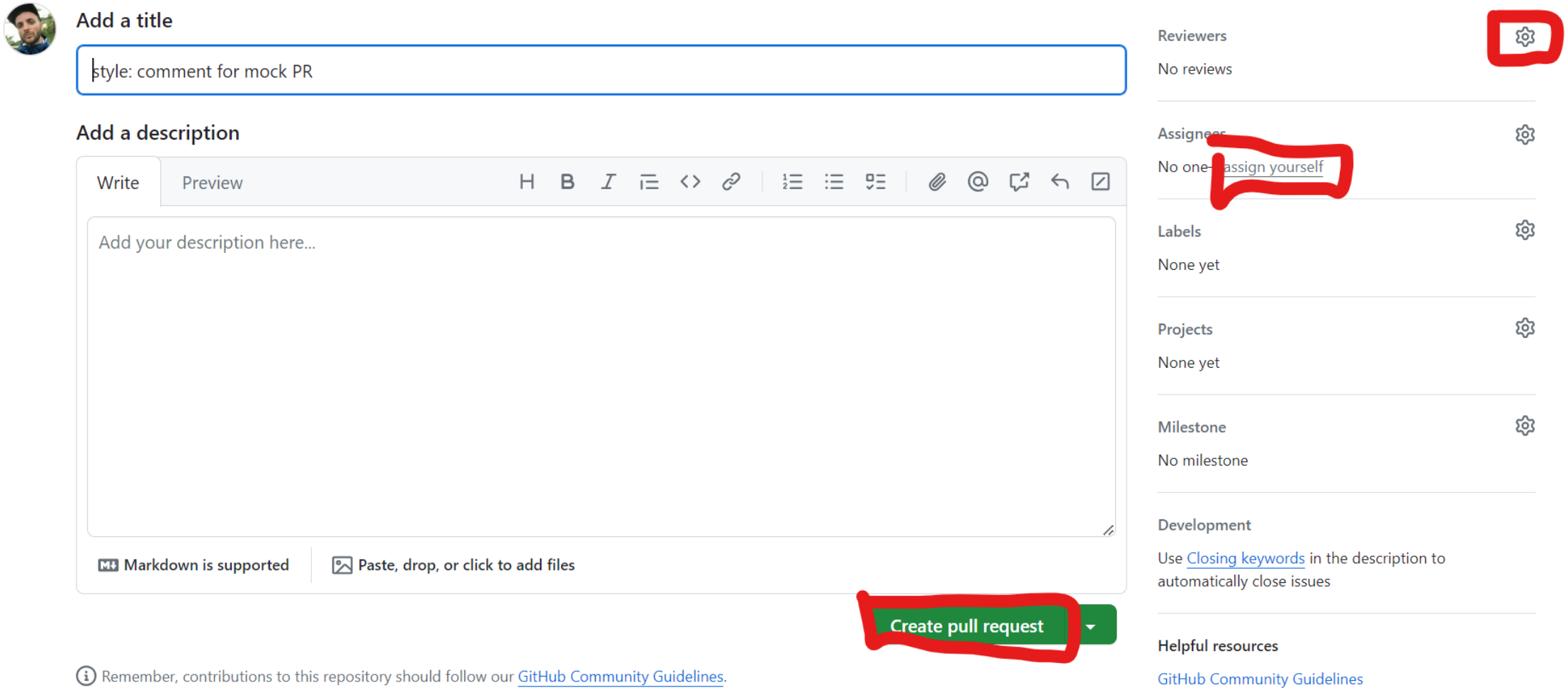
GitHub workflow

- choose `develop` as `base` and your new feature branch for `compare`



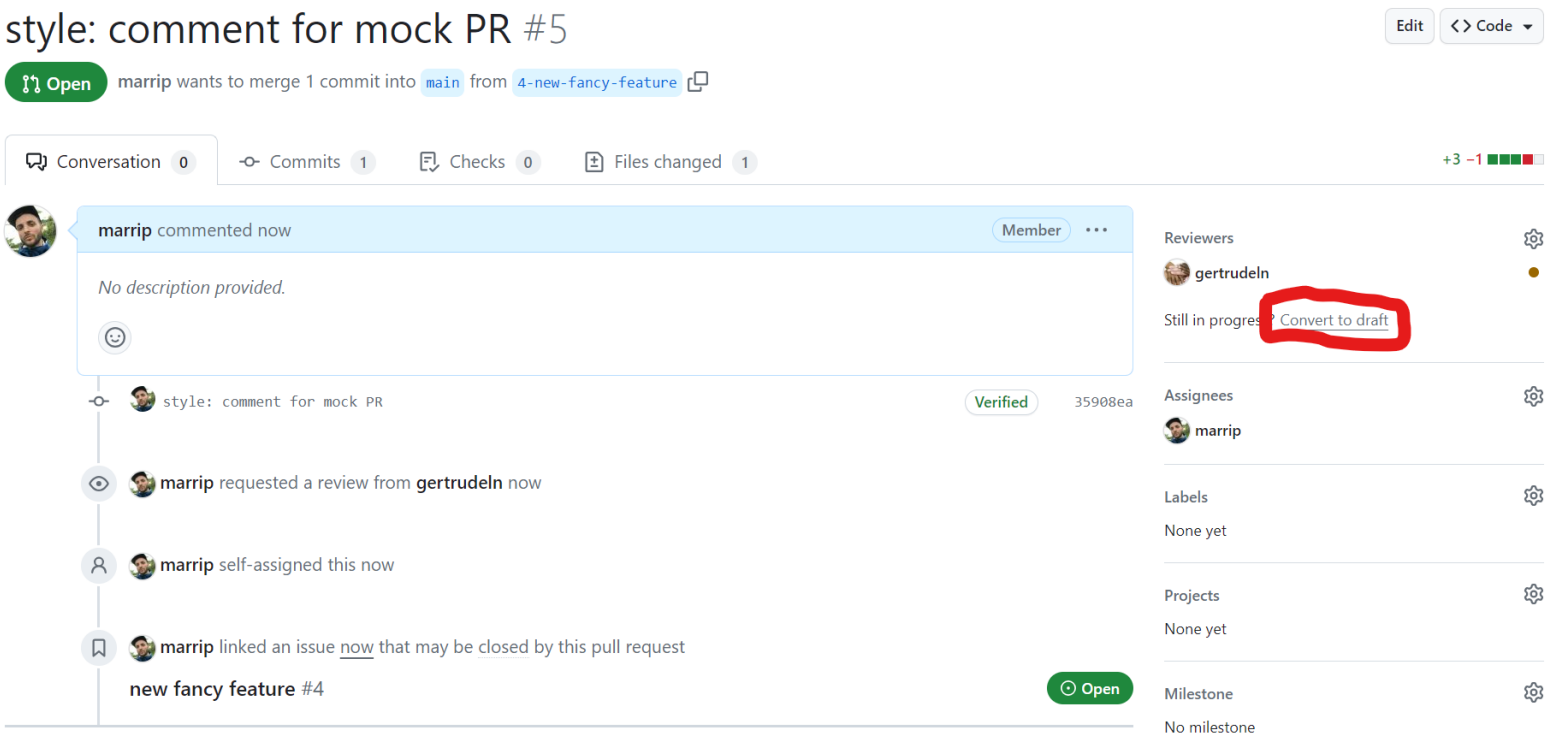
GitHub workflow

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



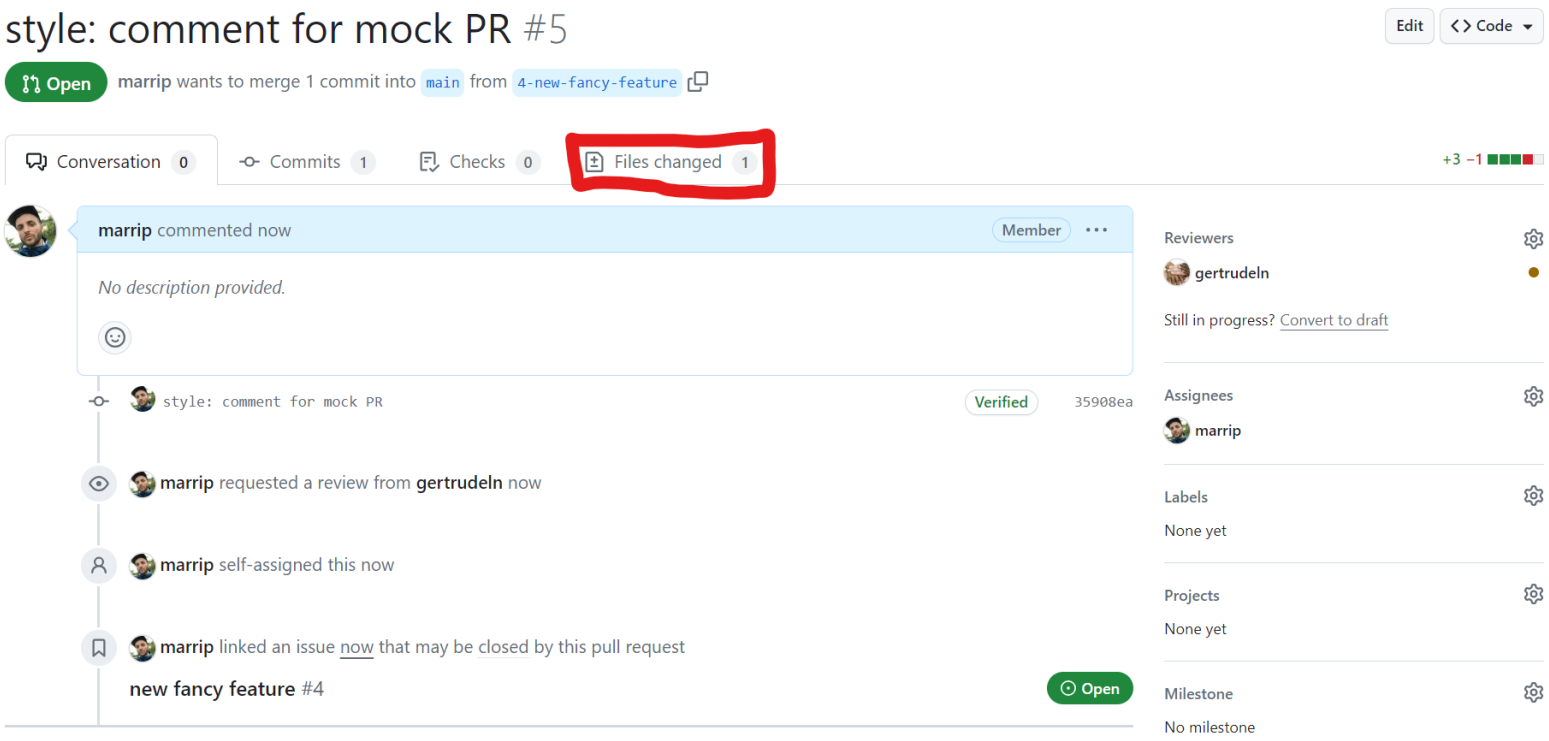
GitHub workflow

- 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



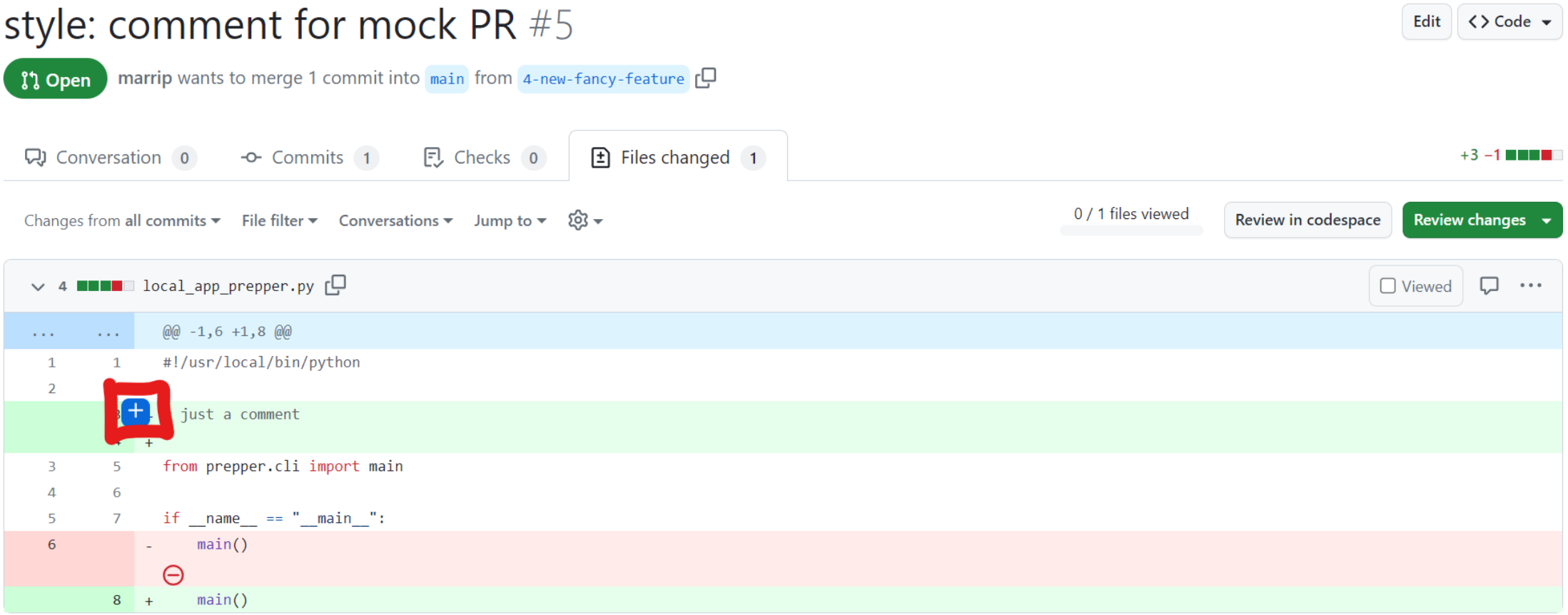
