Scientific Software Development

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Unit 6: Continuous integration - GitHub actions

- GitHub actions basics
- Run your tests and linter automatically through GitHub actions
- How to publish your research and your software
- Optionally: Publish your Python package

The Python package will be completed.
Optional: Publish your package on PyPi.

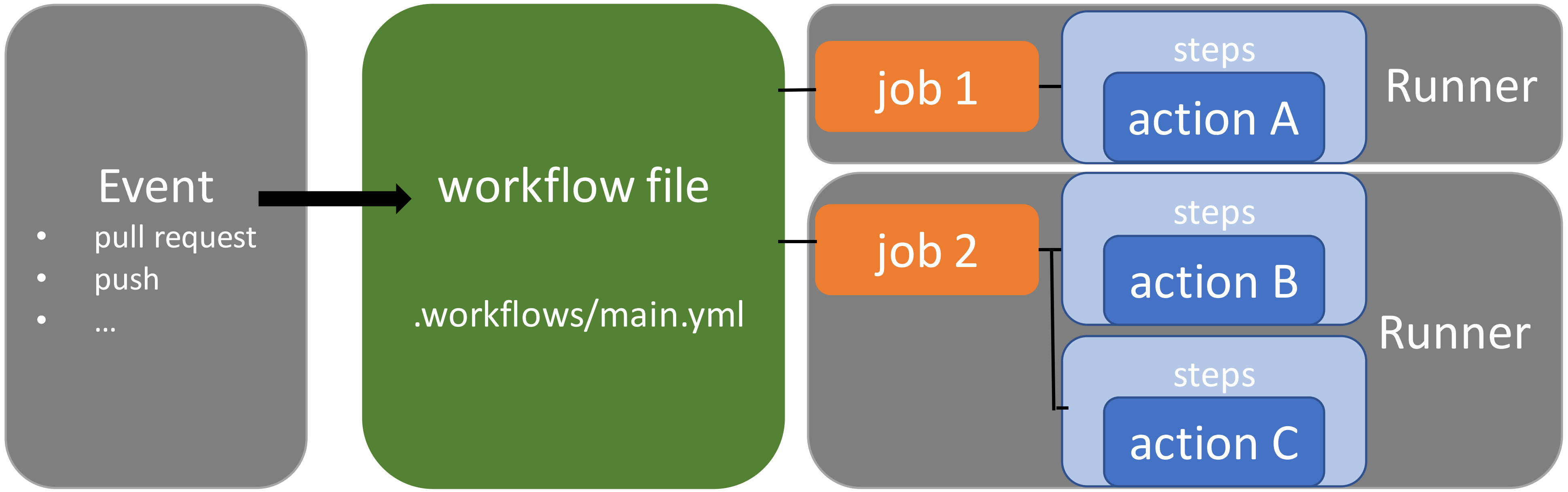
What are GitHub actions?

GitHub actions are a way to automatize syntax checking and testing upon certain events ("whenever something changes"), i.e. pull requests, merging of branches, etc.

This provides a convenient tool to check your code before it is "unleashed" for a more general use.

You only need to set this up once and it will save you time in the long run.

