# Scientific Software Development with Python

Project management and version control



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- 1. Course overview
- 2. Agile software development
- 3. Version control with git
- 4. Project pitches



#### The three fundamental functions of software<sup>1</sup>:

- 1. Performing its given task
- 2. Affording change
- 3. Communicate to its readers

<sup>&</sup>lt;sup>1</sup>Adapted from *Martin, Robert C. Agile software development: principles, patterns, and practices.* 



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Technical

Organisational

Project planning & management

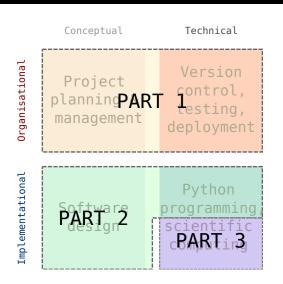
Version control, testing, deployment (DevOps)

Implementational

Software design Python programming, scientific computing

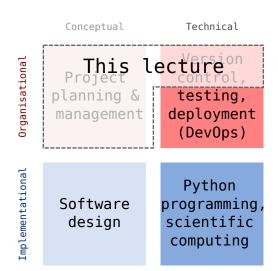
September 9, 2020 4 / 67





September 9, 2020 5 / 67





September 9, 2020 6 / 67



1. Course overview

# 2. Agile software development

3. Version control with git

4. Project pitches

#### **Introductory discussion**



- 1. Discussion in breakout rooms (5 min):
  - Presents yourself to your colleagues
  - Discuss following questions:
    - How big are the projects that your are involved in?
    - How are these projects managed?
- 2. Presentation of results from breakout rooms (< 1 min / room)
  - Select a speaker to summarize results.

September 9, 2020 8 / 67



## 90s and Early 00s:

- Heavyweight development processes prevalent in the software industry:
  - Detailed documentation and planning
  - Sequential process with big, heavy releases
- Problems:
  - Unsuited for complex/explorative projects
  - Can't incorporate change

## Emergence of agile practices:

- 90s: Development of programming and design practices to address problems of heavyweight processes
- 00s: Generalization of agile practices to a management framework.

September 9, 2020 9 / 67



#### **Values**

- 1. Individuals and interactions over processes and tools
- 2. Working software over comprehensive documentation
- **3.** Customer collaboration over contract negotiation
- **4.** Responding to change over following a plan

September 9, 2020 10 / 67



#### **Principles**

- 1. Customer satisfaction highest priority
- 2. Welcome changing requirements
- 3. Deliver working software frequently
- Business people and developers must work together daily throughout the project
- 5. Build projects around motivated individuals
- **6.** Face-to-face conversation to convey information

September 9, 2020 11 / 67



#### Principles — in science

- Customer satisfaction highest priority (✓)
- 2. Welcome changing requirements <
- 3. Deliver working software frequently <
- 4. Business people and developers must work together daily throughout the project
- 5. Build projects around motivated individuals <
- **6.** Face-to-face conversation to convey information (✓)

September 9, 2020 12 / 67



#### **Principles**

- 7. Working software is the primary measure of progress
- 8. Sustainable working pace
- 9. Technical excellence and good design
- 10. Simplicity: Maximizing the amount of work not done
- **11.** The best results emerge from self-organizing teams
- **12.** Regular reflection on how to become more effective

September 9, 2020 13 / 67



#### Principles — in science

- Working software is the primary measure of progress ✓
- **8.** Sustainable working pace ???
- 9. Technical excellence and good design ????
- **10.** Simplicity: Maximizing the amount of work not done ✓
- The best results emerge from self-organizing teams ✓
- **12.** Regular reflection on how to become more effective ???

September 9, 2020 14 / 67



#### Agile principles, summarized

- Self-organizing, cross-functional teams
- Early delivery, evolutionary development
- Flexible response to change

There is considerable overlap between agile principles and research. This makes many agile approaches applicable also for our work.

September 9, 2020 15 / 67

## So, what does it mean?



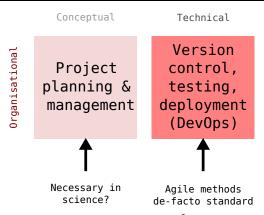
Project planning & management management Conceptual Technical

Version control, testing, deployment (DevOps)

- Organizational-conceptual level: Agile management practices
- Organizational-technical: Agile development techniques

September 9, 2020 16 / 67





- Organizational-conceptual level: ???²
- Organizational-technical: Agile techniques are de facto standard

September 9, 2020 17 / 67

<sup>&</sup>lt;sup>2</sup>I, personally, don't know. Hopefully, we'll find out during the course.

