Scientific Software Development with Python

DevOps 2: Documentation and Continuous Integration

CHALMERS
UNIVERSITY OF TECHNOLOGY

Simon Pfreundschuh
Department of Space, Earth and Environment

Agenda

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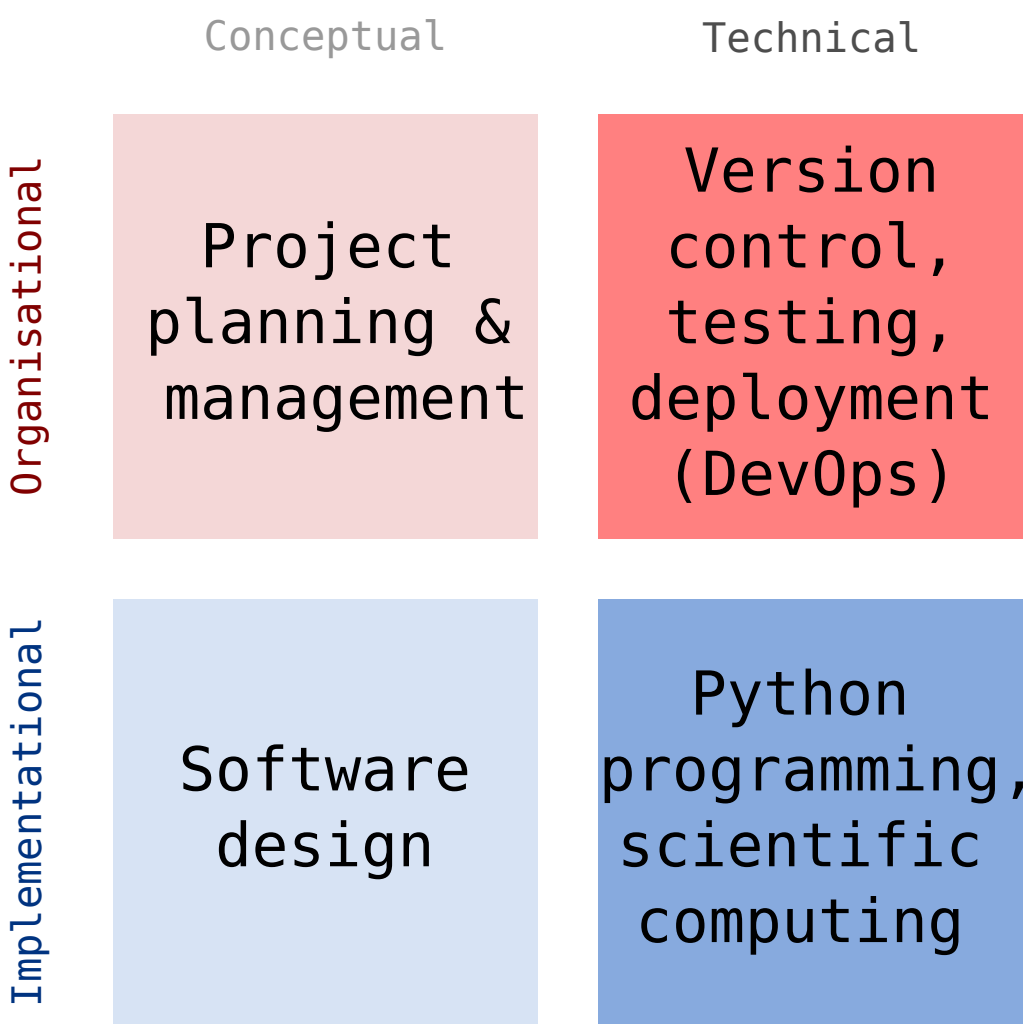
1. Introduction