GitHub actions



GitHub actions

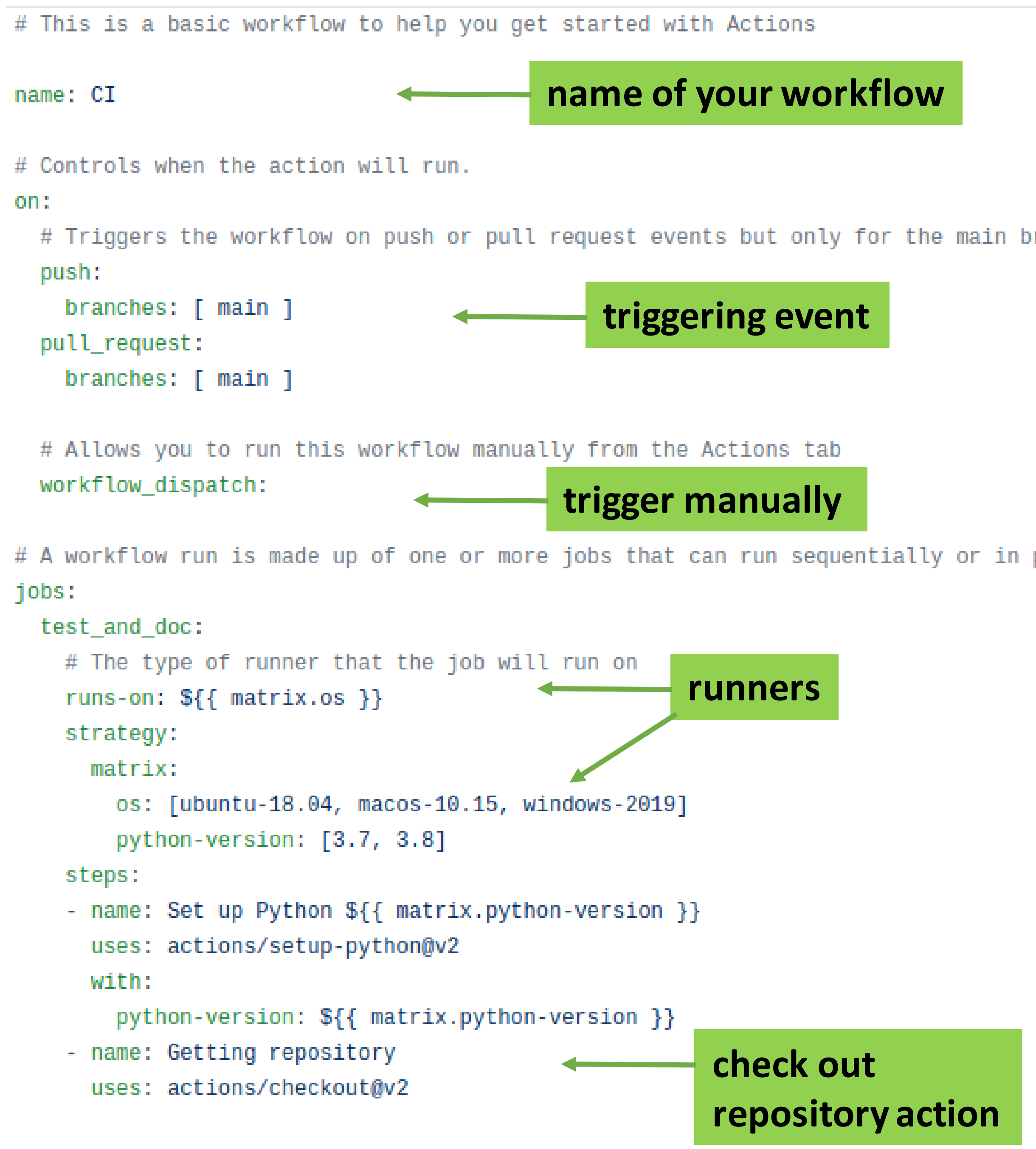
GitHub action pricing:

- Free for public repositories
- For private repositories: ~2000 min/month (execution minutes for hosted runners)
- 1 min actually is 60s on Ubuntu, but: 60s ≙ 2 min on Windows; 60s ≙ 10 min on MacOS

OS	Resources	Price per extra minute
Linux	2 cores, 7 GB	$ 0.008
Windows	2 cores, 7 GB	$0.016
MacOS	2 cores, 7 GB	$ 0.08

The workflow file

- The workflow file is written in YAML (which stands for "YAML Ain't Markup Language") and is a data serialization language; indentation similar to python



```yaml
# This is a basic workflow to help you get started with Actions

name: CI

# Controls when the action will run.
on:
  # Triggers the workflow on push or pull request events but only for the main branch
  push:
    branches: [ main ]
  pull_request:
    branches: [ main ]

  # Allows you to run this workflow manually from the Actions tab
  workflow_dispatch:

# A workflow run is made up of one or more jobs that can run sequentially or in parallel
jobs:
  test_and_doc:
    # The type of runner that the job will run on
    runs-on: ${{ matrix.os }}
    strategy:
      matrix:
        os: [ubuntu-18.04, macos-10.15, windows-2019]
        python-version: [3.7, 3.8]
    steps:
    - name: Set up Python ${{ matrix.python-version }}
      uses: actions/setup-python@v2
      with:
        python-version: ${{ matrix.python-version }}
    - name: Getting repository
      uses: actions/checkout@v2
```

