The art of developing scientific software

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Unit 4: Continuous integration - GitHub actions

- Run your tests and linter automatically through GitHub actions
- Build and publish your documentation on readthedocs
- Optionally: Publish your python module as a package

Recap and presentation of the implementations/discussion lead by the developer teams.
The python module will be completed.
Optional: Publish your modules as a package on PyPi.

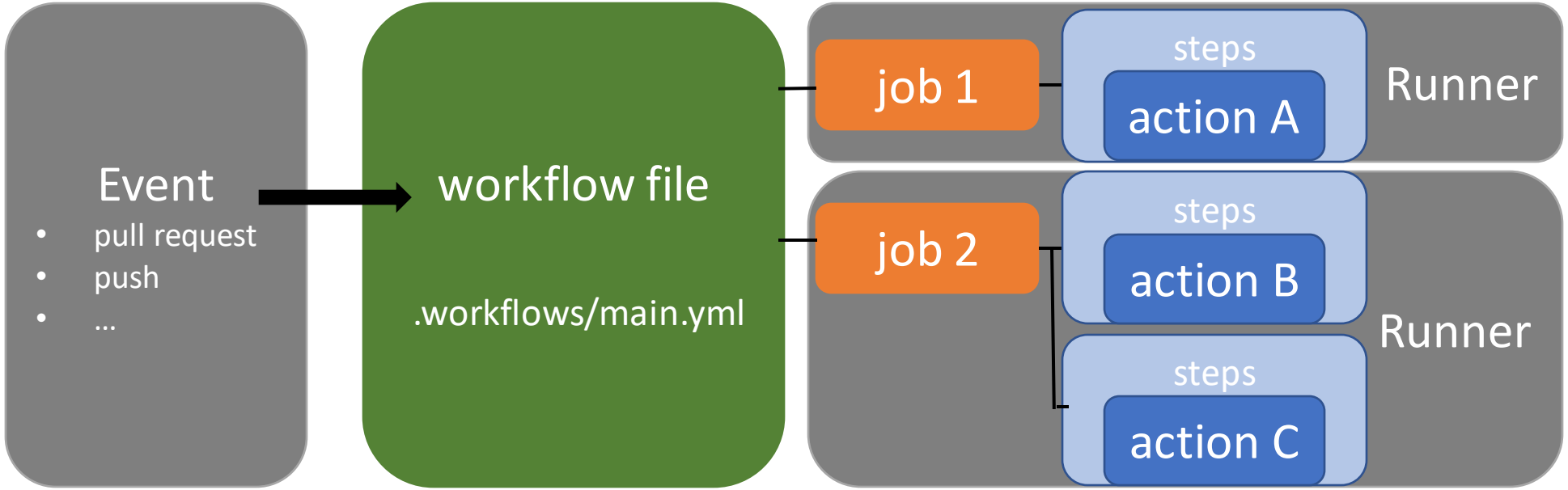
What are GitHub actions?

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
```

name of your workflow

triggering event

trigger manually

runners

check out repository action

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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```

dictionary

list

list

name of your workflow

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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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      with:
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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
```

Build and publish your documentation

- You need a user account on https://readthedocs.org/
- We will connect your github repo with your account on readthedocs in the live session

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.