



PYTHON SEMINAR 2020

JENS HAHN

THEORETICAL BIOPHYSICS

TODAY



I Organisational Matters

II What to Expect

III git

I. ORGANISATIONAL MATTERS

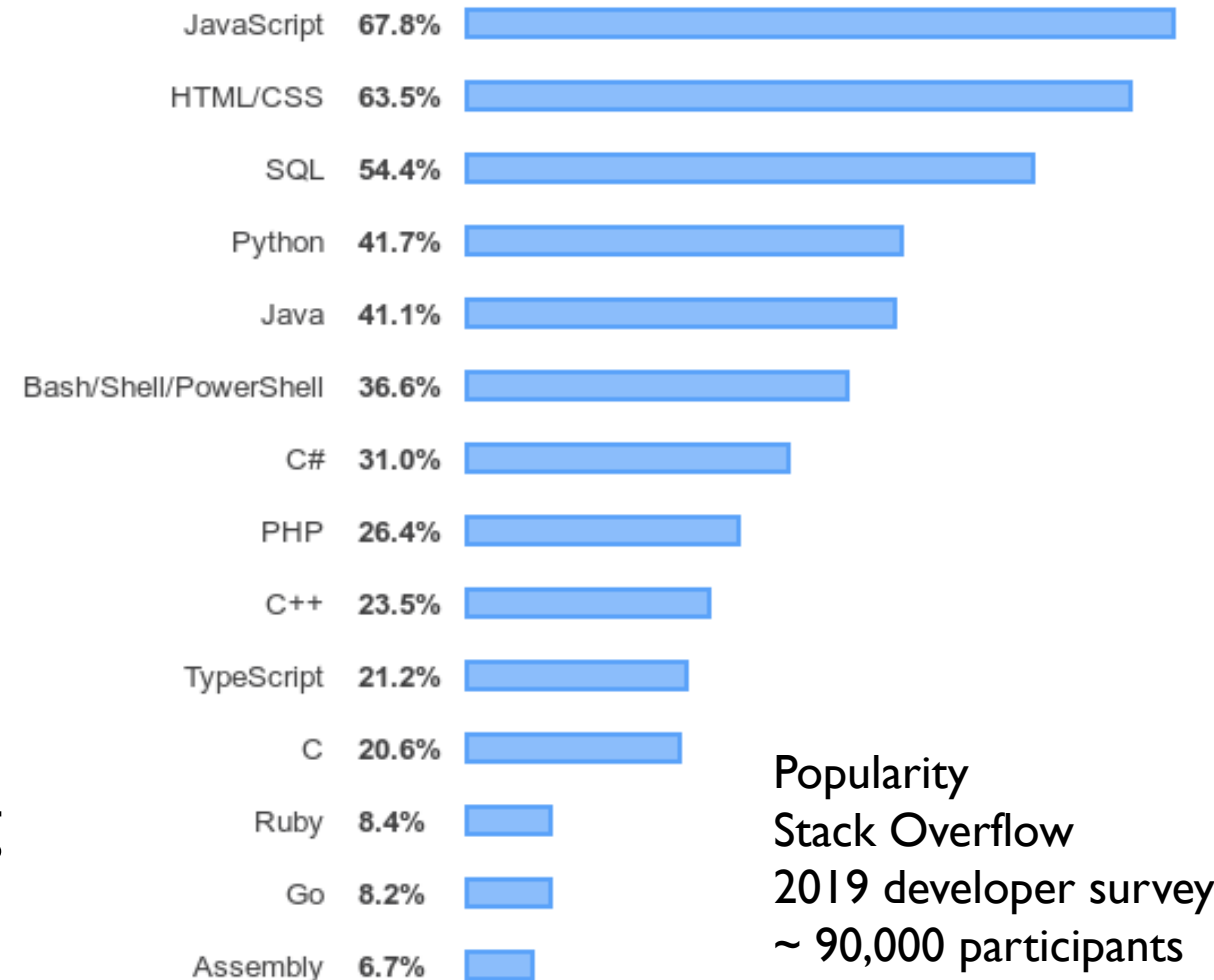


- Not a stand-alone course officially
- No credits, but a certificate
- Mailing list, git and GitHub, no Moodle

II. WHY PYTHON?



- Open-source
- Easy to read
- Large library for scientific purposes
- Flexible
- ‘fastest-growing major programming language today’



II. THIS COURSE



Date	Topic	Tools/software/packages
27/04	Introduction	Git, GitHub
04/05	Python introduction	notebook++, Sublime Text, PyCharm, JupyterLab, ...
11/05	Python basics	Data structures, flow control
18/05	Python basics	Functions, built-ins
25/05	Python basics	Classes, objects
01/06	-	-
08/06	Data analysis	pandas
15/06	Visualisation	matplotlib
22/06	More packages	Collections, numpy
29/06	Modelling	scipy, numpy, matplotlib
13/07	?	?

II. LEARNING PYTHON



More than syntax!

- Online tutorials available (codecademy, ...)
- Python is not Matlab/Octave, Mathematica

This seminar offers

- How to solve problems
- Style guide (code & comments)
- Versioning (project management)
- Testing (efficiency)

II. WHEN TO WRITE A SCRIPT



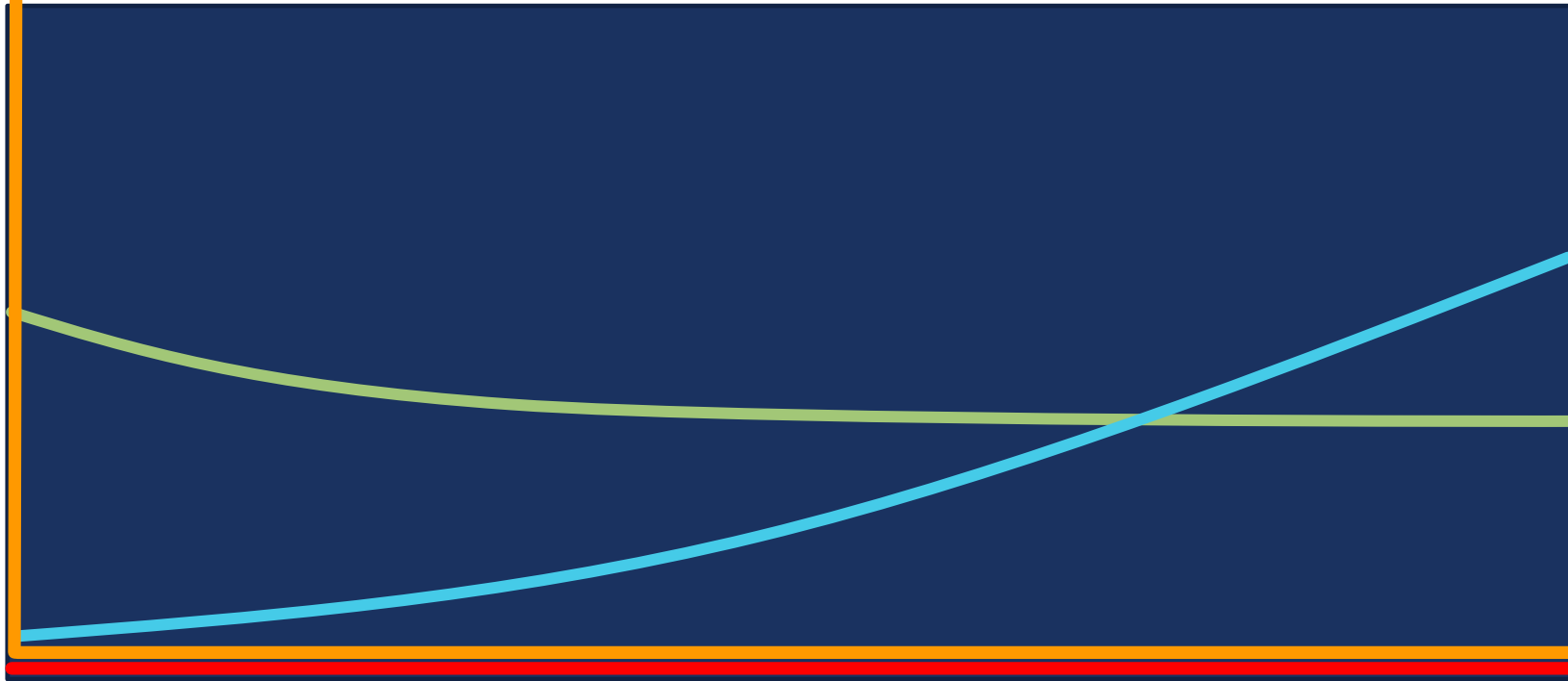
Scripted
Time per task

Manual
Time per task

Mistakes
Manual







Mistakes
Scripted

Task repeats



III. VERSIONING



-  thesis.pdf
-  thesis_final.pdf
-  thesis_final2.pdf
-  thesis_final2_corrected.pdf
-  thesis_new.pdf
-  thesis_new2.pdf