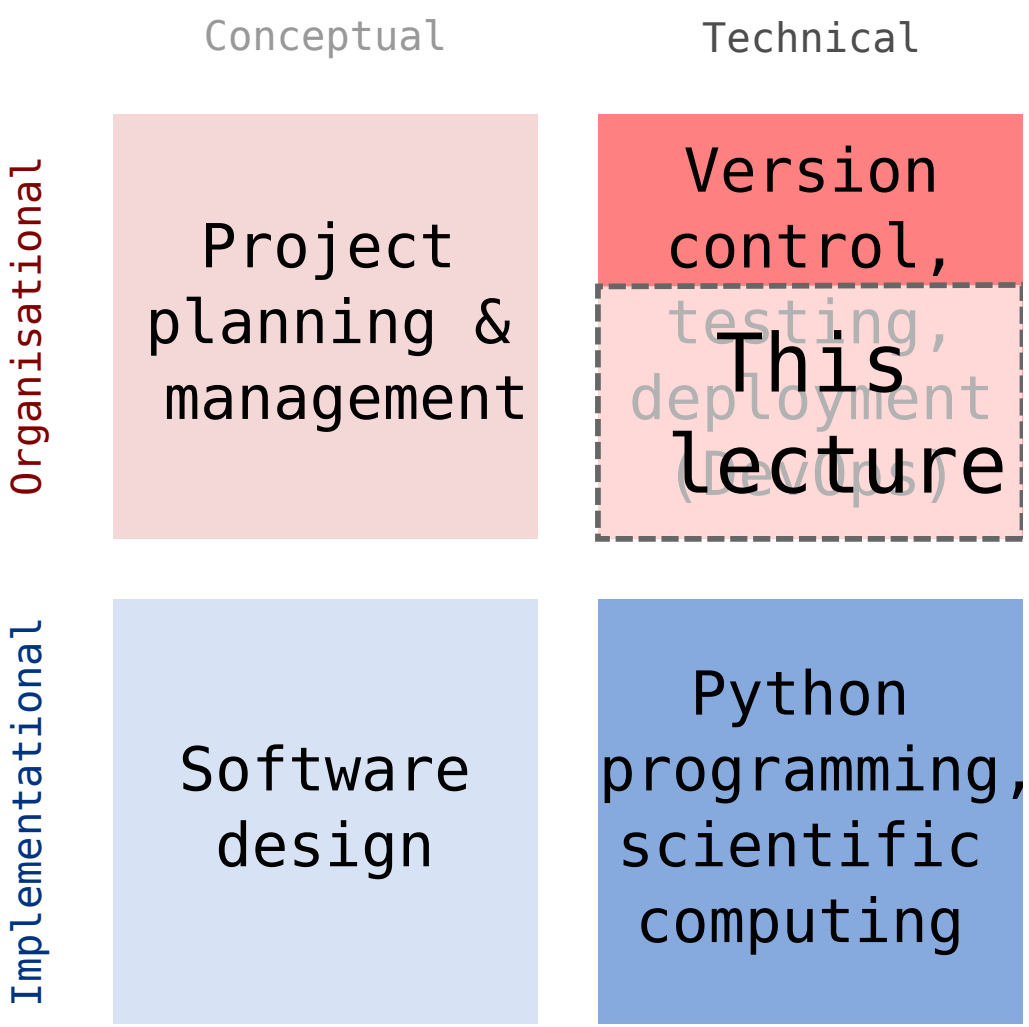
2. Documentation

3. Continuous Integration

Lecture content



Lecture content



This lecture

- Documentation with Sphinx
- Continuous integration with GitHub

Nature Astronomy: The climate issue

- In Australia emissions from super computers stand for largest part of CO_2 emissions
- Running calculations in pure Python emits much more CO_2 than when written in low-level language

Flaws in argumentation

- Emissions in Australia depend on energy mix
- Heavy calculations running on supercomputers are already not using Python
- Emissions from personal computers much lower than from compute clusters
- False dilemma: You should combine programming languages to get the best of both worlds

Nature Astronomy: The climate issue

Comment | Published: 10 September 2020

The ecological impact of high-performance computing in astrophysics

Simon Portegies Zwart

Nature Astronomy **4**, 819–822(2020) | Cite this article

Nature Astronomy: The climate issue

As an alternative, one could run concurrently using multiple cores, rather than a single thread. It is important to share resources and to prevent the monopolization of powerful workstations. To reduce runtime and CO_2 emission, the environmentally concerned researcher might want to reconsider standard Python and either optimize using high-performance libraries or adopt a more environmentally friendly (compiled) alternative. Several interesting alternatives exist, such as Alice, Julia, Rust and Swift. These languages offer the flexibility of Python but with the performance of compiled C++. Educators may want to reconsider teaching Python to university students.