GitHub workflow

- 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



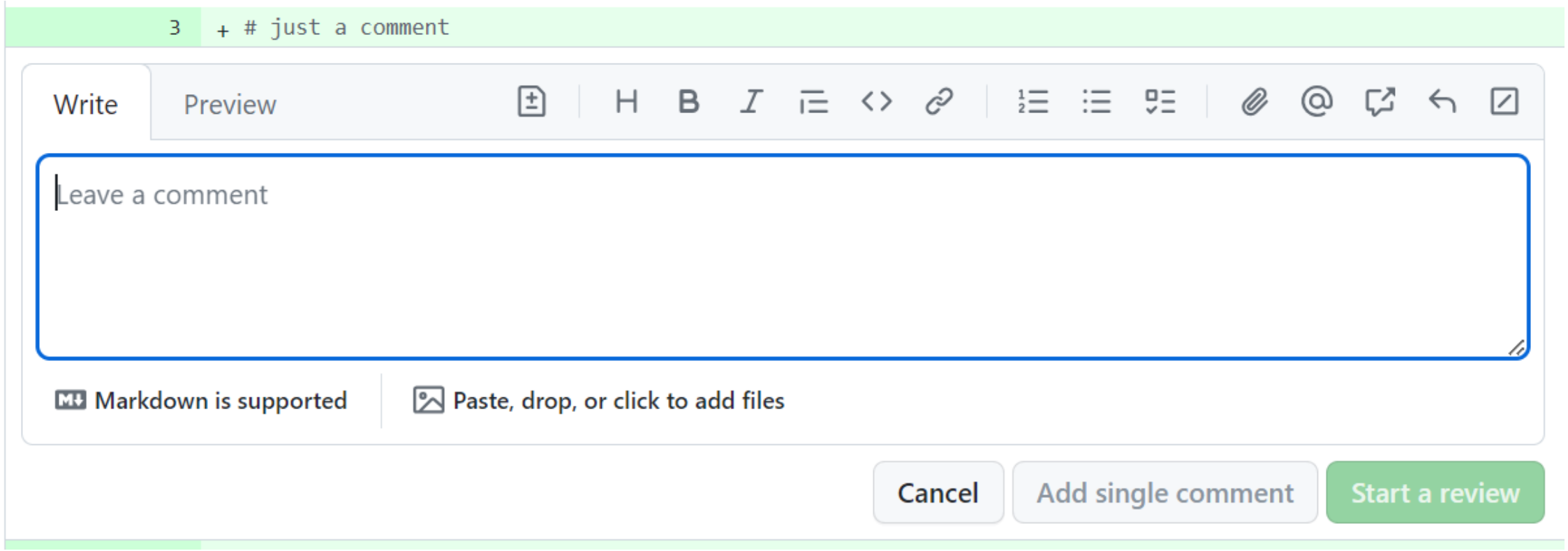
GitHub workflow

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



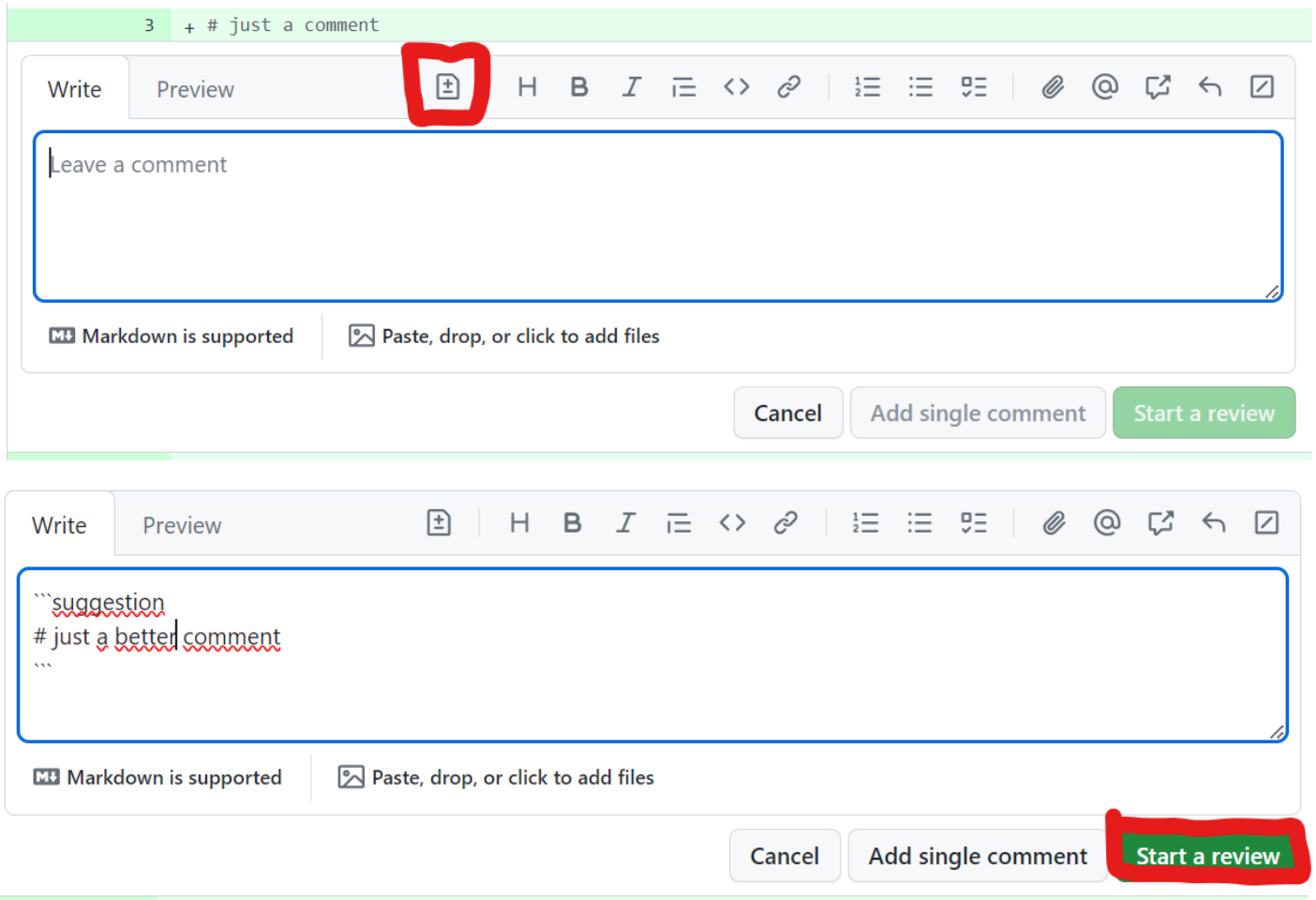
GitHub workflow

- you can type your comment



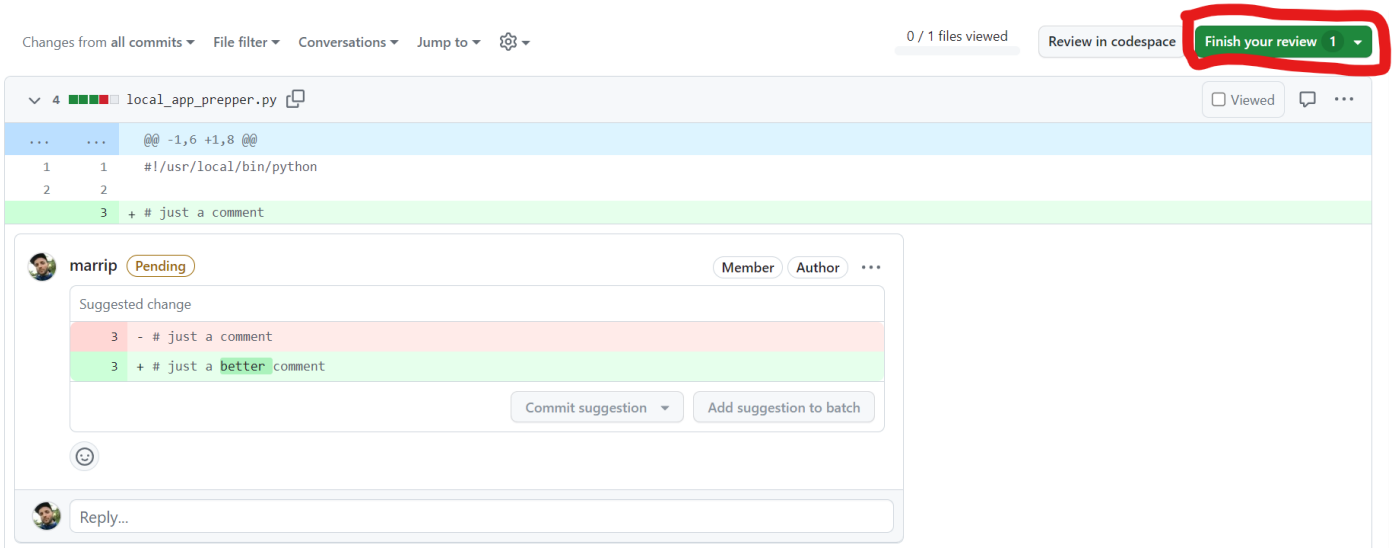
GitHub workflow

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



