Bioinformatics session

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

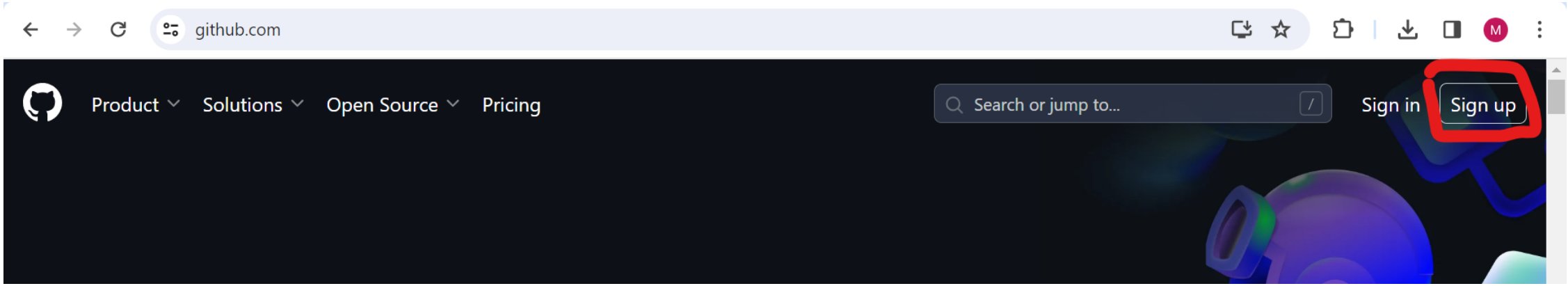
Overview

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`