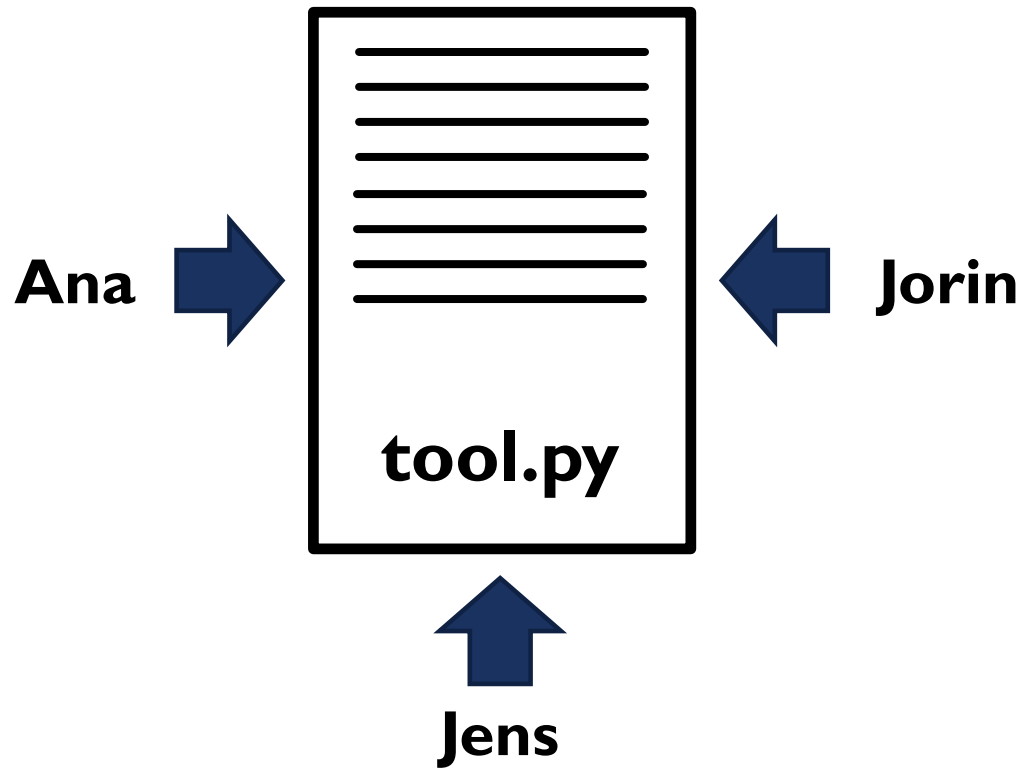
 20170105	 20170110	 20170115	 20170205	 20170210	 20170215	 20170305
 20170310	 20170315	 20170405	 20170410	 20170415	 20170505	 20170510
 20170515	 20170605	 20170610	 20170615	 20170705	 20170710	 20170715
 20170805	 20170810	 20170815	 20170905	 20170910	 20170915	 20171005
 20171010	 20171015	 20171105	 20171110	 20171115	 20171205	 20171210
 20171215	 20180105	 20180110	 20180115	 20180205	 20180210	 20180215
 20180305	 20180310	 20180315	 20180405	 20180410	 20180415	 20180505
 20180510	 20180515	 20180605	 20180610	 20180615	 20180705	 20180710
 20180715	 20180805	 20180810	 20180815	 20180905	 20180910	 20180915
 20181005	 20181010	 20181015	 20181105	 20181110	 20181115	 20181205
 20181210	 20181215					

III. VERSIONING



- Cooperation
- Project documentation (descriptions, explanations, manual)
- Task list (assigned co-worker, due date)
- Keep everything together

III. COOPERATION



Date	Author	Change
05/03/2018 – 4.03 pm	Jens	Create draft
05/03/2018 – 4.10 pm	Ana	Added chapter I
05/03/2018 – 6.08 pm	Jorin	Added feature X
05/03/2018 – 6.30 pm	Jorin	Debugged feature X
06/03/2018 – 11.40 am	Ana	Added feature Y
06/03/2018 – 2.30 pm	Ana	Merged
07/03/2018 – 6.01 pm	Jens	Added feature Z

III. GIT

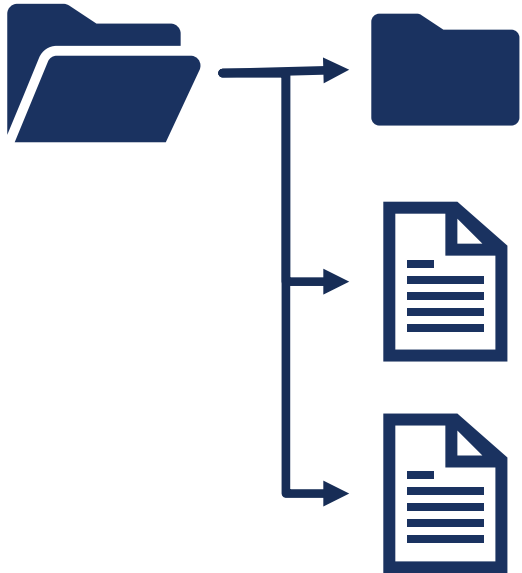


- Open source
 - Track and save all changes (with short description)
-
- Secure cloud storage
 - Wiki, issue tracking
 - Project management
 - Cooperation