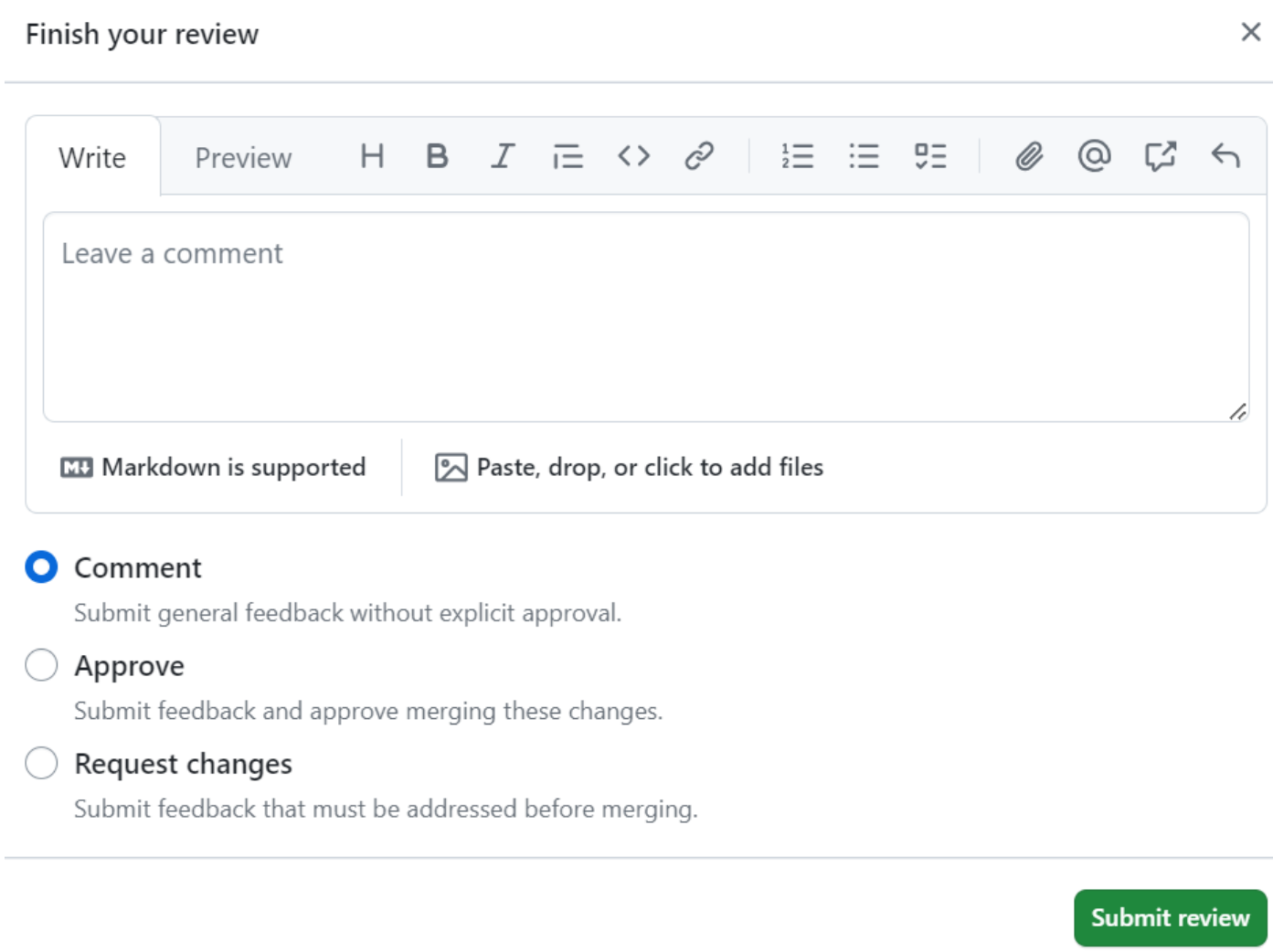
GitHub workflow

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



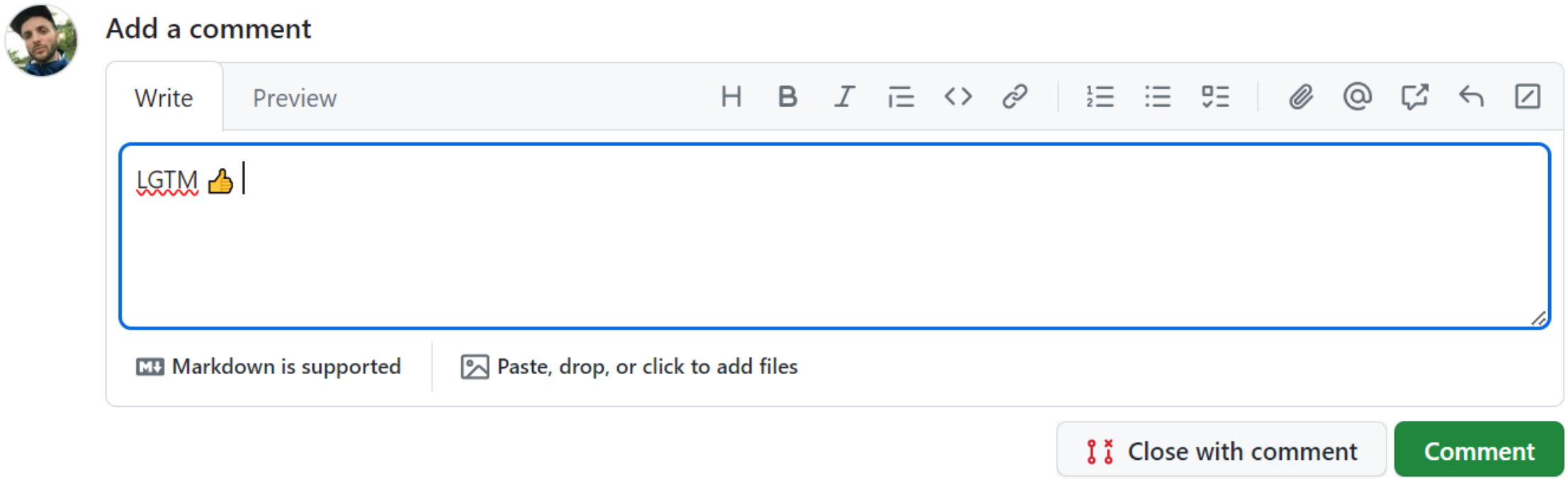
GitHub workflow

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



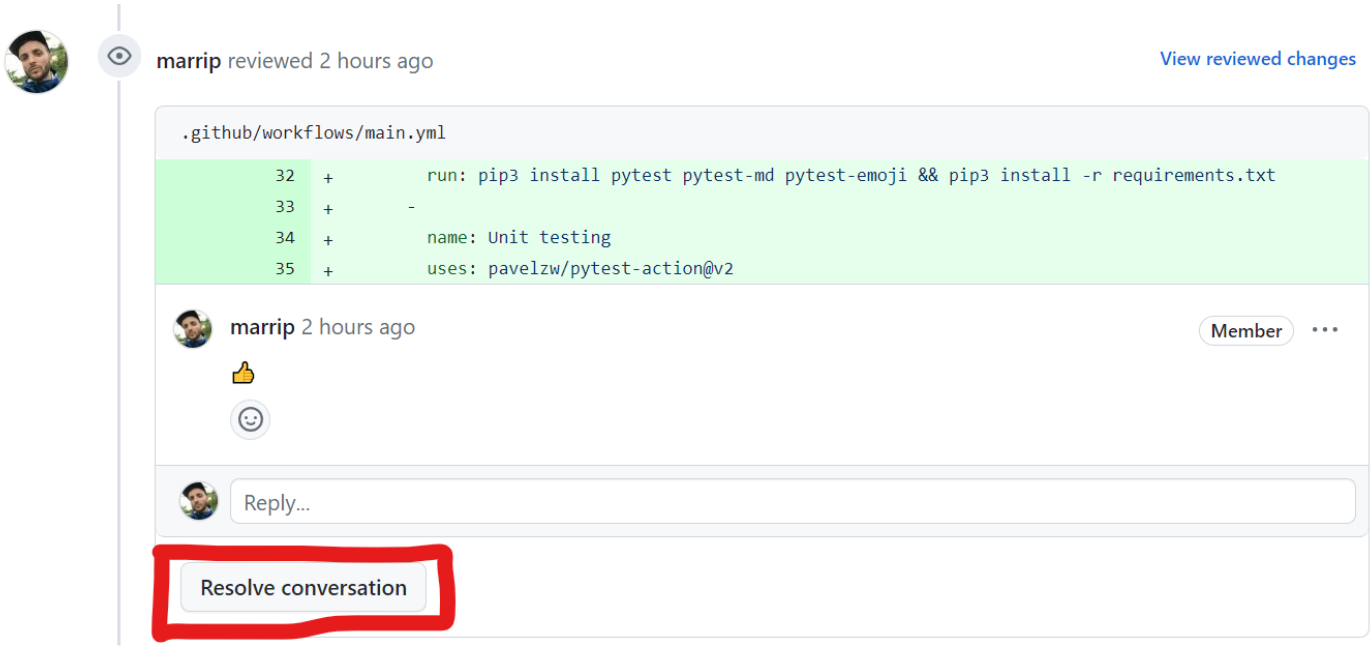
GitHub workflow

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