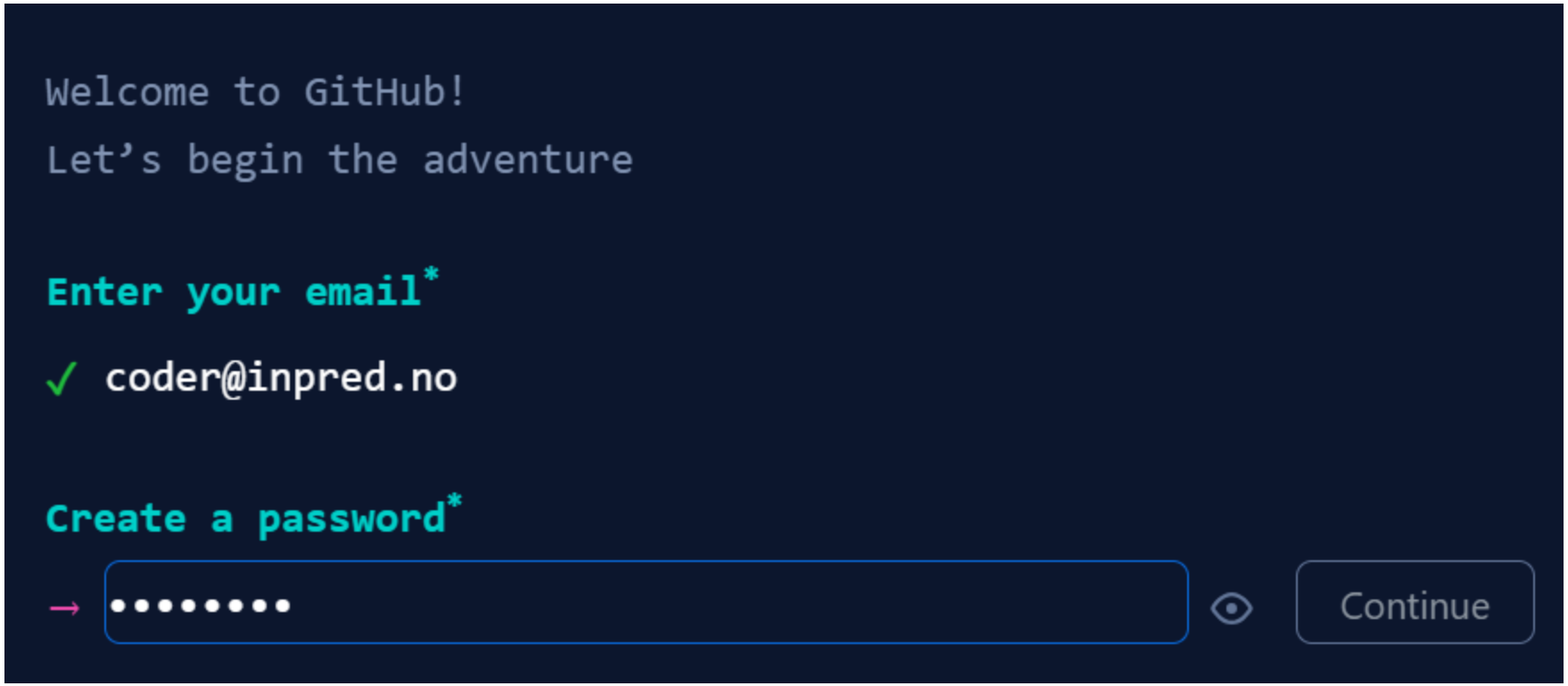


Create a GitHub account

- enter your email

Create a GitHub account

- set a password

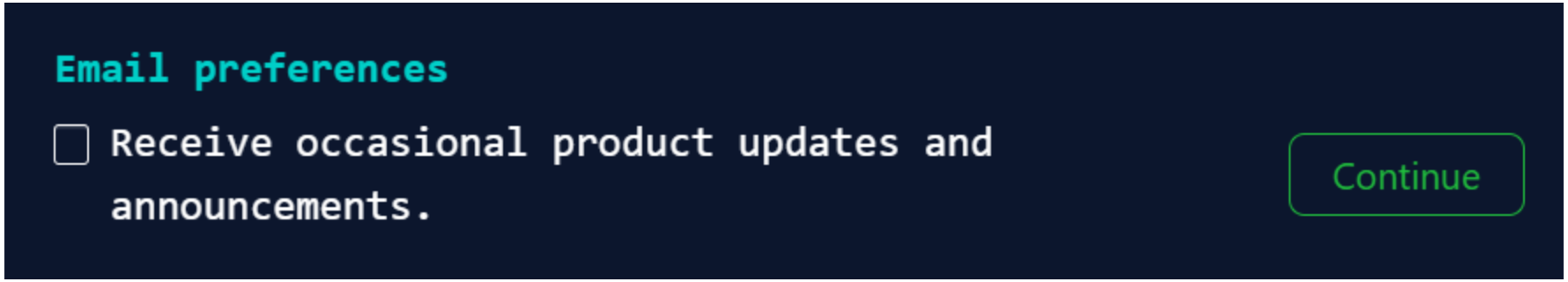


Create a GitHub account

- choose a username