Nature Astronomy: The climate issue

CO_2 production as a function of the time to solution for a variety of popular computational techniques employed in astrophysics (turquoise data points), and other activities common among astronomers[2,3] (green data points). The solid red curve gives the individual world-average production in 2017, whereas the dotted red curve give the maximum per-capita country average. The Laser Interferometer Gravitational-Wave Observatory (LIGO) carbon production is taken over its first 106-day run (using ~180 kW)[17], and for the Atacama Large Millimeter/submillimeter Array (ALMA) a 1-year average[18]. A Falcon 9 launch lasts about 32 minutes during which ~110,000 litres of highly refined kerosene is burned. The tree-code running on a GPU was performed using $N = 2^{20}$ particles. The direct N-body code on a CPU (right-most turquoise data point) was run with $N = 2^{13}$ particles[15], and the other codes with $N = 2^{16}$ particles. All performance results were scaled to $N = 2^{20}$ particles. The calculations were performed for 10 N-body time units[19]. The energy consumption was computed using the scaling relations of ref. [20] and converted from KWh to CO_2 using 0.283 kWh kg^{-1}. The turquoise dotted curve shows the estimated carbon emission when these calculations would have been implemented in Python running on a single core. The burgundy curve shows how the performance and carbon production changes while increasing the number of compute cores from 1 to 10^6 (out of a total of 7,299,072 of the world's fastest computer, left-most point) using the performance model of ref. [21]. Figure created with Matplotlib[22].

Issues with argumentation

- Large impact of emission

Execise 1

- Complete exercise 1 on task sheet.
- Time: 10 minutes.

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Purposes

1. Communication with users
2. Communication between developers

Types of documentation

- Problem-oriented (How?):
  - User guide
- Information-oriented (What?)
  - Source-code documentation

Publishing documentation

- In principle, publishing documentation makes only sense for code that is intended to be used by others (interfaces)
- **But:** Python makes it very easy to reuse functions from arbitrary modules
- Small- and medium-sized projects: Makes sense to publish all documentation in single document.
  - Keeping everything in one place makes it easier to keep things up to date.
  - Examples can serve as integration tests, which will keep them from becoming outdated

Sphinx

- Originally developed for the Python documentation
- Install using `pip`:

```
$ pip install sphinx
```

How it works:

- Write documentation using ReStructuredText (`*.rst`) markup language
- Sphinx defines special directives that allow cross references between files.
- Build documentation in desired output format (HTML, PDF, ...)

Typical folder structure

```
project_dir/
├── module/
│   └── __init__.py
├── test/
│   └── test_module.py
└── docs
```

Getting started

```
$ cd docs
$ sphinx-quickstart
```

Minimal setup

- Generated by `sphinx-quickstart`:

```
project_dir/
├── module/
│   └── __init__.py
├── test/
│   └── test_module.py
└── docs
    ├── Makefile
    ├── source/
    │   ├── conf.py
    │   └── index.rst
    └── build/
```

Minimal setup

- I recommend separating source and build path for docs
- `source/conf.py`: Python source file to configure documentation settings
- `source/index.rst`: Root document for documentation
- `Makefile`: Makefile to build documentation

The default `index.rst`

```
.. weather_app documentation master file, created by
   sphinx-quickstart on Sat Sep 19 08:20:42 2020.
   You can adapt this file completely to your liking, but it should at least
   contain the root `toctree` directive.

Welcome to weather_app's documentation!
=======================================

.. toctree::
   :maxdepth: 2
   :caption: Contents:



Indices and tables
==================

* :ref:`genindex`
* :ref:`modindex`
* :ref:`search`
```

The generated `index.html`

- Not much to see, so far

ReStructuredText

```
A section heading
=================

A subsection heading
--------------------

A subsubsection heading
~~~~~~~~~~~~~~~~~~~~~~~