III. REPOSITORIES



File on my computer

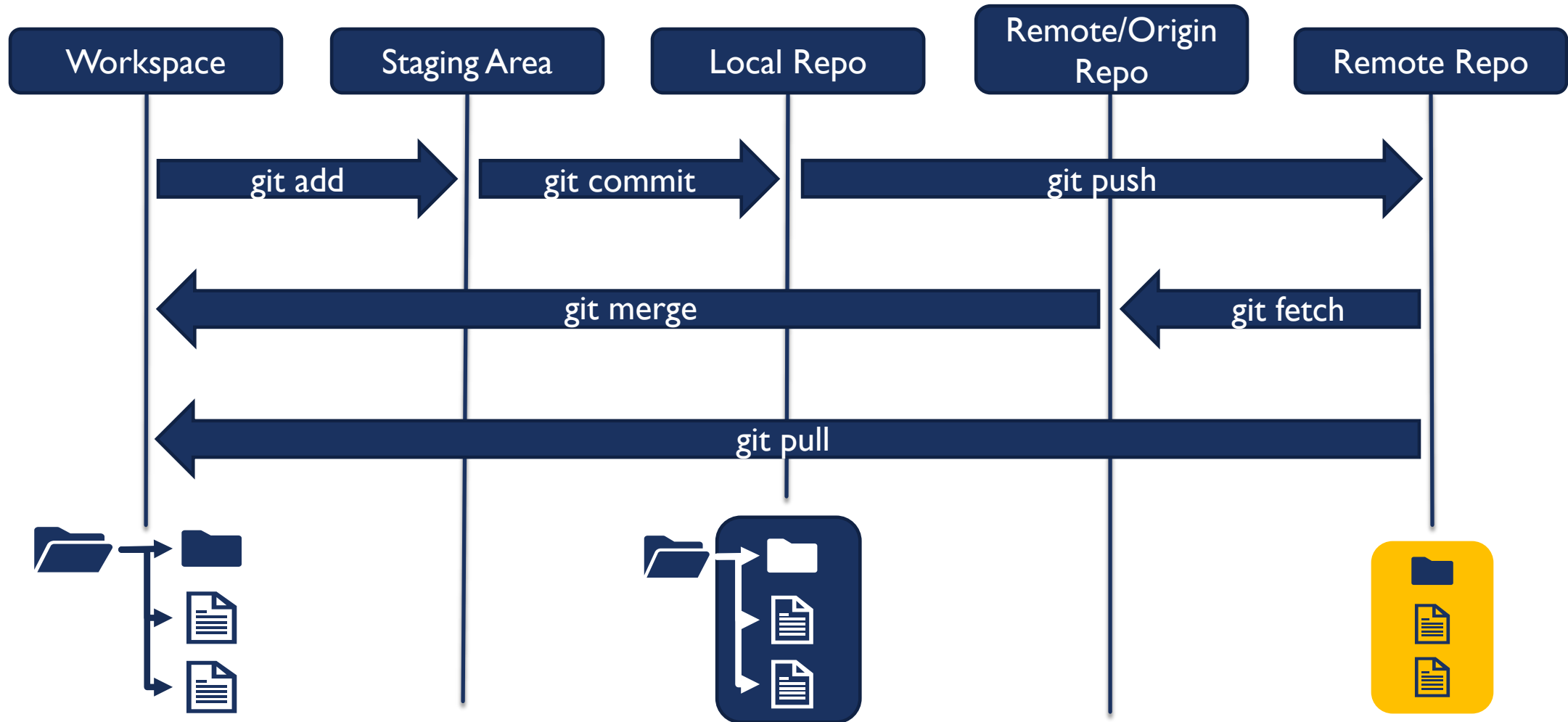


Turn into repository



- git will track changes
- changes can be saved
- changes can be reverted
- different 'versions' of folder

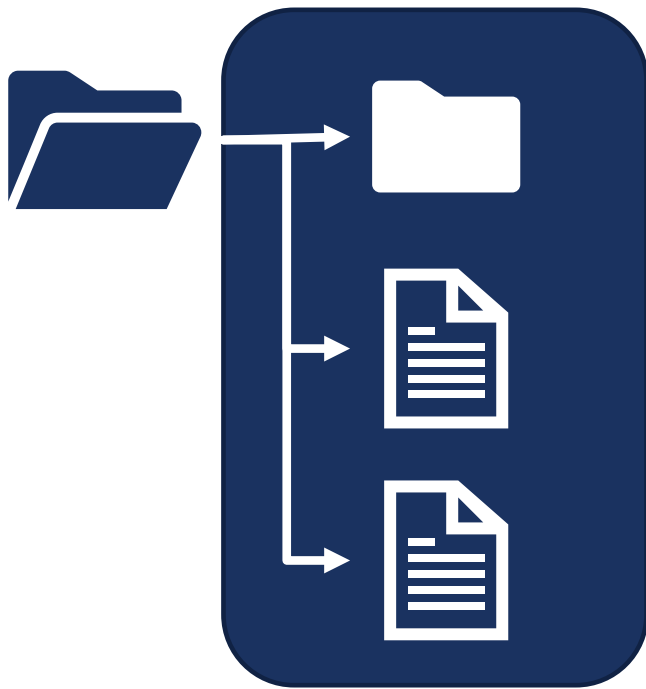
III. GIT STAGES



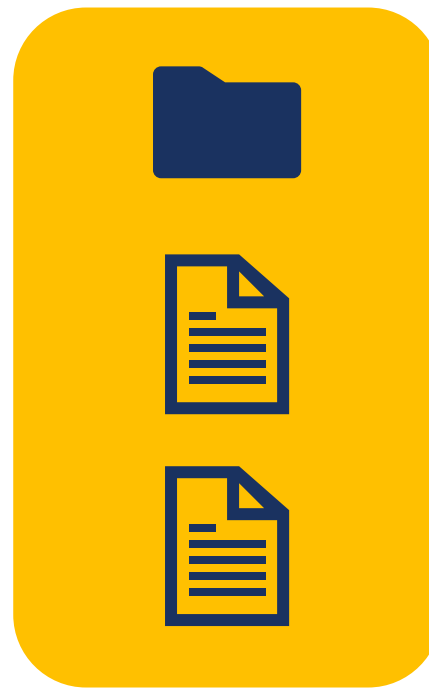
III. REPOSITORIES



On your computer



On server



Collaborator's PC



III. GIT FROM AN EXISTING REPO



Get files from
git repository

`git clone ...`



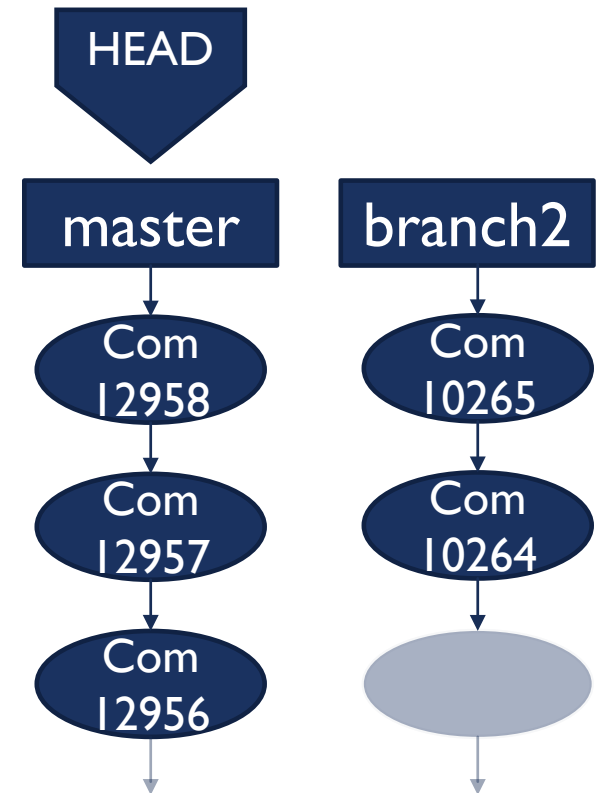
Add files to repo
Add to tracking

`git add ...`



Save state of
tracked files

`git commit ...`



III.

bitbucket.com



WCM



Source



Commits



Branches



Pull requests



Pipelines



Issues



Wiki



Downloads



Boards



Settings

WCM-Team / Untitled project

WCM

Clone



default



Filter files



/

Name

Size

Last commit

Message



GUI



_deprecated



_parked



html



python_models



python_models_for_testing



sbml_models



sbtabs



src



.hgignore

1.11 KB

2015-02-03

Minor



CDC_core.pkl

41.77 KB

2016-02-06

added script to change id to name (S...



ReadSBML.py

11.86 KB

2015-07-24

CDC conversion to reactions finished

PythonSeminar2019

- Project
- Details
- Activity
- Releases
- Cycle Analytics

- Repository
- Issues 0
- Merge Requests 0
- CI / CD
- Operations
- Registry
- Wiki
- Snippets
- Settings

TheoreticalBiophysics > PythonSeminar2019 > Details

PythonSeminar2019

Project ID: 11854950

Star0

Fork0

Clone

GNU GPLv3 1 Commit 1 Branch 0 Tags 0 Bytes Files

Repository of the Python Seminar 2019



Auto DevOps

It will automatically build, test, and deploy your application based on a predefined CI/CD configuration.