Create a GitHub account

- choose email preferences

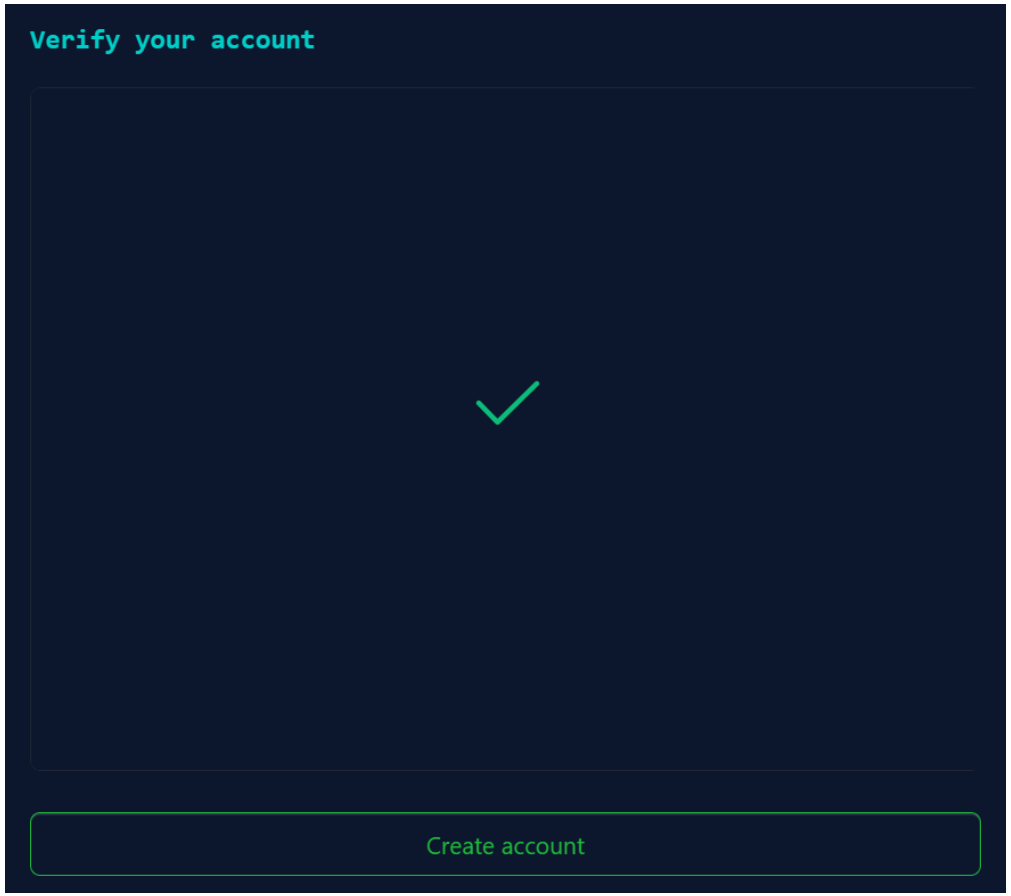


Create a GitHub account

- solve the puzzle

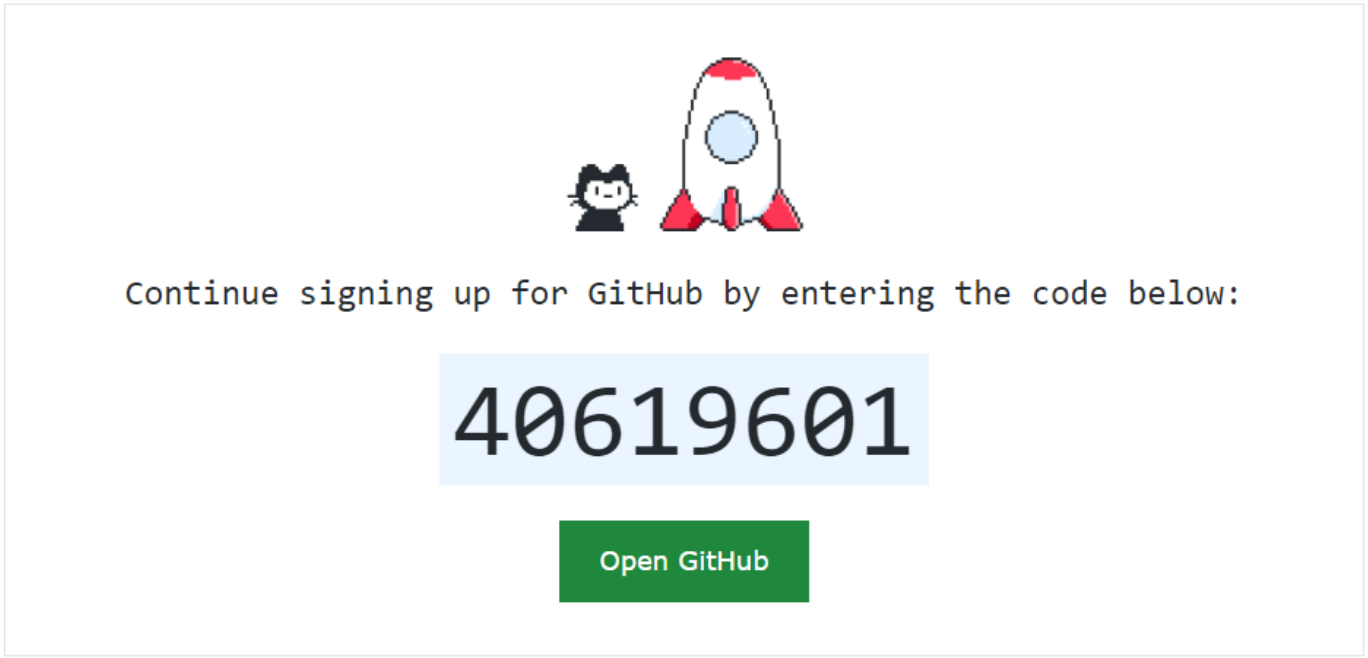
Create a GitHub account