*Italics*, **Bold**, ``code``

* A bullet ...
* ... list

1. A numbered ...
2. ... list

# Also a numbered ...
# ... list

Good to know: Paragraphs must always start on the same indentation
level.
```

Directives

- General syntax:

```
.. directive_name:: argument_1 ...
   :option_1: value_1
   :option_2: value_2

   Content ...
```

- Option directly follow directive declaration
- Blank line to separate options from content
- Content must be on same indentation level as options

The `toctree` directive

```
.. toctree::
  :maxdepth: 2
  :caption: Contents:

  file_1
  file_2
```

- Links content from other `.rst` files
- Content should be list of `.rst` filenames without the file ending
- Depth option determines up to which header levels should be listed

The `code-block` directive

```
- Used to display code in documentation
.. code-block:: python

  def say_hi():
      print("hi")
```

- Expects name of language as argument

Building the documentation

- To build HTML documentation in `build` folder:

```
$ cd docs
$ make html
```

Extended `index.rst`

```
The weather_app package
=======================

The ``weahter_app`` Python package provides a Python API to access the current
SMHI weather forecast as well as a command line application to check the
forecast for the next 24 hours at your location in Sweden.


.. toctree::
  :maxdepth: 2
  :caption: Contents:

  installation
  usage
  api_reference

Indices and tables
==================

* :ref:`genindex`
* :ref:`modindex`
* :ref:`search`
```

- Expects name of language as argument

The generated `index.html`

weather_app

Navigation

Contents:

Installation
Usage
API Reference

Quick search

Go

The weather_app package

The `weahter_app` Python package provides a Python API to access the current SMHI weather forecast as well as a command line application to check the forecast for the next 24 hours at your location in Sweden.

Contents:

- Installation
  - Stable version
  - Development version
- Usage
  - Command line application
  - Python module
- API Reference
  - The weather_app module
  - The weather_app.api module
  - The weather_app.render module

Indices and tables

- Index
- Module Index
- Search Page

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Execise 2

- Complete exercise 2 on task sheet.
- Time: 15 minutes.

Including Python docstrings

- Sphinx provides the `autodoc` extension to automatically include docstrings
- The `napoleon` extension allows using Google and numpy docstrings, which are much are easier to read and write then plain `.rst`.
- In `conf.py`:

```
...
# Add any Sphinx extension module names here, as strings. They can be
# extensions coming with Sphinx (named 'sphinx.ext.*') or your custom
# ones.
extensions = [ 'sphinx.ext.autodoc', 'sphinx.ext.napoleon' ] ...
...
```

To include docstrings from module

- Need to create `*.rst` file and reference it from other document
- Use `automodule` directive to include docstrings from whole module.
- In `*.rst` file:

```
.. automodule:: weather_app.api
  :members:
```

Including docstrings

- `autodoc` provides more directives for more fine-grained control
- Process is semi-automatic: Need to create files for all modules
- Can be automated using `sphinx-apidoc` command

Execise 3

- Complete exercise 3 on task sheet.
- Time: 15 minutes.

GitHub Pages

- Simple web hosting service for GitHub repositories
- Hosts static web page locates in `docs` folder or specific branch called `gh-pages`

Example workflow

- Generate documentation
- Push generated documents to `gh-pages` branch

Things to consider

- Don't want to keep track of history
- Need to make sure all files are included
- Need `.nojekyll` to tell GitHub to use Sphinx's `.css` files.

Example workflow