# Agile project management



#### Iterative development

- · Release early and often
- Work is performed in sprints.
- A sprint consists of three phases:
  - 1. Planning
  - 2. Implementation
  - 3. Reflection

September 9, 2020 18 / 67



#### **Project planning**

- Acknowledge uncertainty:
  - Not all can be known details from the start
  - Requirements are likely going to change during the process
- Keep it simple:
  - Focus on functionality from user perspective (features)
  - Omit implementation details
- Be flexible:
  - The project plan may change during the project

September 9, 2020 19 / 67



#### **User story**

- informal, natural language description of a feature
- Represents a requirement

#### **Backlog**

- Collection of user stories that define the project
- Task pool for next development iteration
- Can be extended throughout the project

The backlog defines the project scope. It is the essential planning tool of agile project management.

September 9, 2020 20 / 67



## 1. Sprint planning

- Defines the work to be done in a sprint by selecting user stories from the backlog
- The team decides how the stories should be implemented
- Amount of work based on *velocity* estimates from previous iteration
- Defines how increment should be delivered

Result of the sprint planning should be a tangible **sprint goal**, which the team commits to as a whole.

September 9, 2020 21 / 67



#### **During the sprint**

- The team self-organizes its work to reach the sprint goal
- Short but regular meetings to optimize the probability to reach the sprint goal
- During meeting, each team member explains<sup>3</sup>:
  - 1. What did I do since the last meeting that helped the team meet the sprint goal?
  - 2. What will I do now to help the team reach the sprint goal?
  - **3.** Do I see any impediments that may prevent the development team from reaching the sprint goal?

September 9, 2020 22 / 67

<sup>&</sup>lt;sup>3</sup>Adapted from https://www.scrumguides.org/docs/scrumguide/v2016/2016-Scrum-Guide-US.pdf



#### After the sprint

- Sprint review:
  - Which user stories have been implemented?
  - What problems occured?
  - What is the current state of the backlog?
  - How to proceed?
    - Input for next sprint planning
- 2. Retrospective
  - The team reflects on its development process
  - The team identifies ways to:
    - Make work more effective and enjoyable
    - Increase product quality
  - The team decides which improvements it wants to implement in the next iteration

September 9, 2020 23 / 67

## Your project work



- Project work will be done in four sprints
- After each sprint, all teams will present their progress (retrospectives in schedule)<sup>3</sup>

The purpose of the retrospectives is to learn from each other. Share your experiences. Focus on your learnings and problems.

September 9, 2020 24 / 67



- 1. Course overview
- 2. Agile software development
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#### git

- Created by Linus Torvalds for the development of the Linux kernel
- Distributed version-control system:
  - Keeps track of changes in source code
  - Allows synchronizing changes with repositories in arbitrary locations
- Usage:

```
$ git <command> <args>
```

September 9, 2020 26 / 67



#### GitHub

- One of several hosting services for git repositories
- Additional features:
  - Simple web hosting
  - Communication platform
  - Issue tracking

If you don't have an account, get one at https://github.com!

September 9, 2020 27 / 67



Branch

## **Principles**

- git tracks development as a sequence of changes in repositories
- Examples of changes:
  - Adding a file
  - Removing/renaming a file
  - Changing its content

September 9, 2020 28 / 67



Branch

#### **Principles**

- A single sequence of changes is called a branch
- the current state of your directory is defined by which branch is checked out (grey rectangle)
- The currently checked out files are referred to as the working tree

September 9, 2020 29 / 67



```
$ git status
```

• Prints all relevant information about the current repository:

```
On branch main
Your branch is up to date with
Changes not staged for commit:
                           to update what will be committed)
  (use
                               to discard changes in working directory)
  (use
  modified: README.md
Untracked files:
                           to include in what will be committed)
  (use
  STUDENT_LIST.md
no changes added to commit (use
                                           and/or
```

September 9, 2020 30 / 67



#### Your identity

```
$ git config --global user.name
$ git config --global user.email your_email@chalmers.se
```

#### Your editor

```
$ git config --global core.editor vim # or emacs, nano, ...
```

#### **Default branch name**

Change default branch name to main<sup>4</sup>:

```
$ git config --global init.defaultBranch main
```

September 9, 2020 31 / 67

<sup>4</sup>https://tools.ietf.org/id/draft-knodel-terminology-00.html

# Creating an empty repository



Branch

main

## Creating an empty repository

#### \$ git init

 Creates and initializes an empty repository in the current directory

September 9, 2020 32 / 67

# **Committing changes**



Branch

main

#### **Committing changes**

- Staging: git add marks changed or new files for the next commit
- **2. Commiting**: git commit adds the changes from the staged files as an atomic change to the repository<sup>5</sup>

September 9, 2020 33 / 67

<sup>&</sup>lt;sup>5</sup>Explicit staging can be skipped by using git commit followed by a list of file names.