Learn more in the [Auto DevOps documentation](#)

Enable in settings

master pythonseminar2019 / + History Find file Web IDE

Add LICENSE

Jens Hahn authored 8 hours ago

bc53b334

- README
- Add CHANGELOG
- Add CONTRIBUTING
- Add Kubernetes cluster
- Set up CI/CD

Name	Last commit	Last update
LICENSE	Add LICENSE	8 hours ago
README.md	Initial commit	8 hours ago

README.md

[Pull requests](#)[Issues](#)[Marketplace](#)[Explore](#)[tbphu](#) / [Python_course](#)[Unwatch](#)

13

[★ Star](#)

2

[Fork](#)

33

[Code](#)[Issues](#) 0[Pull requests](#) 0[Projects](#) 0[Wiki](#)[Insights](#)[Settings](#)Python Seminar - Theoretical Biophysics - Humboldt-Universität zu Berlin <https://rumo.biologie.hu-berlin.de/tb...>[Edit](#)[Manage topics](#)[76 commits](#)[1 branch](#)[0 releases](#)[6 contributors](#)Branch: [master](#)[New pull request](#)[Create new file](#)[Upload files](#)[Find File](#)[Clone or download](#)**abulovic** Some interesting links (prog, viz & otherwise)

Latest commit dc14c37 on Jul 16, 2018

[examples](#)

Some interesting links (prog, viz & otherwise)

9 months ago

[slides](#)

added slides for ode

9 months ago

[solution](#)

Add assignment 2 (data types, flow control)

11 months ago

[20180710_pandas_example.ipynb](#)

added pandas solution

9 months ago

[20180716_ODEexample.ipynb](#)

added ODE example

9 months ago

[agentbased.py](#)

added agentbased model

10 months ago

[agentbased_expanded.py](#)

Add expanded version of the agent-based model

10 months ago

[assignment_1.py](#)

changed assignments and solution for assignments lecture

11 months ago

[assignment_2.py](#)

Add assignment 2 (data types, flow control)