- create your account



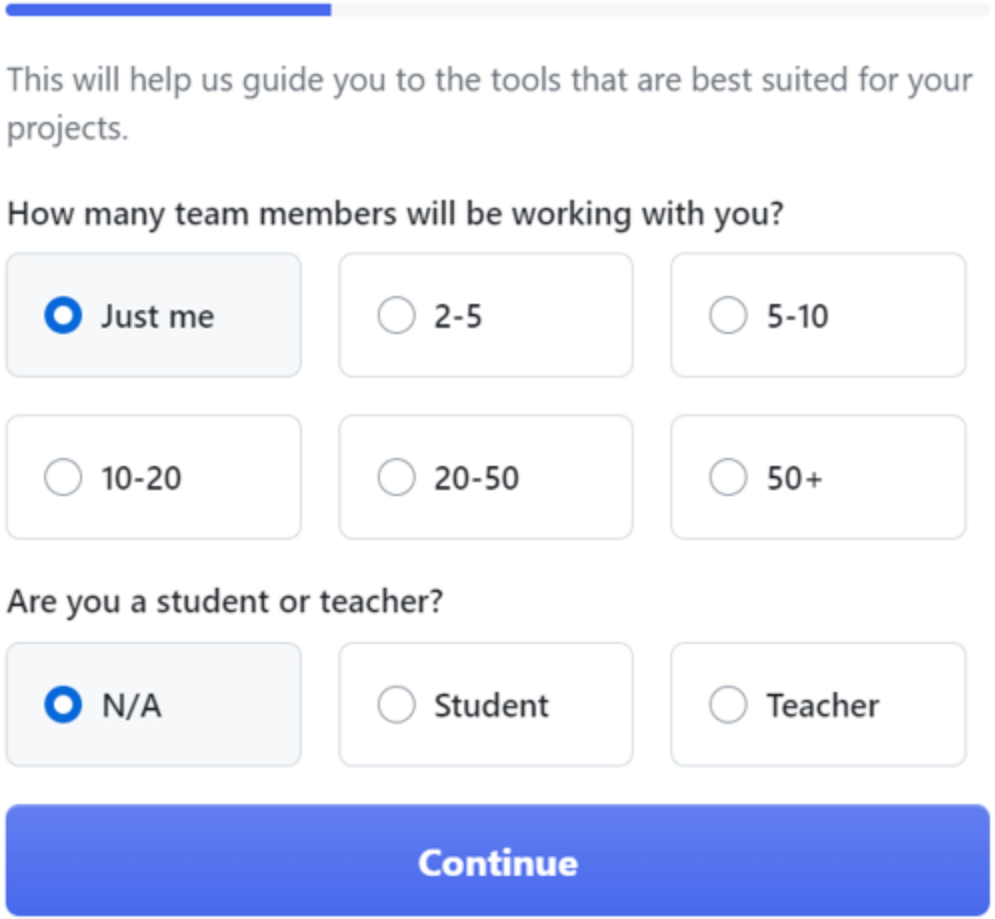
Create a GitHub account

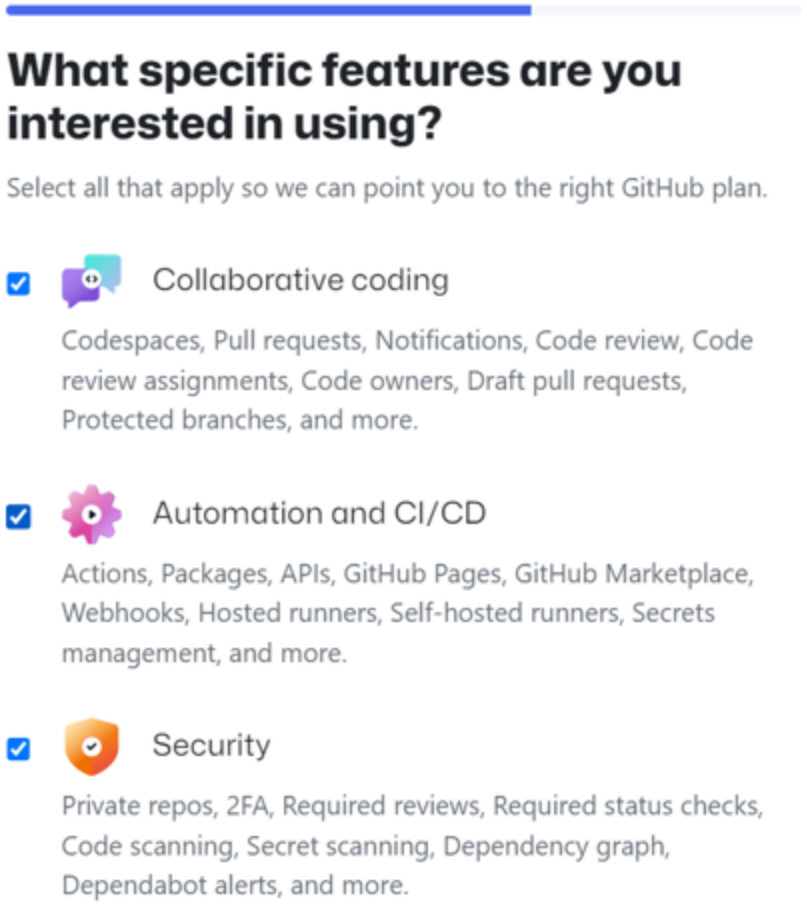
- find the activation code in the email you received