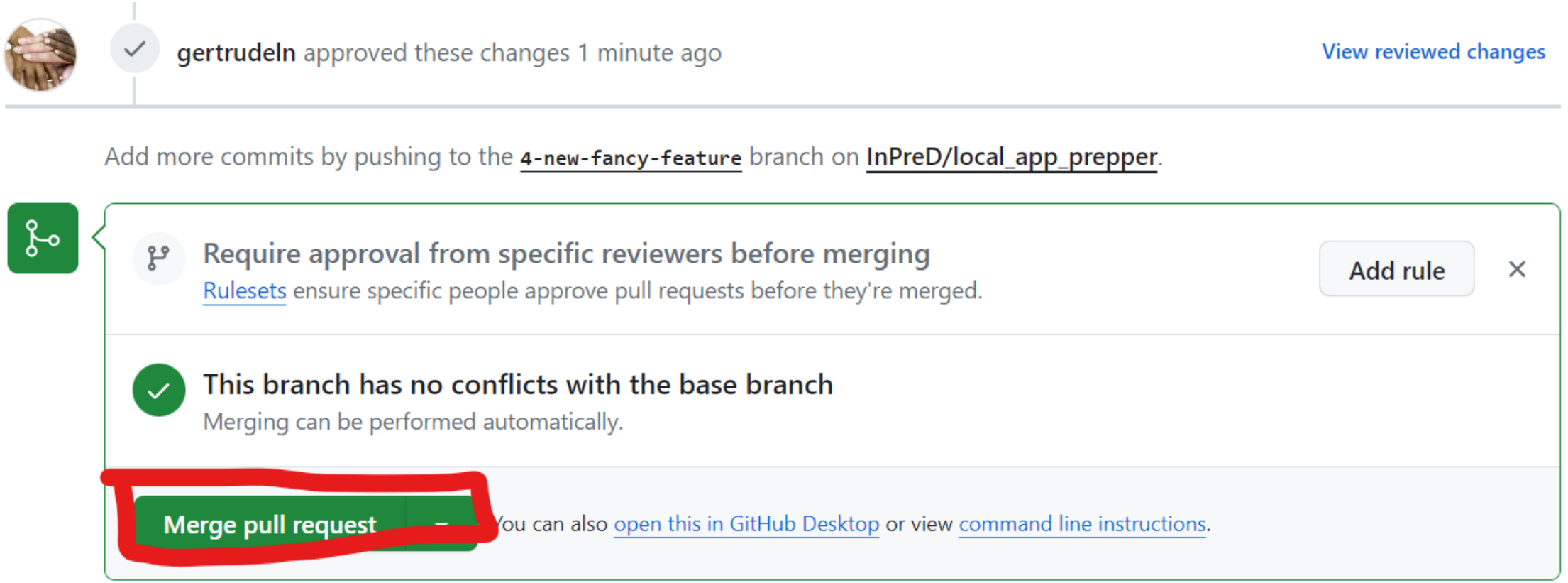
GitHub workflow

- 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



GitHub workflow

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



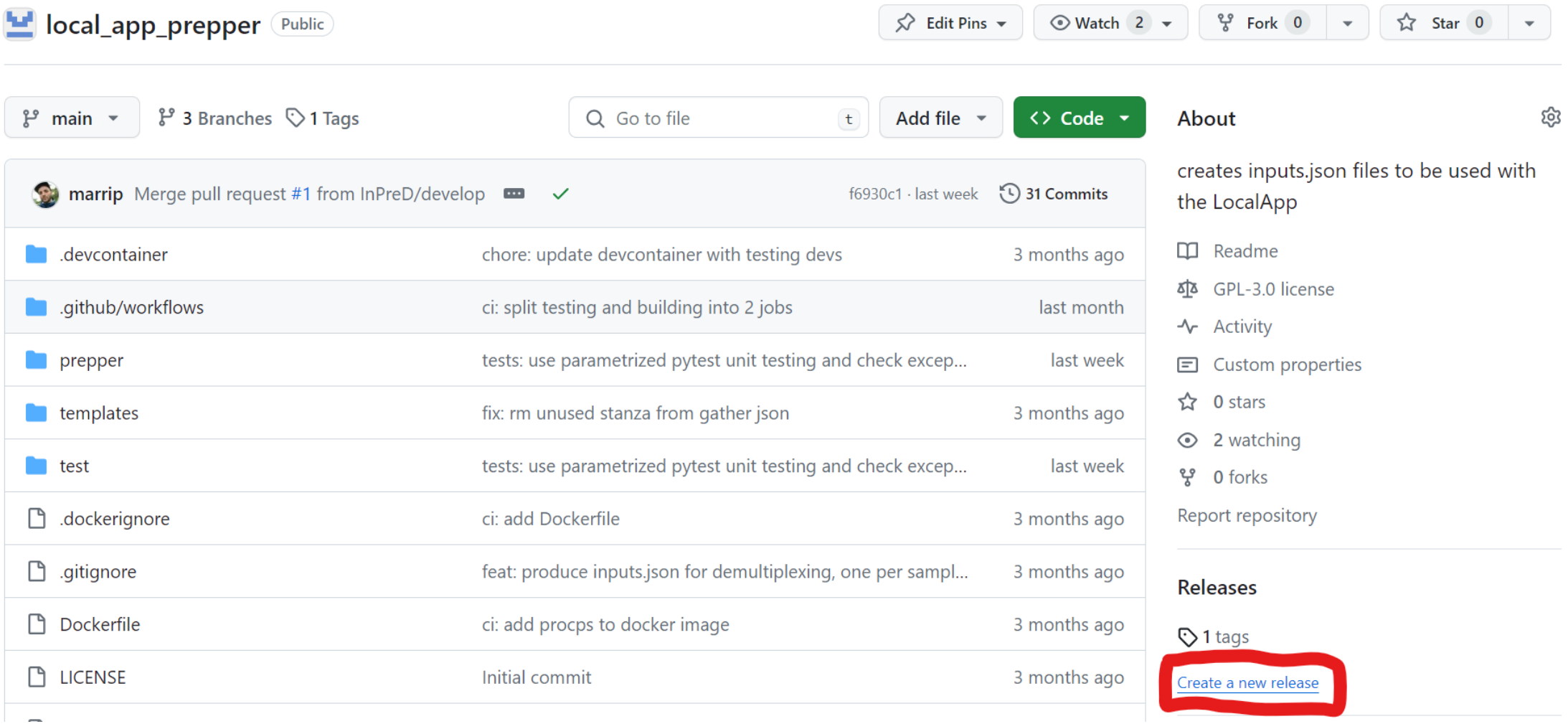
2. Development & Collaboration

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

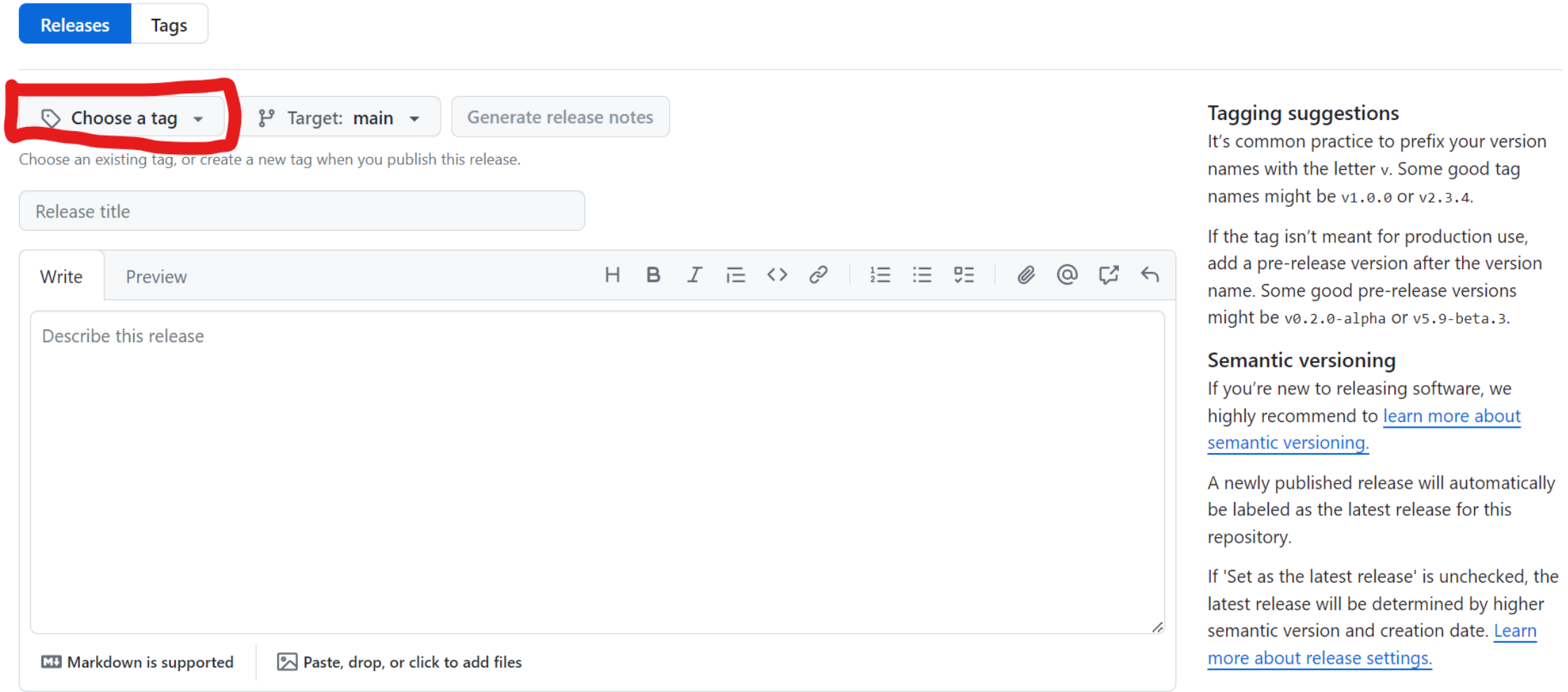
Release

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