11 months ago

III. GIT IN ACTION



local repository

remote repository

local repository

Ana

Server

Jens



git clone



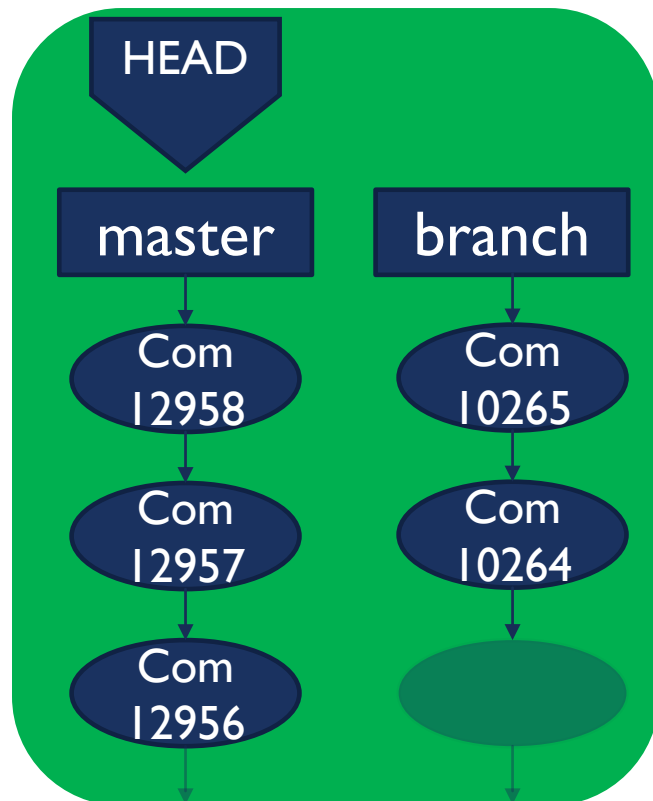
git clone



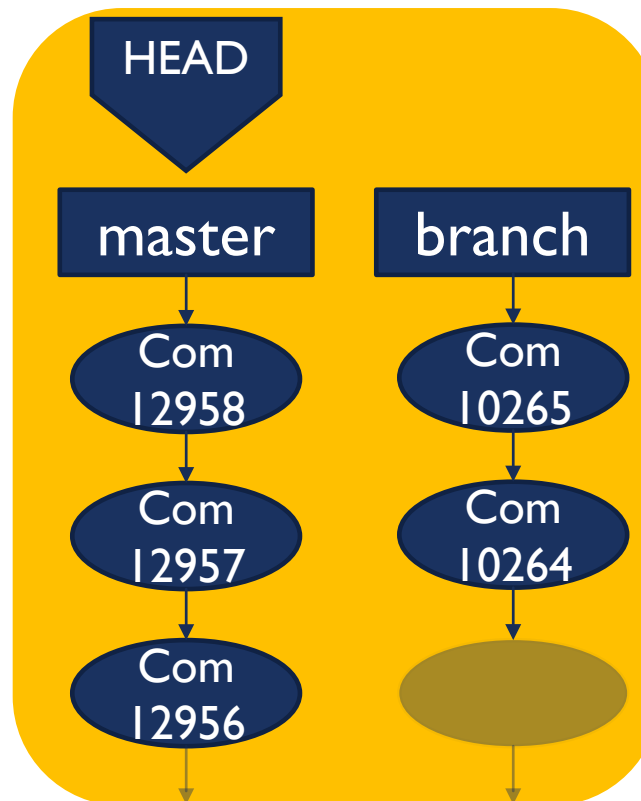
III. GIT IN ACTION



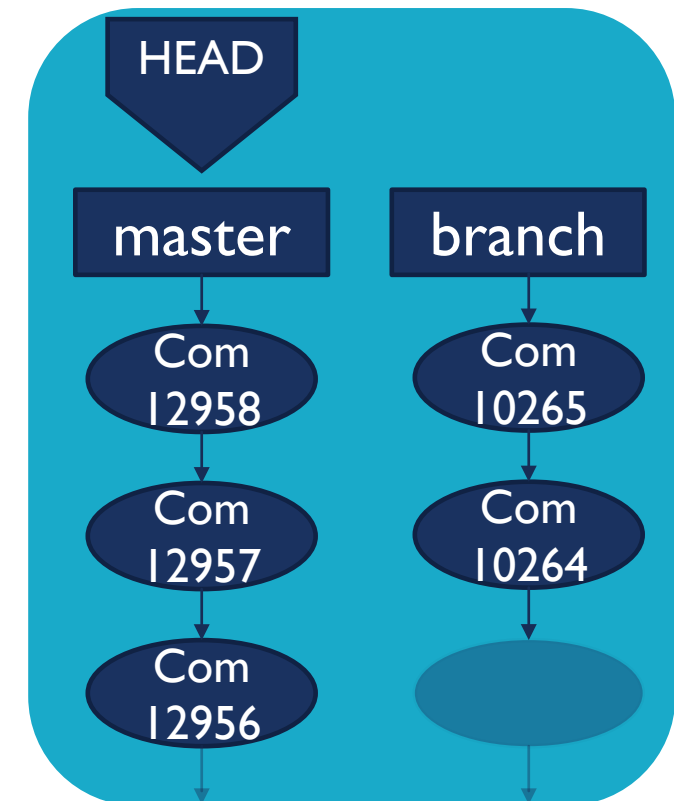
Ana



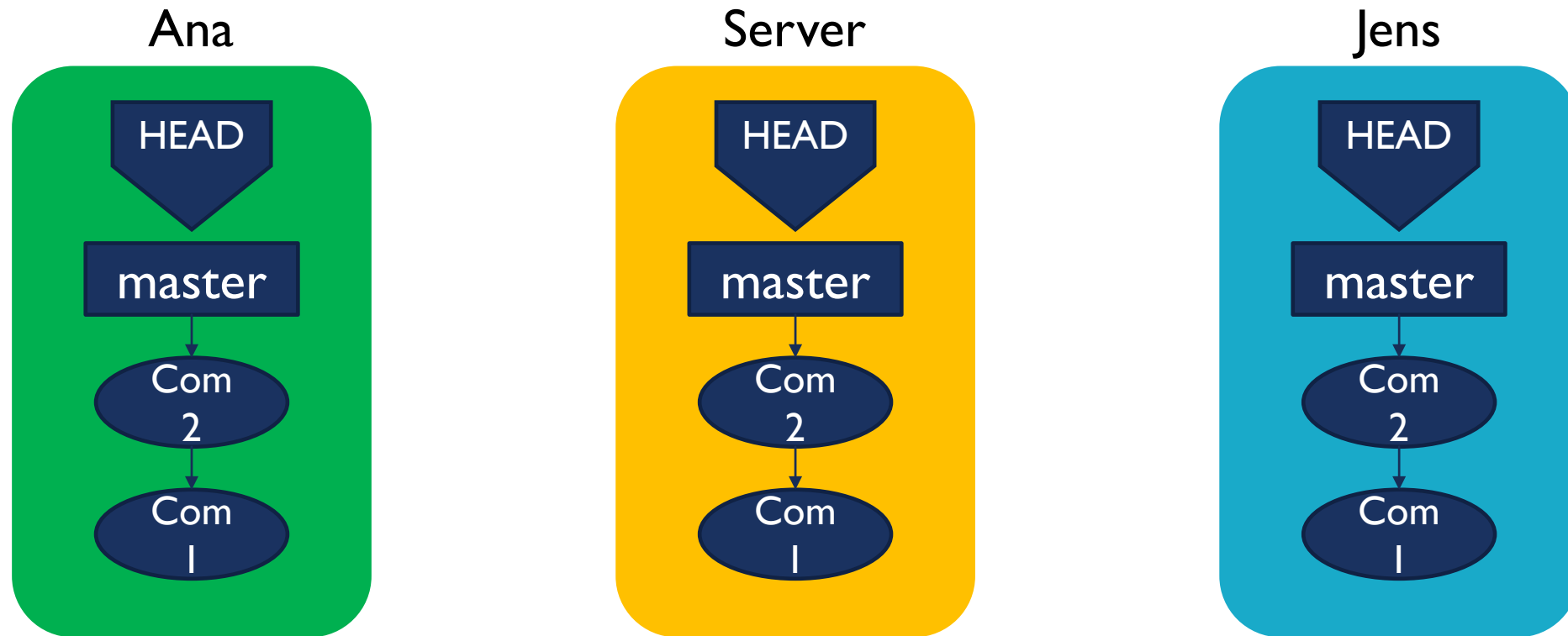
Server



Jens



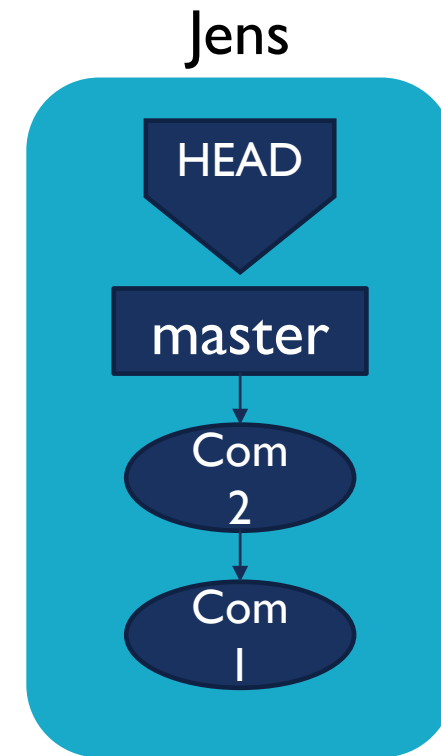
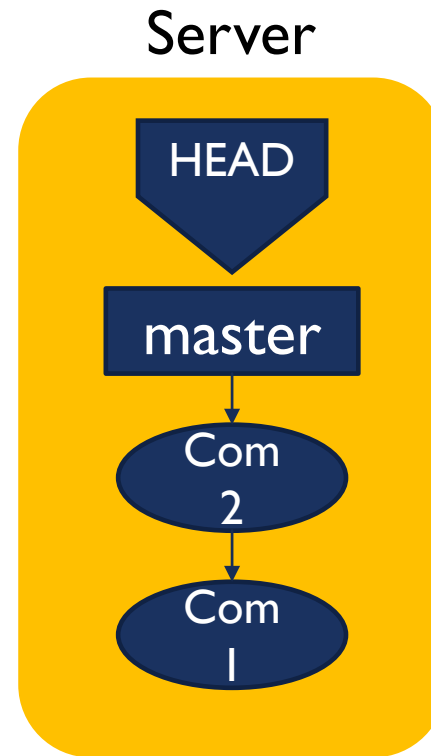
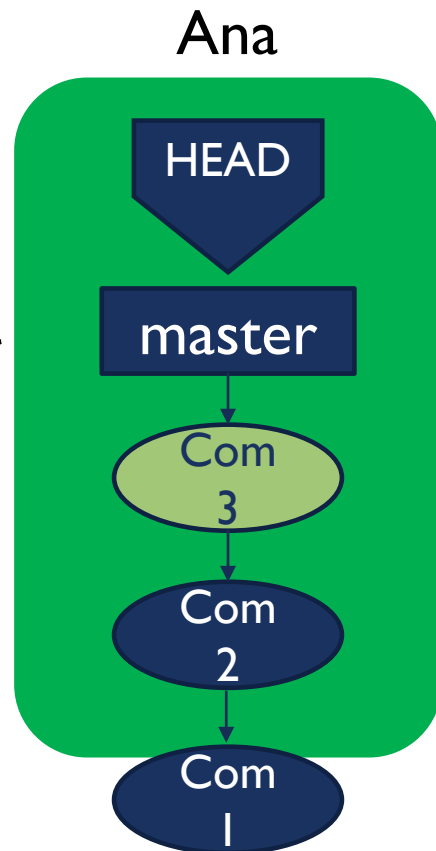
III. GIT IN ACTION