Create a GitHub account

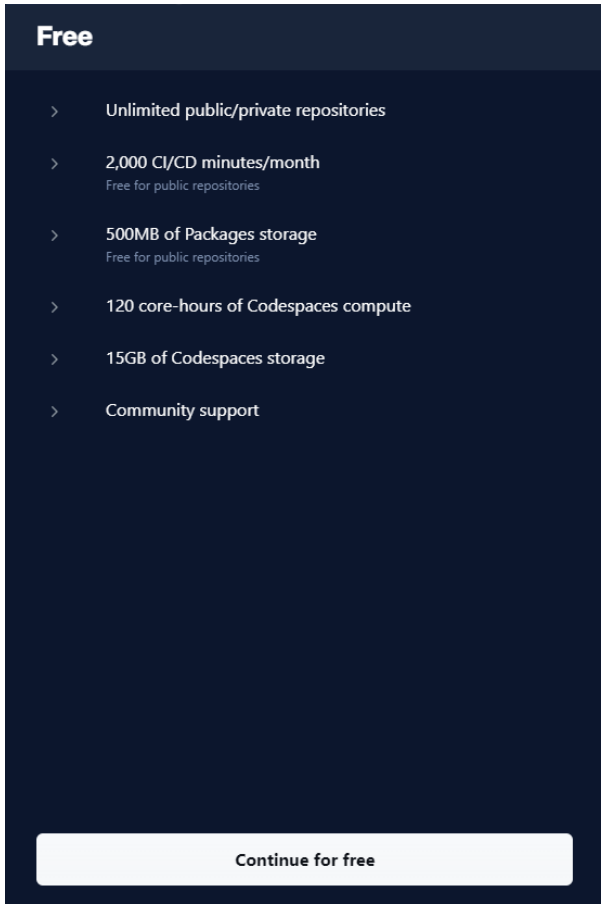
- select the desired options





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

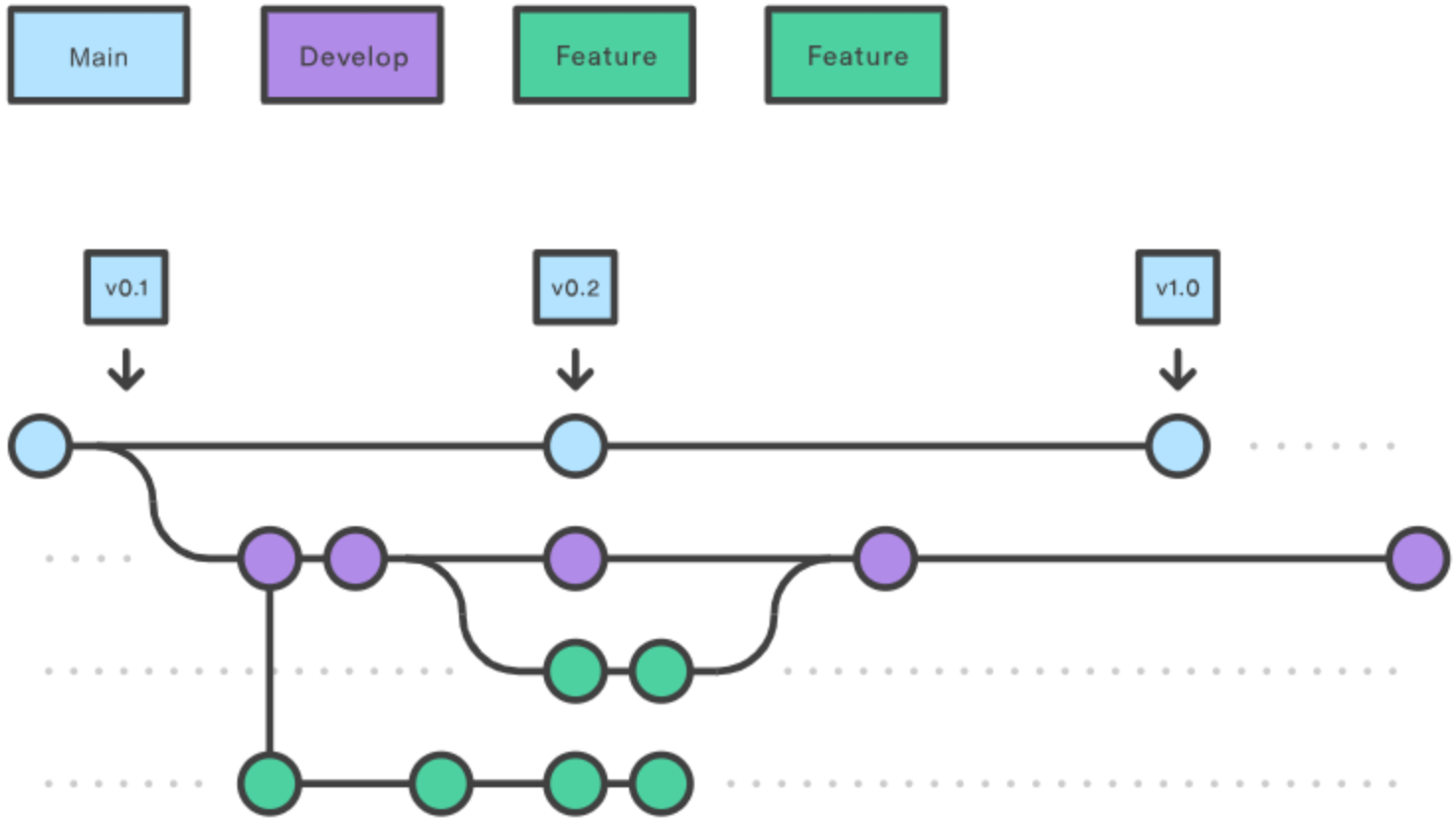
`git push` : upload changes to remote counterpart