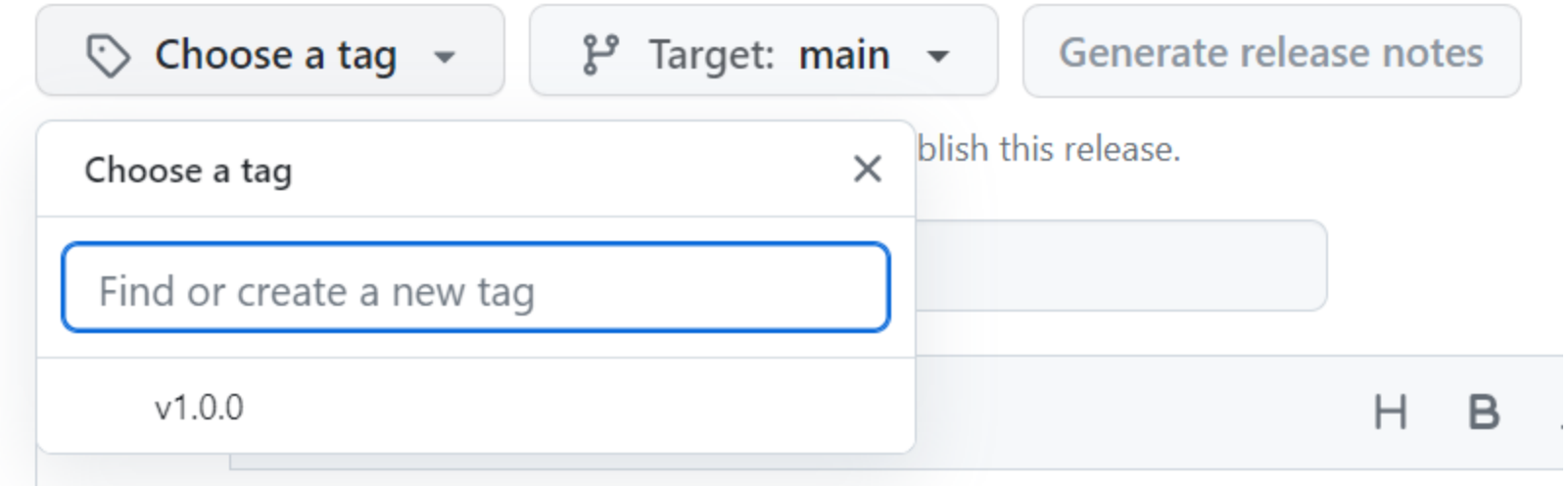
Release

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



Release

- ideally, you choose a tag according to semantic versioning



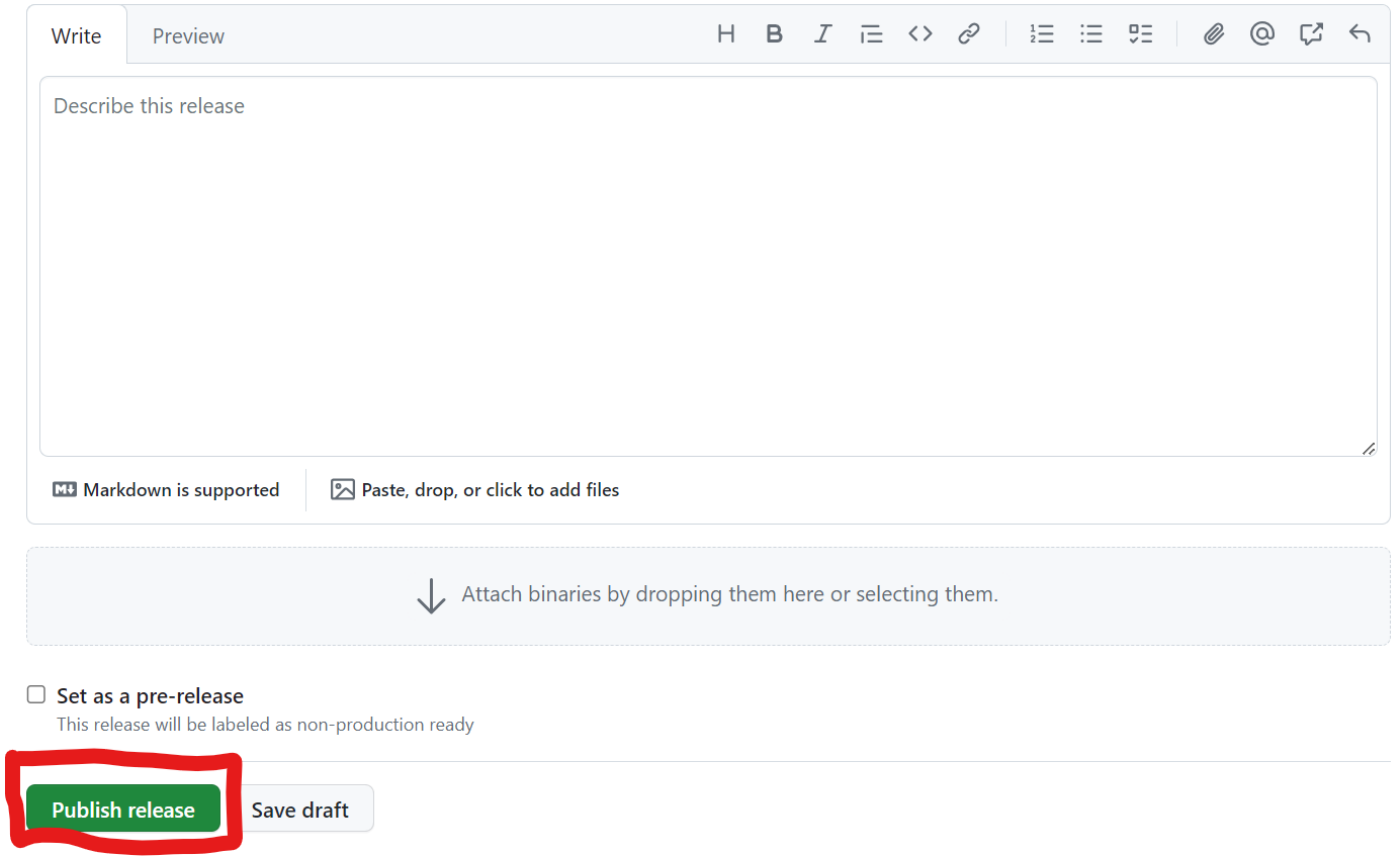
Release

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

Release

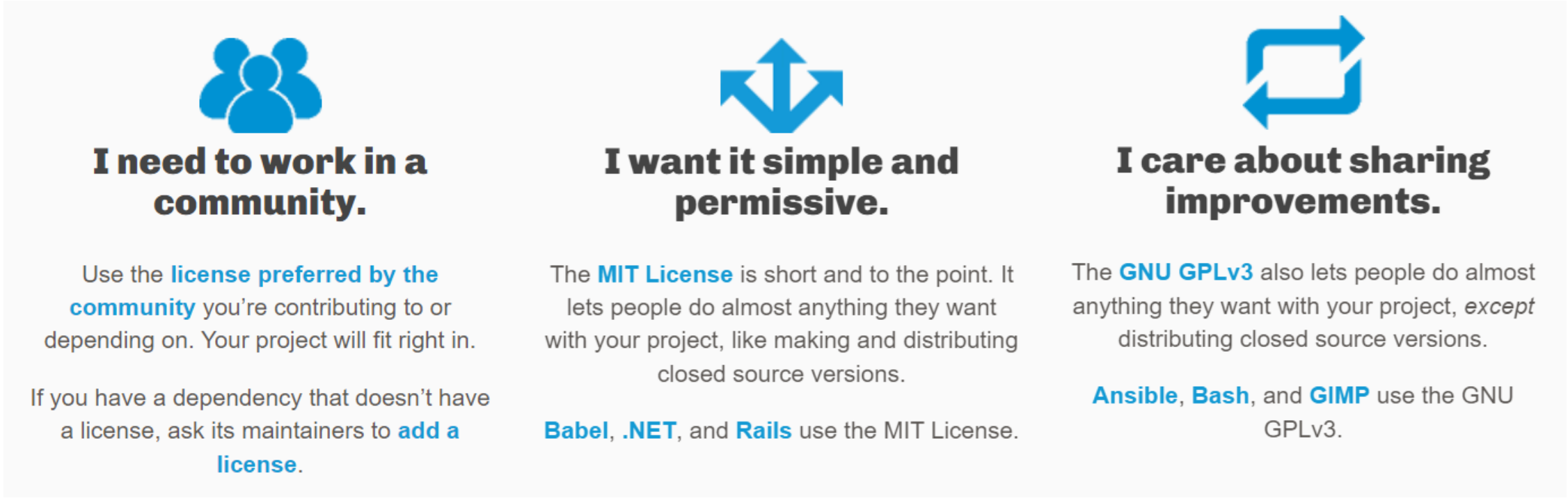