```
git branch -d gh-pages          # Delete branch if exists
git checkout --orphan gh-pages # Use --orphan to discard history
git rm -rf .                    # Removes staged files contained in branch
cp -r docs/build/html/* .       # Copy generated documentation
touch .nojekyll                 # Create .nojekyll file
git add *.html *.js *.inv _static _sources .nojekyll
git commit
git push -u <remote-name>
```

- Need to make sure GitHub pages service is activated for repository
- Documentation available at `<user_name>.github.io/<repository_name>`

Read the docs

- Online service to automatically build and host Sphinx documentation
- Automatic versioning
- Popular

Summary

- Sphinx is de-facto standard for Python documentation
- Can be used both for user-facing documentation and developer documentation

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DevOps so far:

- Steps required to integrate code changes:
  - Testing
  - Packaging
  - Generating documentation

Problem

These are too many manual steps. How can we assure that we perform them every time?

Continuous integration (CI)

- Regularly integrate and release code changes
- Advantages:
  - Flexibility: Respond to changing requirements
  - Reactiveness: Being able to fix things quickly
  - Learning: Direct feedback ensure learning from mistakes

The key to continuous integration is automating all manual DevOps steps.

Continuous integration with GitHub

- GitHub offers free CI functionality
- Other services/products: Jenkins, Travis
  - Functionality is similar
- Principle:
  - Define workflow to automate with special file in repository
  - Workflow is executed in the cloud and results are accessible through we interface

Workflows and actions

- Workflow: Sequences of steps executed on a given event (e. g. push)
- Actions:
  - Steps executed in workflow
  - Can be parametrized and reused, there's even a "marketplace" for them
- Actions and workflows can be defined within the repository:

```
project_dir/
└── .github/
    ├── actions
    │   └── action.yml
    └── workflows
        └── workflow.yml
```

Workflow example

- File: `.github/workflows/install_and_test.yml`

```yaml
name: install_and_test
on: [push]
jobs:
  install_job:
    runs-on: ubuntu-latest
    steps:
      - uses: actions/checkout@v2
        with:
          ref: 'main'
      - uses: actions/setup-python@v2
        with:
          python-version: '3.6'
      - run: pip install .
      - run: pip install pytest
      - run: pytest test/
```

Workflow example

- Runs whenever code is pushed to repository
- Runs on server with latest ubuntu
- Executed steps:
  1. Checkout latest changes from repository (Predefined action)
  2. Setup Python on server (Predefined action)
  3. Install the package
  4. Install pytest
  5. Run tests

Testing in different environments

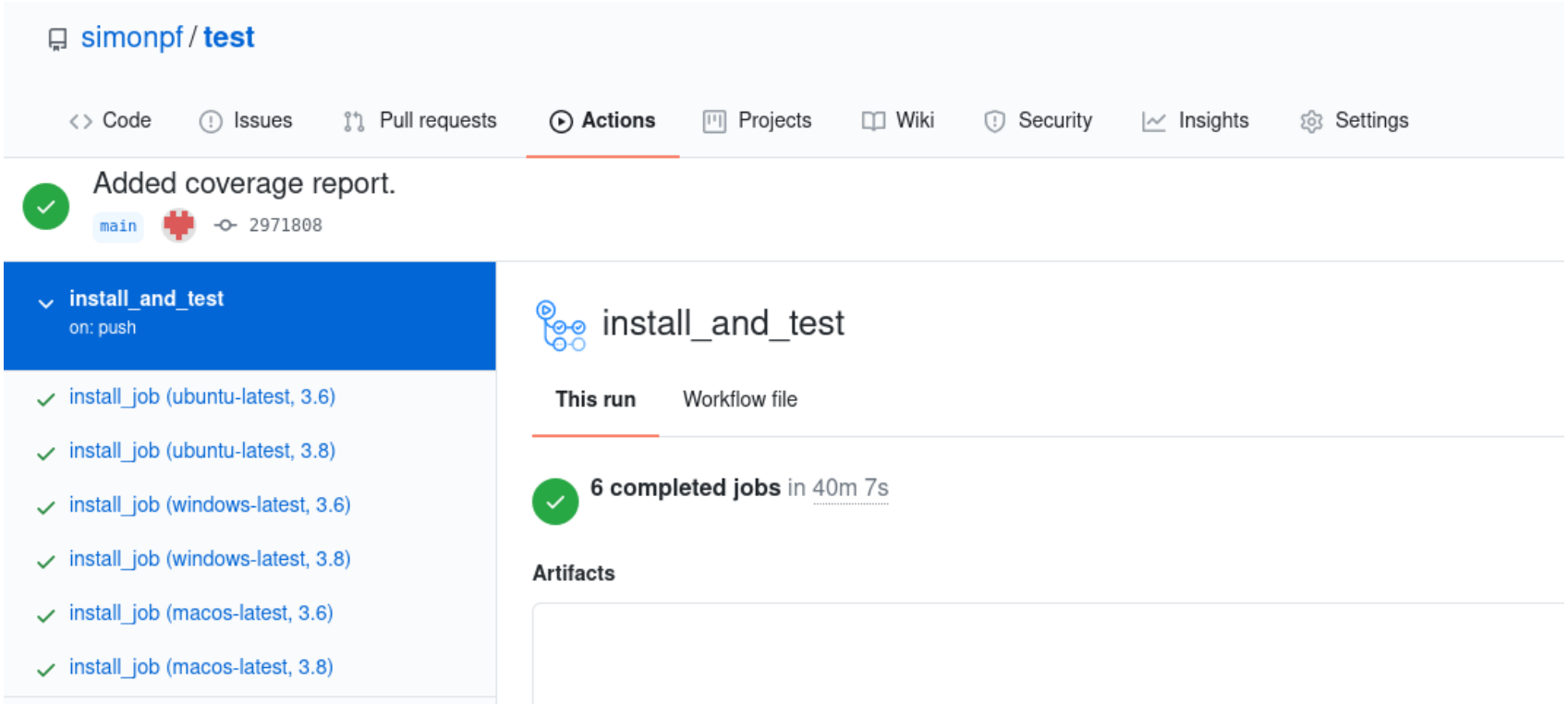
```yaml
name: install_and_test
on: [push]
jobs:
  install_job:
    strategy:
      matrix:
        os: [ubuntu-latest, windows-latest, macos-latest]
        python: [3.6, 3.8]
    runs-on: ${{ matrix.os }}
    steps:
      - uses: actions/checkout@v2
        with:
          ref: 'main'
      - uses: actions/setup-python@v2
        with:
          python-version: ${{ matrix.python }}
      - run: pip install .
      - run: pip install pytest
      - run: pytest test/
```