# **Committing changes**



#### Branch

```
Change 1 -------main
```

New file: README.md New file: LICENSE.md

#### **Committing changes**

or

```
$ git commit README.md LICENSE.md
```

September 9, 2020 34 / 67



#### Branch

```
Change 1 - main

New file: README.md

New file: LICENSE.md
```

- Use git log to list the most recent changes in branch
- Commits are identified by their checksum (the long, seemingly random number on the second line)

```
$ git log
commit 21959efd7528a00fab48062473f0409acd74e113 (HEAD -> main)
Author: Simon Pfreundschuh <simon.pfreundschuh@chalmers.se>
Date: Mon Sep :09:44 +0200

Added README and LICENSE files.
```

September 9, 2020 35 / 67



Branch

Change 1 Change 2 main





- Branching allows experimenting with new features at the same time as keeping a snapshot of the currently working code
- Use git branch to create a new branch:

```
$ git branch new_feature
```

September 9, 2020 37 / 67





- However, currently we are still on the main branch<sup>6</sup>
- All git commands affect the branch that is currently checked out, i.e. main.

September 9, 2020 38 / 67

 $<sup>^{\</sup>rm 6} Indicated$  by grey rectangle in figure. Use git  $\,$  status to verify.





• To switch to the new branch we need to *check it out*<sup>7</sup>:

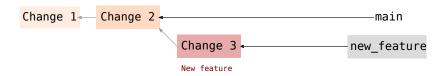
```
$ git checkout new_feature
```

 Since the development in both branches is identical, the working directory doesn't change.

September 9, 2020 39 / 67

<sup>&</sup>lt;sup>7</sup>Alternatively, use git checkout -b <br/>branch\_name> to create new branch and to check it out immediately.





• We can now add the new feature to the branch:

```
$ git add new_feature.py
$ git commit
```

September 9, 2020 40 / 67

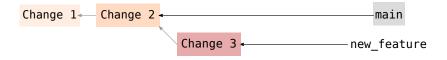




- Integrating changes from another branch is called merging
- To merge the changes in new\_feature into main:

September 9, 2020 41 / 67



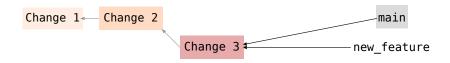


- Integrating changes from another branch is called merging
- To merge the changes in new\_feature into main:
  - 1. Checkout main

\$ git checkout main

September 9, 2020 42 / 67





- Integrating changes from another branch is called merging
- To merge the changes in new\_feature into main:
  - 1. Checkout main

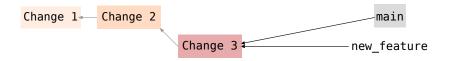
```
$ git checkout main
```

2. Merge:

```
$ git merge new_feature
```

September 9, 2020 43 / 67





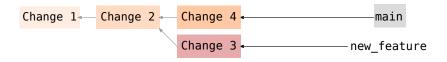
## Fast forwarding

• The special case where the branch to merge is simply ahead of the other branch is called **fast forwarding**.

Fast forwarding is trivial

September 9, 2020 44 / 67



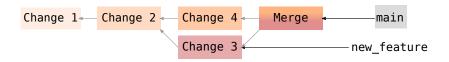


## **Diverging branches**

- However, typically the branches will diverge
- In this case a merge operation is required, which itself is a change committed to the repository

September 9, 2020 45 / 67





## **Diverging branches**

- However, typically the branches will diverge
- In this case a merge operation is required, which itself is committed to repository
- If the changes to merge affect identical lines in the same files, a conflict occurs, which has to be resolved manually.

September 9, 2020 46 / 67



Local Change 1  $\leftarrow$  Change 2  $\leftarrow$  Change 3  $\leftarrow$  Change 4  $\leftarrow$  main

### Remotes

- Distributed version control: Every repository can be synchronized with multiple other repositories in different locations.
- A separate repository setup to track the same development is called a remote

September 9, 2020 47 / 67

# **Working with remotes**



Branch



### Remote

github.com/see-mof/ssdp

## Adding a remote

```
$ git remote --add <remote_name> https://github.com/see-mof/ssdp
```

• If the remote is a newly created repository it is still empty.