- when you are satisfied with your release, `Publish release`



2. Development & Collaboration

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. Resources

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

3. Nextflow

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
- **nf-core**: project/community that develops framework for nextflow including guidelines, tools, modules, subworkflows, pipelines and test data

3. Nextflow

Requirements

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

3. Nextflow

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. Nextflow

Something

- stubbing

3. Nextflow

nf-core template

3. Resources

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

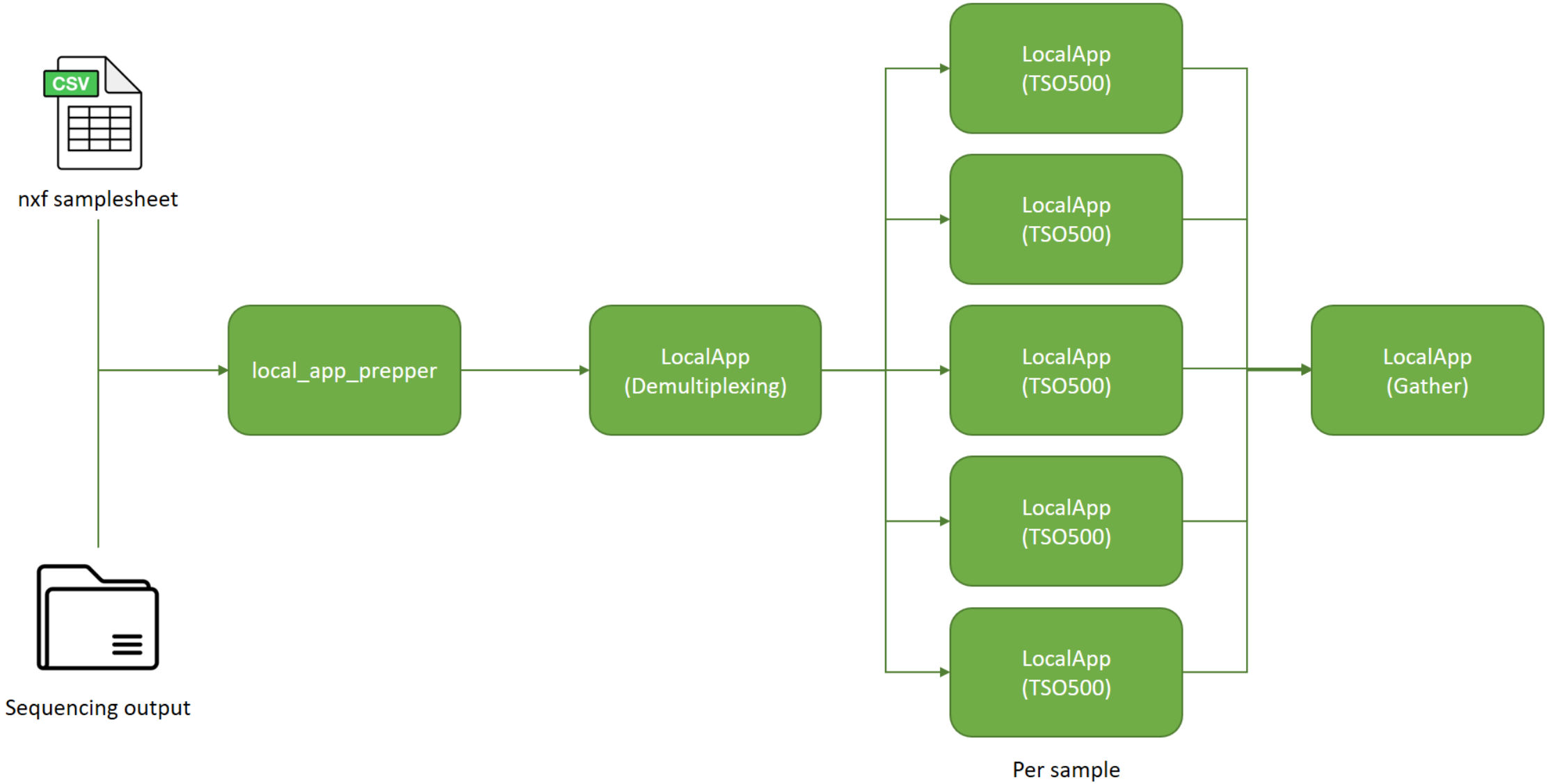
4. `tso500_nxf_workflow`

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. `tso500_nxf_workflow`

Overview



4. `tso500_nxf_workflow`

Demonstration

4. `tso500_nxf_workflow`

Outlook

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

4 Resources

- repository
- local_app_prepper
- samplesheet_generator

5. Python

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

Resources

- nf-core
- pytest unittesting