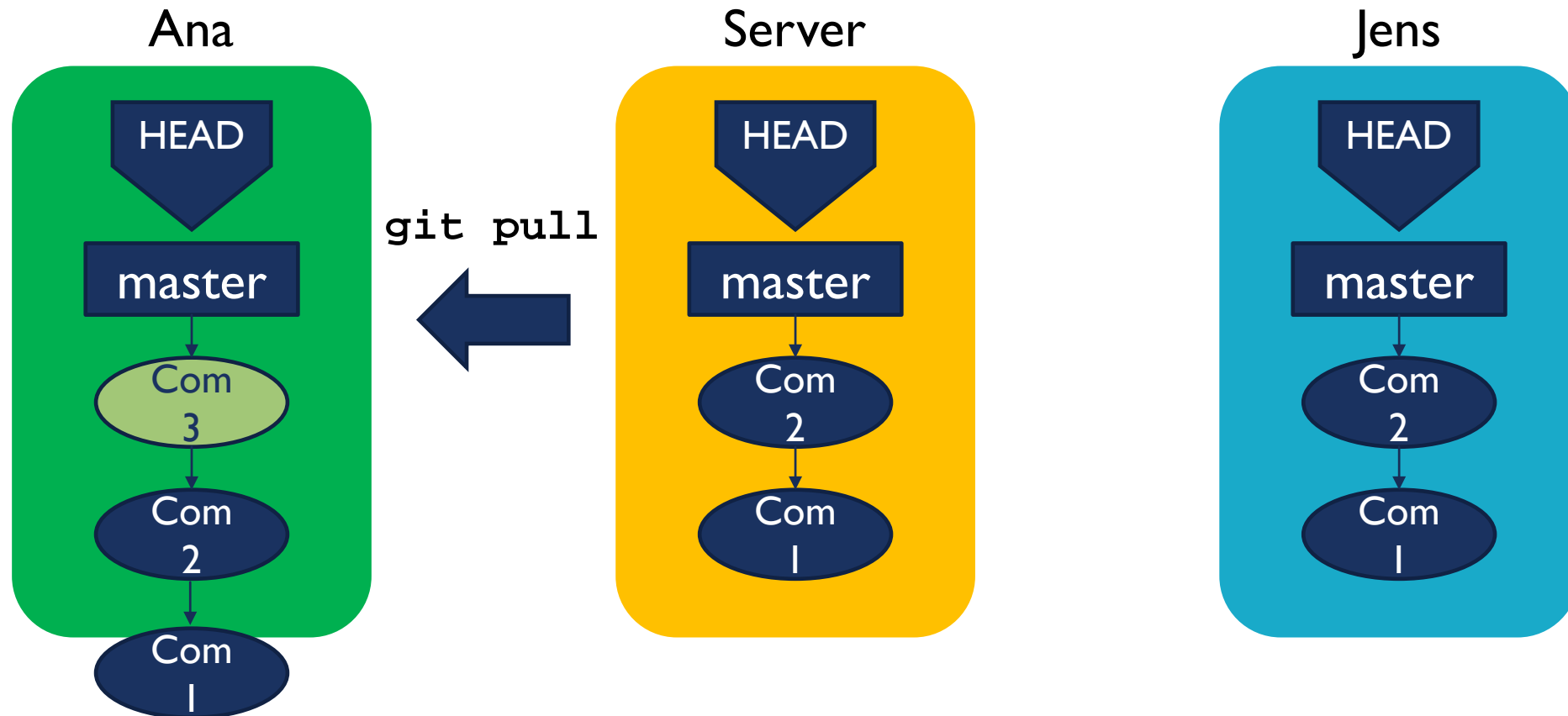
III. GIT IN ACTION



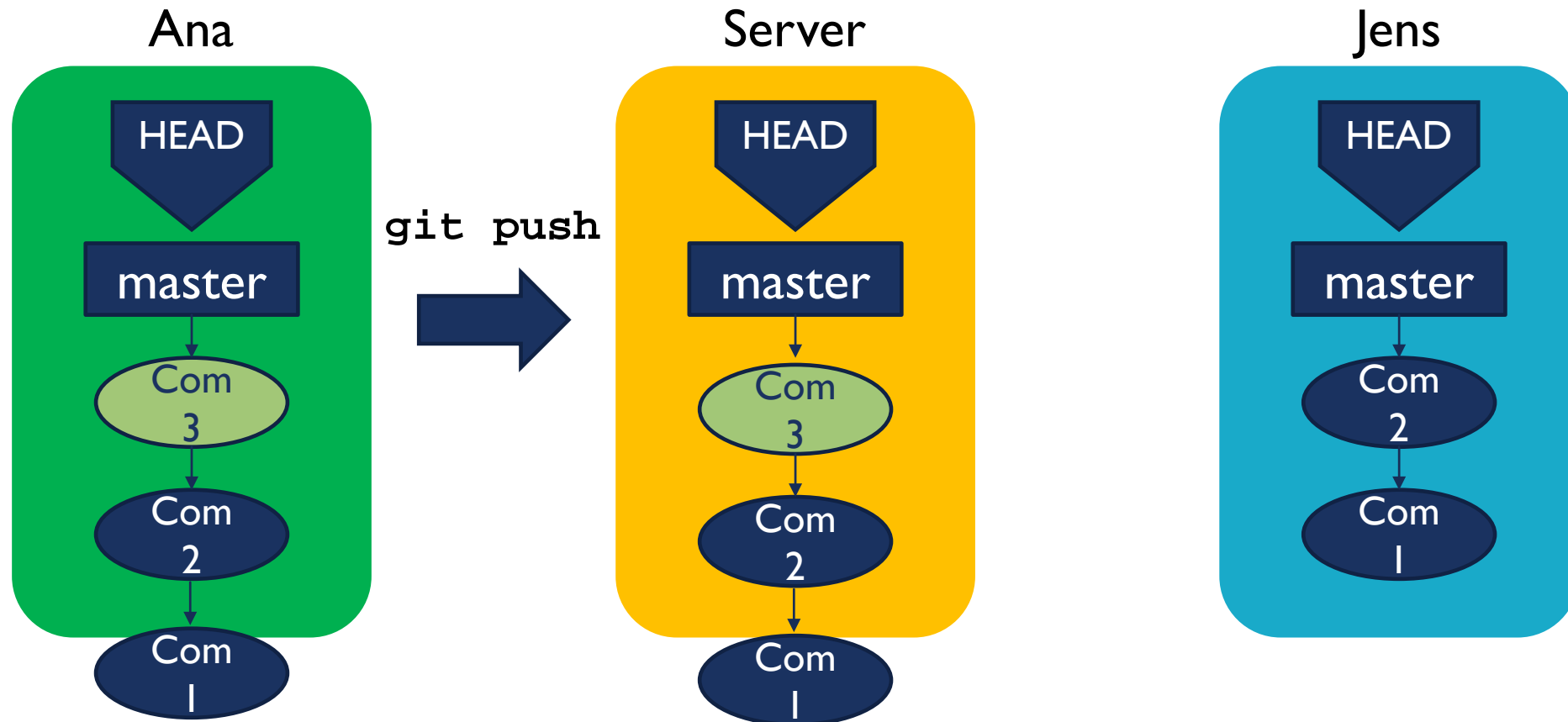
git commit



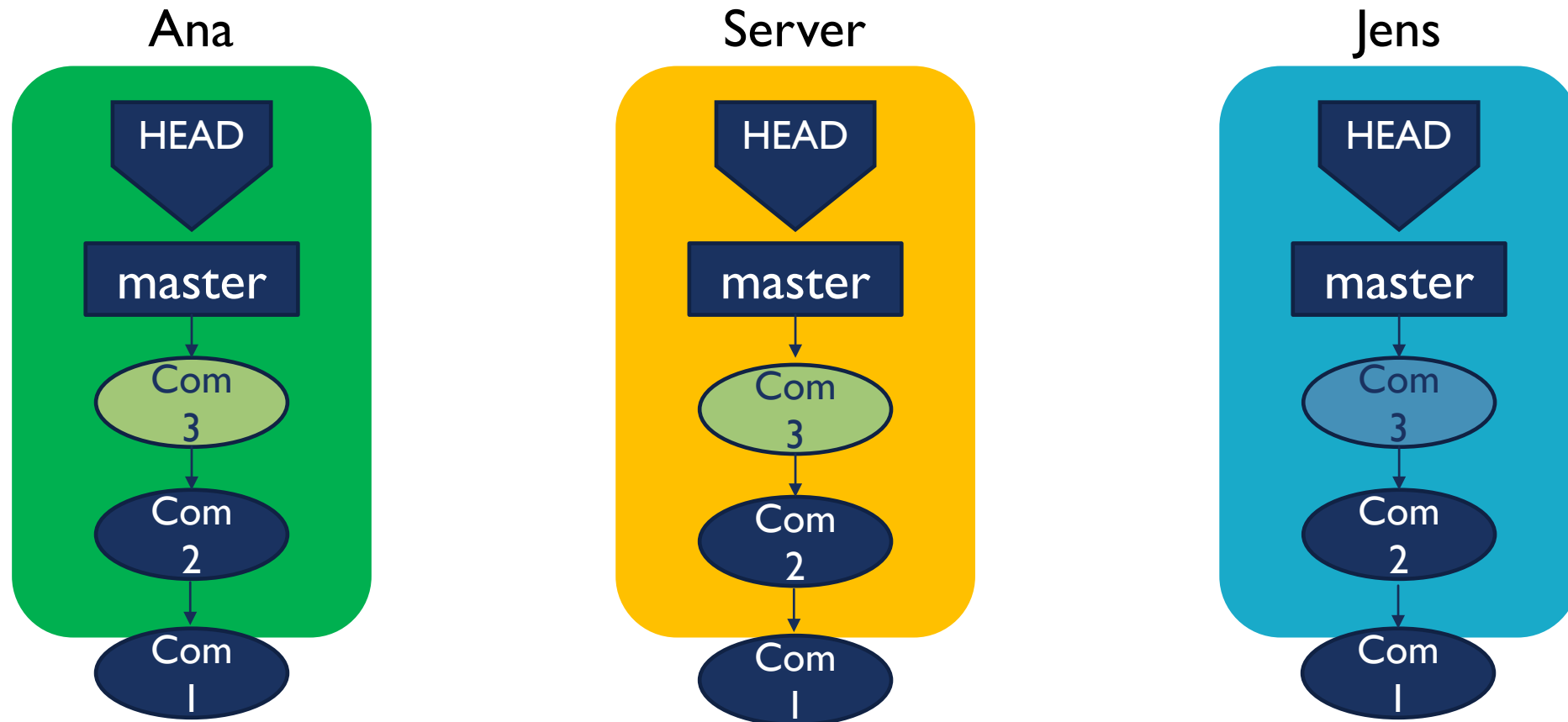
III. GIT IN ACTION



III. GIT IN ACTION