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

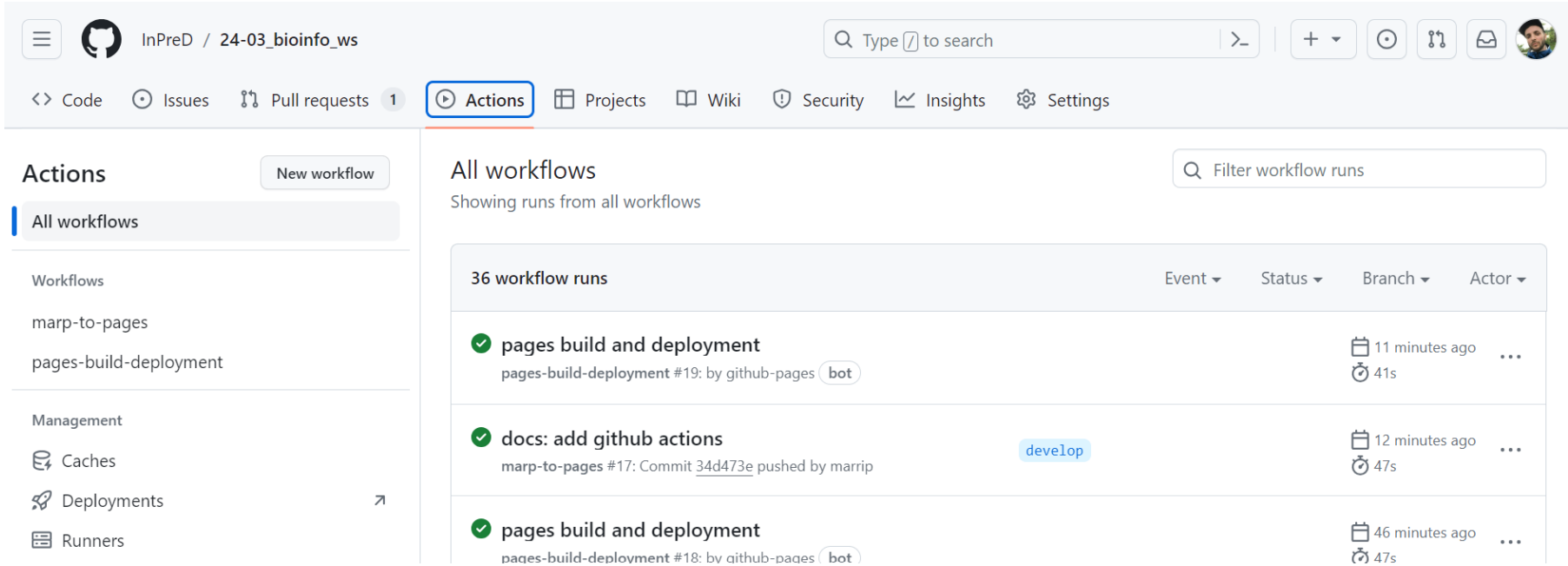
```yaml
name: Docker Build
on:
  push:
    branches:
      - main
      - develop
    tags:
      - '*.*.*'

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
  ...
```