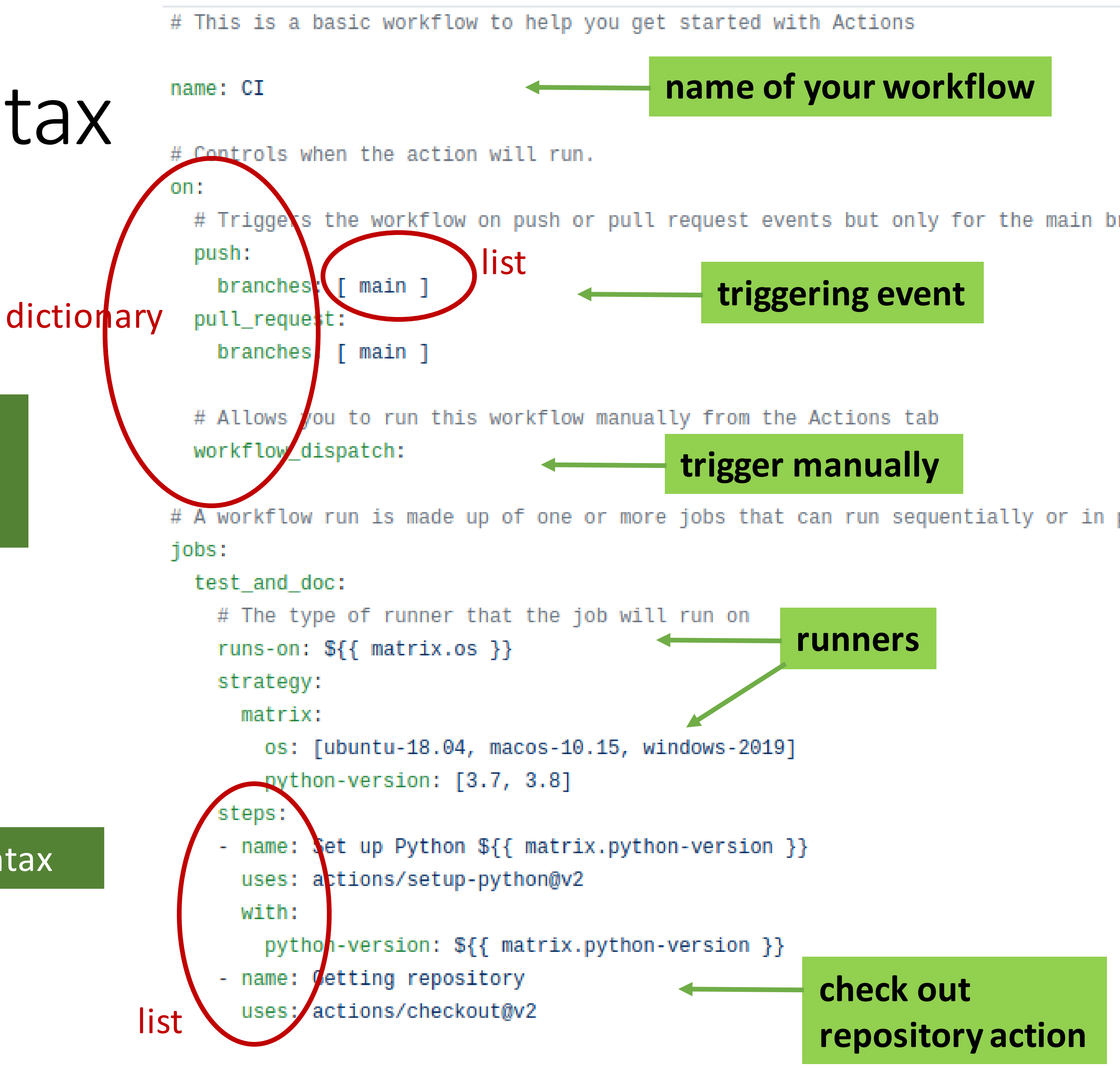
Workflow syntax

key: value

list or collection:
  - list item 1
  - list item 2

my multi-line value: |
  instruction 1
  instruction 2

- understands JSON syntax



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Workflow syntax

https://docs.github.com/en/actions/reference/workflow-syntax-for-github-actions

- file needs .yml or .yaml extension
- has to be stored in .github/workflows

`name:`
the name of your workflow

`on:`
the action that triggers the workflow

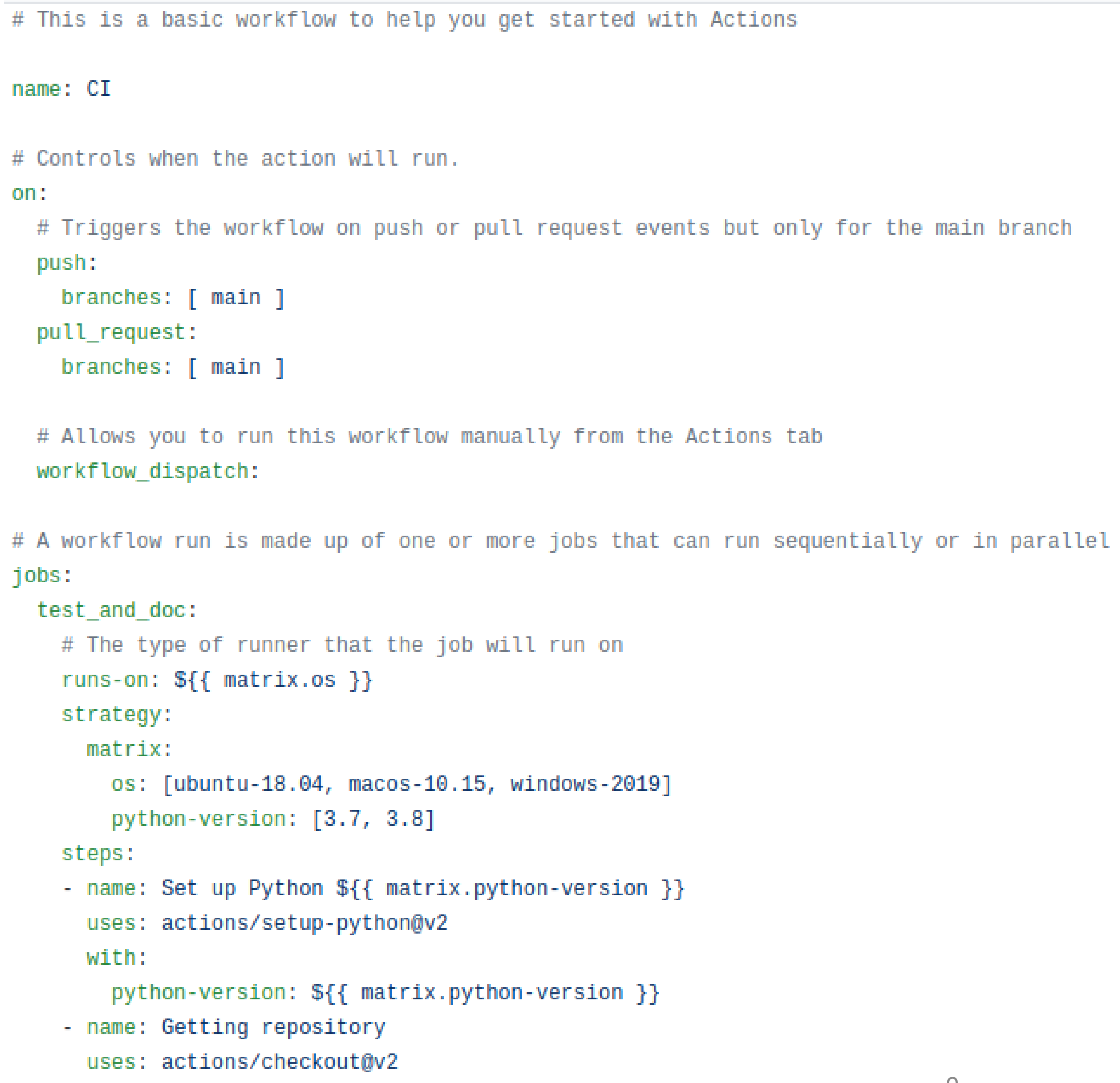
`jobs:`
the jobs that constitute the workflow

Workflow syntax

```
on: [push, pull_request]
```

```
job:
  job_id:
    name: my job name
    needs: job1 # this ensures job1 is run first
    runs-on: myOS # the architecture that should be used
    steps:
      ...
```

Virtual environment	YAML workflow label
Windows Server 2019	windows-latest or windows-2019
Ubuntu 20.04	ubuntu-latest or ubuntu-20.04
Ubuntu 18.04	ubuntu-latest or ubuntu-18.04
Ubuntu 16.04	ubuntu-16.04
macOS Big Sur 11.0	macos-11.0
macOS Catalina 10.15	macos-latest or macos-10.15



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Workflow syntax

strategy:
creates a build matrix
for the job to run in

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Workflow syntax: The actions