September 9, 2020 48 / 67



## **Publishing local development**

 The -u option tells git, which remote branch main should track

```
$ git push -u <remote_name> <branch> # here: git push -u origin main
```

• This becomes the default location for future pushes:

```
$ git push # Same as: git push origin/main
```

September 9, 2020 49 / 67



```
Branch

Local Change 1 ← Change 2 ← main

tracks

Remote Change 1 ← Change 2 ← origin/main
```

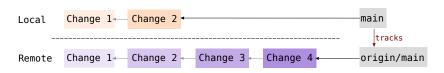
## Fetching changes from remote

- git keeps local copy of remote branches
- They are denoted by <remote\_name>/<branch\_name>
- git fetch updates the local copy of the remote branch:

```
$ git fetch origin main
```

September 9, 2020 50 / 67





## Fetching changes from remote

- git keeps local copy of remote branches
- The are denoted as <remote\_name>/<branch\_name>
- git fetch <remote\_name> <branch\_name> updates the local copy of the remote branch:

```
$ git fetch origin main
```

September 9, 2020 51 / 67



## Merging the local branch

 To update the local branch main, merge the local copy of the remote branch

```
$ git merge origin/main
```

September 9, 2020 52 / 67



## Pulling changes from remote

• git pull combines the fetch and merge commands:

```
$ git pull origin main
```

or

```
$ git pull # sufficient, if local branch tracks remote
```

September 9, 2020 53 / 67

# Working with remotes



#### Branch

## Cloning a repository

```
$ git clone https://github.com/see-mof/ssdp
```

 This creates a new local repository, adds the target as remote and pulls all branches

September 9, 2020 54 / 67

## git exercise



- Solve tasks 1 and 2 from the git task sheet
- Time 10 minutes
- Help each other in breakout rooms

September 9, 2020 55 / 67

# Working with remotes



#### Branch

## Multiple remotes

It is possible to have multiple remotes<sup>8</sup>:

```
$ git add remote fork https://github.com/simonpf/ssdp
$ git push fork
```

September 9, 2020 56 / 67

<sup>&</sup>lt;sup>8</sup>For example a personal fork of a public repository.

# Distributed development workflow



				Branch
Local	Change 1	Change 2	•	—main
Remote	Change 1←	Change 2		—origin/main

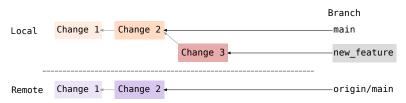
# Contributing to a public repository

1. Clone public repository

September 9, 2020 57 / 67

# Distributed development workflow



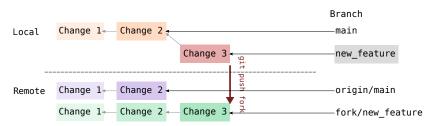


# Contributing to a public repository

- 1. Clone public repository
- 2. Add feature in new branch

September 9, 2020 58 / 67



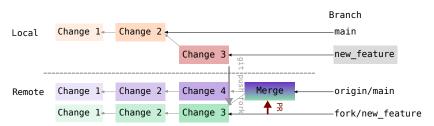


## Contributing to a public repository

- 1. Clone public repository
- 2. Add feature in new branch
- 3. Push new branch to personal fork of public repository

September 9, 2020 59 / 67



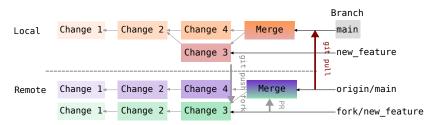


## Contributing to a public repository

- 1. Clone public repository
- 2. Add feature in new branch
- 3. Push new branch to personal fork of public repository
- 4. Make pull request (PR) from fork

September 9, 2020 60 / 67





## Contributing to a public repository

- 1. Clone public repository
- 2. Add feature in new branch
- 3. Push new branch to personal fork of public repository
- 4. Make pull request (PR) from fork
- 5. Update local main branch

September 9, 2020 61 / 67





### Forks and pull requests

- To fork a repository, click the fork symbol in the upper right corner
- To make a pull request, click on Pull requests and then New pull request

September 9, 2020 62 / 67

## git exercise



- Solve tasks 3 and 4 from the git task sheet
- Time: 10 minutes
- Help each other in breakout rooms

September 9, 2020 63 / 67

### git status revisited



```
On branch main
Your branch is up to date with
Changes not staged for commit:
  (use
                           to update what will be committed)
                               to discard changes in working directory)
  (use
 modified: README.md
Untracked files:
                           to include in what will be committed)
  (use
 STUDENT_LIST.md
no changes added to commit (use
                                          and/or
```

September 9, 2020 64 / 67



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## **Project requirements**



- Final project published a Python package
- Installable via pip
- Automated test suite with high coverage (> 90%)
- Automated deployment
- Online documentation hosted on GitHub or Read The Docs.

September 9, 2020 66 / 67

# **Project pitches**



- Maximum 5 minutes per presentation
- Ideally more than two persons per project
- If you work alone, please find someone to discuss your progress with and review code

September 9, 2020 67 / 67