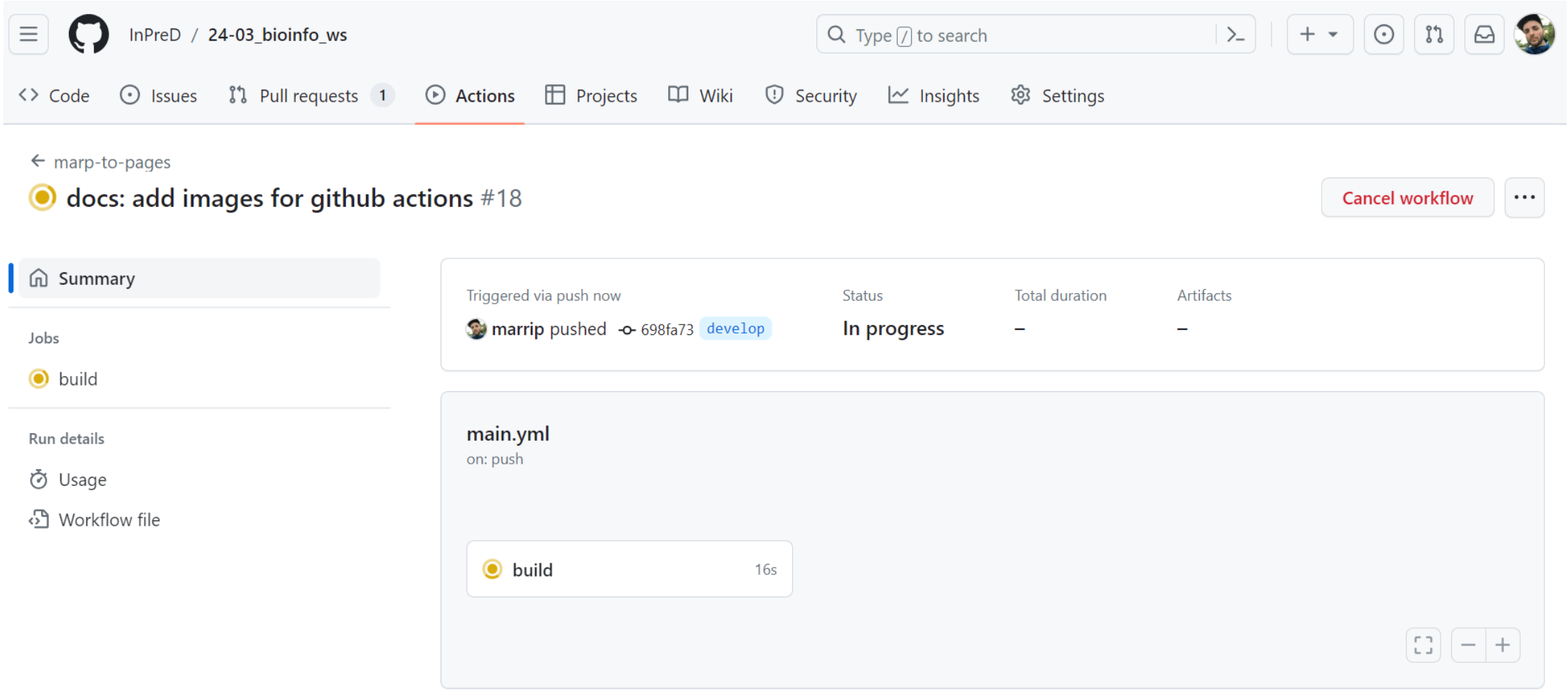
GitHub Actions

```
...
  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 }}
```