- The actions are individual tasks that can be written in different languages
- Write your own or use available ones

```
job:
  job_id:
    name: my job name
    needs: job1 # this ensures job1 is run first
    runs-on: myOS # the architecture that should be used
    steps:
      - name: checkout the repo
        uses: specify an action
```

← specify version number of the referenced action
otherwise updates to the action may break your workflow

https://github.com/actions
https://github.com/marketplace?type=actions
https://hub.docker.com/

actions are either JavaScript files or Docker containers
for Docker containers, job must be run in linux environment

relevant actions: `{owner}/{repo}/{path}@{ref}` or `docker://{image}:{tag}`
`actions/checkout@v2` *# checks out your repository on the runner – you will always need this if you run tests/linter*
`actions/setup-python@v2 # sets up python environment`

`sonarsource/sonarcloud-github-action@master # code quality analysis through sonarcloud`

Workflow syntax: run

```
job:
  job_id:
    name: my job name
    needs: job1 # this ensures job1 is run first
    runs-on: myOS # the architecture that should be used
    steps:
      - name: build the documentation
        run: | # run a script, execute a command-line command
          cd doc
          build html
      - name: run the linter
        run: flake8
```

Example running a script using bash

```
steps:
  - name: Display the path
    run: echo $PATH
    shell: bash
```

Example running a script using Windows cmd

```
steps:
  - name: Display the path
    run: echo %PATH%
    shell: cmd
```

Example running a script using PowerShell Core

```
steps:
  - name: Display the path
    run: echo ${env:PATH}
    shell: pwsh
```

Example: Using PowerShell Desktop to run a script

```
steps:
  - name: Display the path
    run: echo ${env:PATH}
    shell: powershell
```

Example running a python script

```
steps:
  - name: Display the path
    run: |
      import os
      print(os.environ['PATH'])
    shell: python
```

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Linter in GitHub actions

- Create a workflow file in `.github/workflows/main.yml`
- Run the linter through the workflow

```
- name: Run linter
  run: flake8
```

Take care of proper indentation! Yaml syntax is very strict.

Linter in GitHub actions

- Trigger the workflow and see what happens.

Unit tests in GitHub actions

- Add the following lines to your GitHub actions file:

```
- name: Run tests
      run: |
        cd src/package
        python -m pytest
```

- Take care of proper indentation!

Unit tests in GitHub actions

- Trigger the workflow and see what happens.

Linter and tests in GitHub actions

- Meddle with your code so that the linter/unit tests will fail. Commit to a branch and open a Pull Request. What happens?

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How to publish research and software

Scenario 1:
You publish your research but not the data nor the software.
Data availability statement:
".. data is available from the authors upon reasonable request..."

Please consider to publish a preprint on a preprint server like arxiv (after submission of your paper to a journal but before its publication)

How to publish research and software

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Please consider to publish a preprint on a preprint server like arxiv (after submission of your paper to a journal but before its publication)

Scenario 2:
You publish your research and data but not the software.
Data availability statement:
".. data is available at DOI..."

- publish preprint
- publish data on a platform like zenodo, and obtain a DOI

How to publish research and software

Scenario 3:
You publish your research, data and software.
Data availability statement:
".. data and software is available at DOI ..."

- publish preprint
- publish data with DOI
- publish software with DOI (ie zenodo)

How to publish research and software

Scenario 3:
You publish your research, data and software.
Data availability statement:
".. data and software is available at DOI ..."

- publish preprint
- publish data with DOI
- publish software with DOI (ie zenodo)

Scenario 4:
You publish your research and data separate from the software, both in a journal/data in a database.
Data availability statement:
".. data is available at DOI..."
Software is referenced via its publication.

- publish preprint
- publish data with DOI
- publish software in dedicated, peer-review journal*

*List of possible journals: https://www.software.ac.uk/which-journals-should-i-publish-my-software

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Publish a Python package on PyPi

- Work through:
- https://packaging.python.org/tutorials/packaging-projects/

Publish a Python package

- You need a file __init__.py in your package source directory so that the directory can be imported as a package
- Unit tests are in tests/
- Create the file pyproject.toml - this file communicates with build tools like pip and build

```
[build-system]
requires = [
    "setuptools>=42",
    "wheel"
]
build-backend =
"setuptools.build_meta"
```

list of packages needed to build your package

Configure the metadata

- Static metadata setup.cfg: Always the same. Try to keep it static rather than dynamic.

- Dynamic metadata setup.py: Determined at install-time. Only use when absolutely necessary.

Live lesson

- In the live lesson, we will set up GitHub actions for your Python package.