```yaml
...
  strategy:
    matrix:
      os: [ubuntu-latest, windows-latest, macos-latest]
      python: [3.6, 3.8]
...
  runs-on: ${{ matrix.os }}
...
    - uses: actions/setup-python@v2
      with:
        python-version: ${{ matrix.python }}
```

Testing in different environments

- Define strategy matrix:
  - `variable: [values, ...]`
- Access variable values using `{{ matrix.variable }}`
- Different job launched for each combination of variable values

Testing in different environments



Adding a test badge to your repository page

- GitHub provides badge graphics showing the status for every workflow under the URL:
  `https://github.com/<username>/<repository>/workflows/<name>/badge.svg`
- Can be embedded in `README.md` which is rendered on the front page of your repository:

```
![workflow name](https://github.com/<username>/<repository>/workflows/<name>/badge.svg)
```

Uploading distribution packages to PyPI

- Problem:
  - Need username and password to upload to PyPI
  - **Repository is public, so can't want to store sensitive data there**
- Solution:
  - GitHub secrets: Stores sensitive data in encrypted form to be accessed from within workflows
  - API Token: Unique identifier that GitHub can use to

Uploading distribution packages to PyPI

- Steps:
  - Generate API token on pypi.org
    - Account settings -> Add API token
  - Store API token as secret in your GitHub repository
    - Repository settings -> secrets -> new secret
    - Use secret in workflow `{{ secret.name }}`

Example workflow

```yaml
name: release
on:
  push:
    tags:
      - '*'
jobs:
  release_job:
    runs-on: ubuntu-latest
    steps:
      - uses: actions/checkout@v2
        with:
          ref: 'main'
      - uses: actions/setup-python@v2
        with:
          python-version: '3.8'
      - run: pip install .
      - run: pip install wheel twine
      - run: python setup.py sdist bdist_wheel
      - run: python -m twine upload -u __token__ -p ${{ secrets.TWINE_TOKEN }} dist/*
```

Example workflow

- PyPI requires all binaries to have unique versions, so you can't release everything that you push
- Better policy is to release when a tag is pushed to the repository
- Tags are named references to specific revisions of the repository:

```
git tag -a v0.0.1 # Mark current version with a name
git push origin v0.0.1 # Push tag to GitHub
```

Summary

- CI requires automation of all relevant DevOps tasks
- Basic CI functionality provided by GitHub even for free accounts