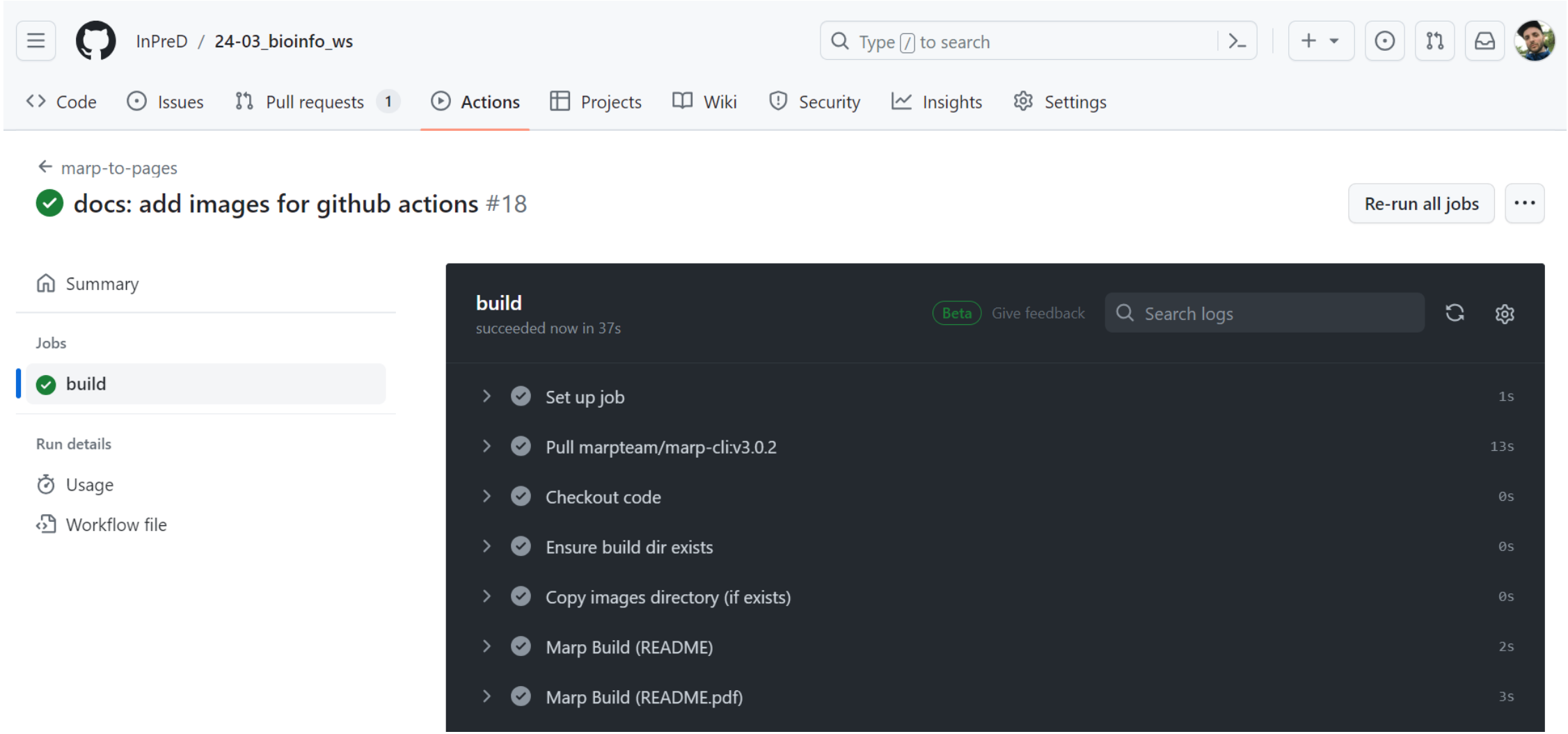
GitHub Actions



GitHub Actions



GitHub Actions



- pull requests (best practice)
- 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