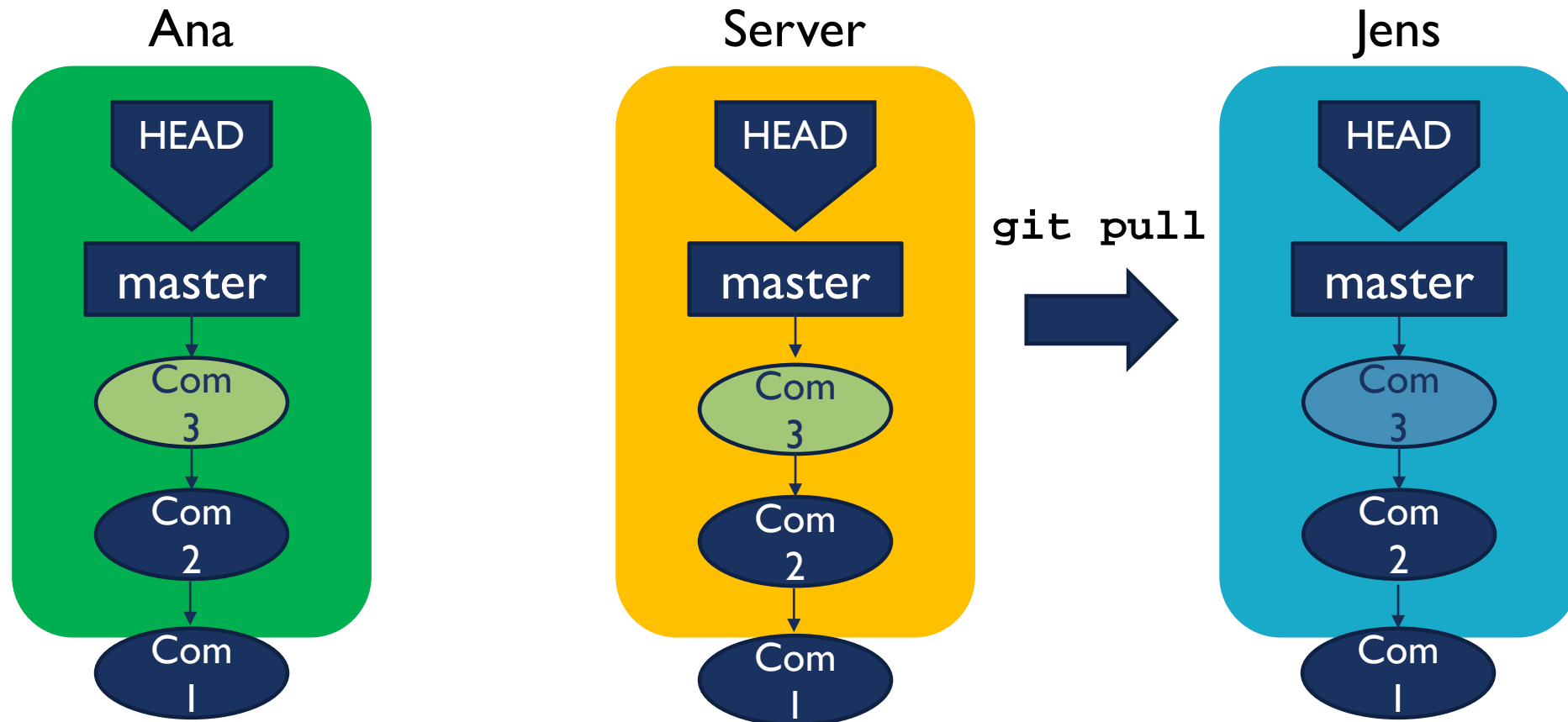


III. GIT IN ACTION

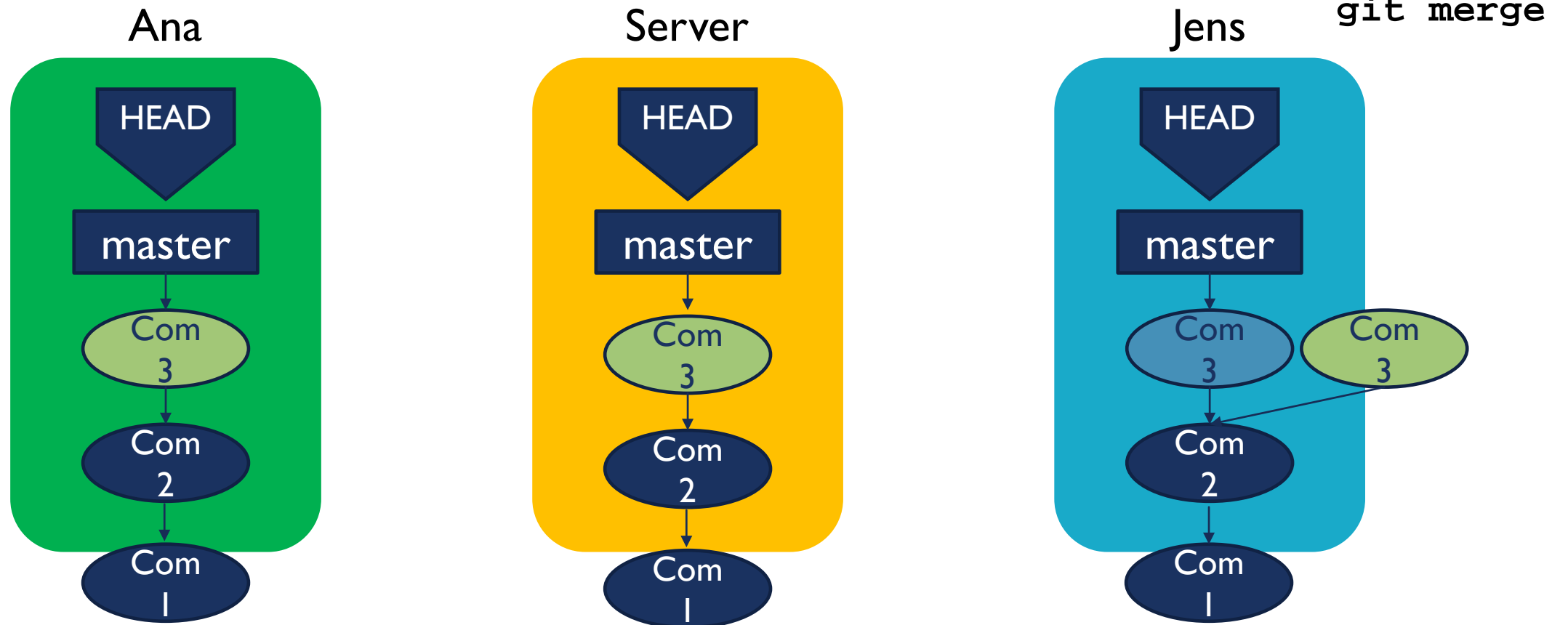


git commit

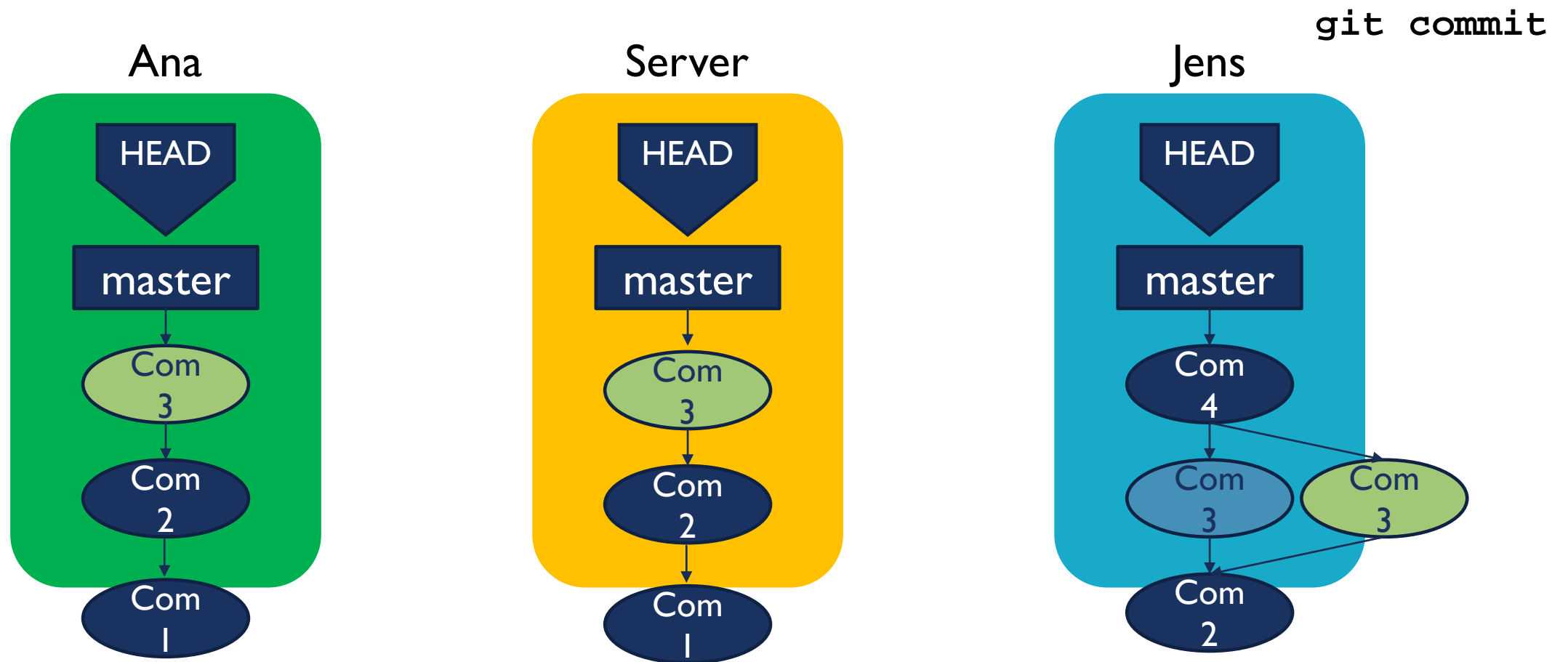
III. GIT IN ACTION



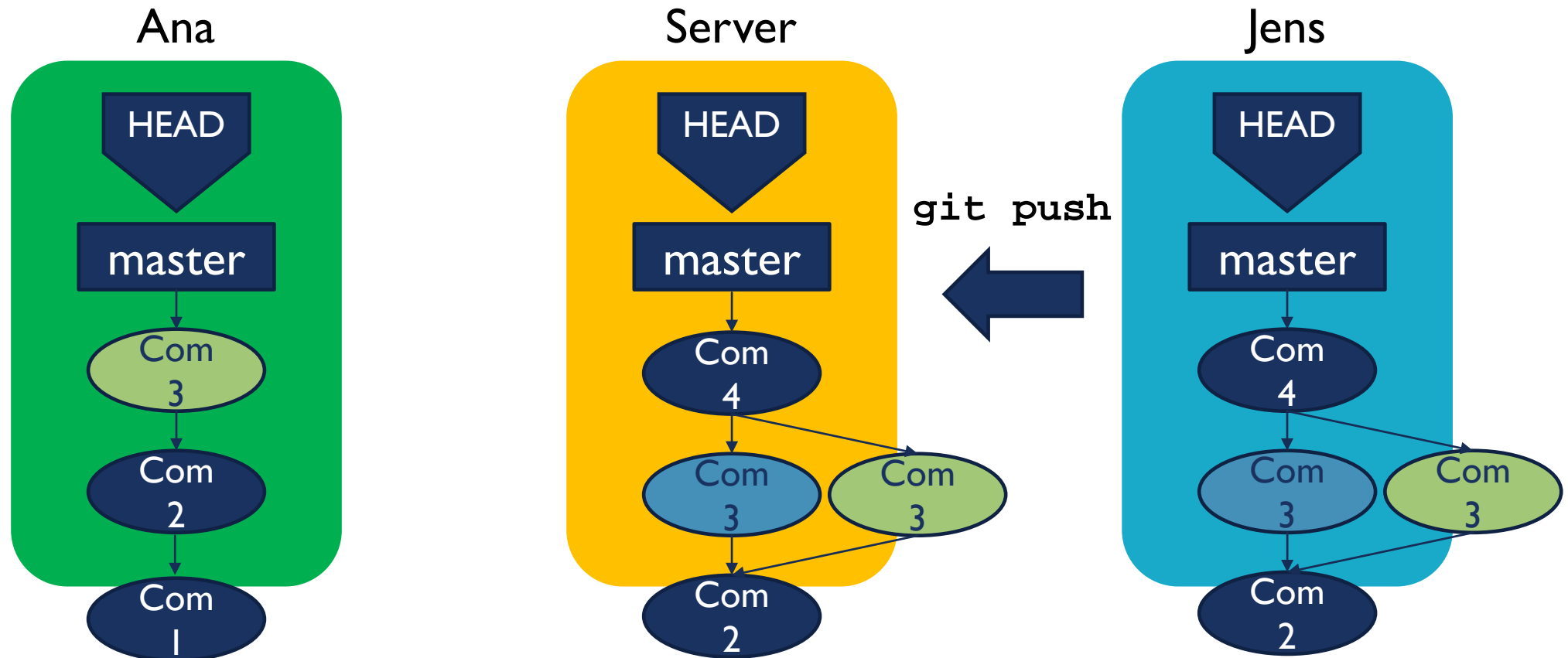
III. GIT IN ACTION



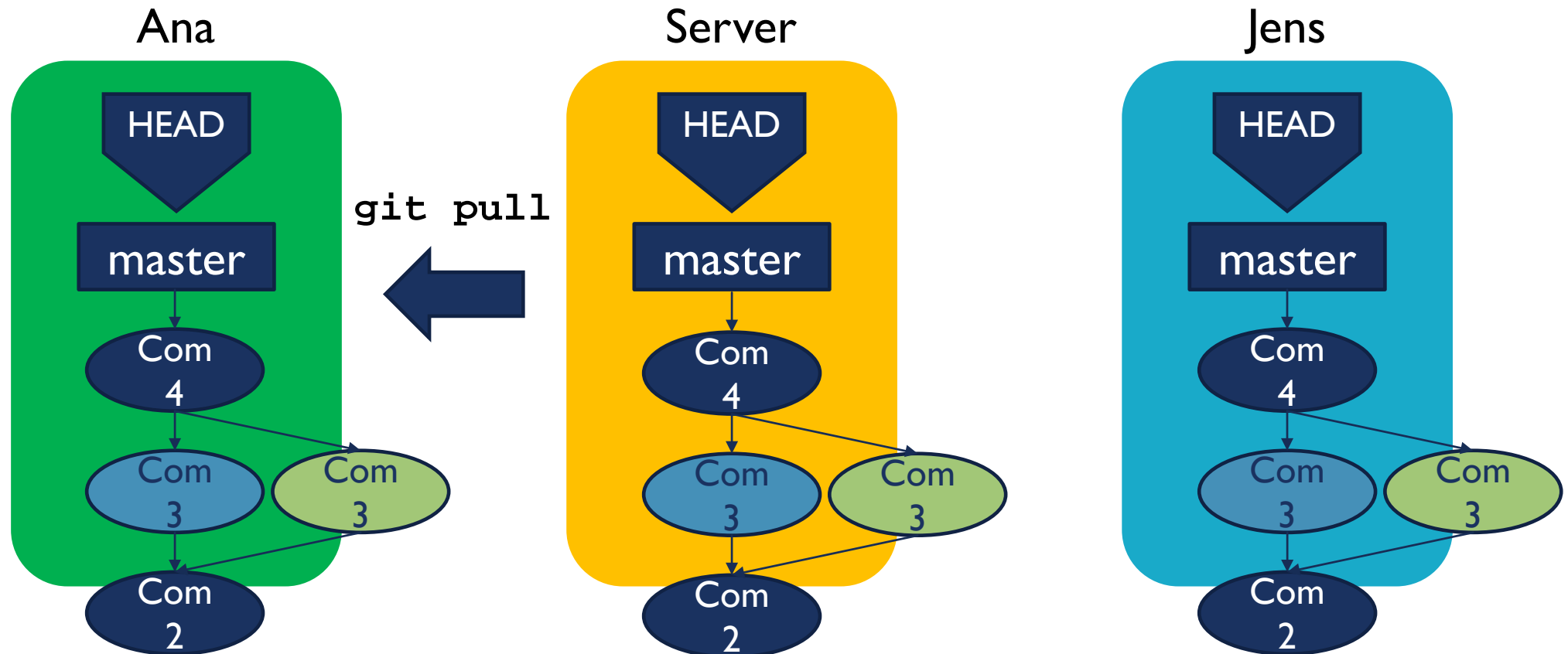
III. GIT IN ACTION



III. GIT IN ACTION



III. GIT IN ACTION



III. HANDS ON



- Get an account at <https://github.com/>
- Create a repo online

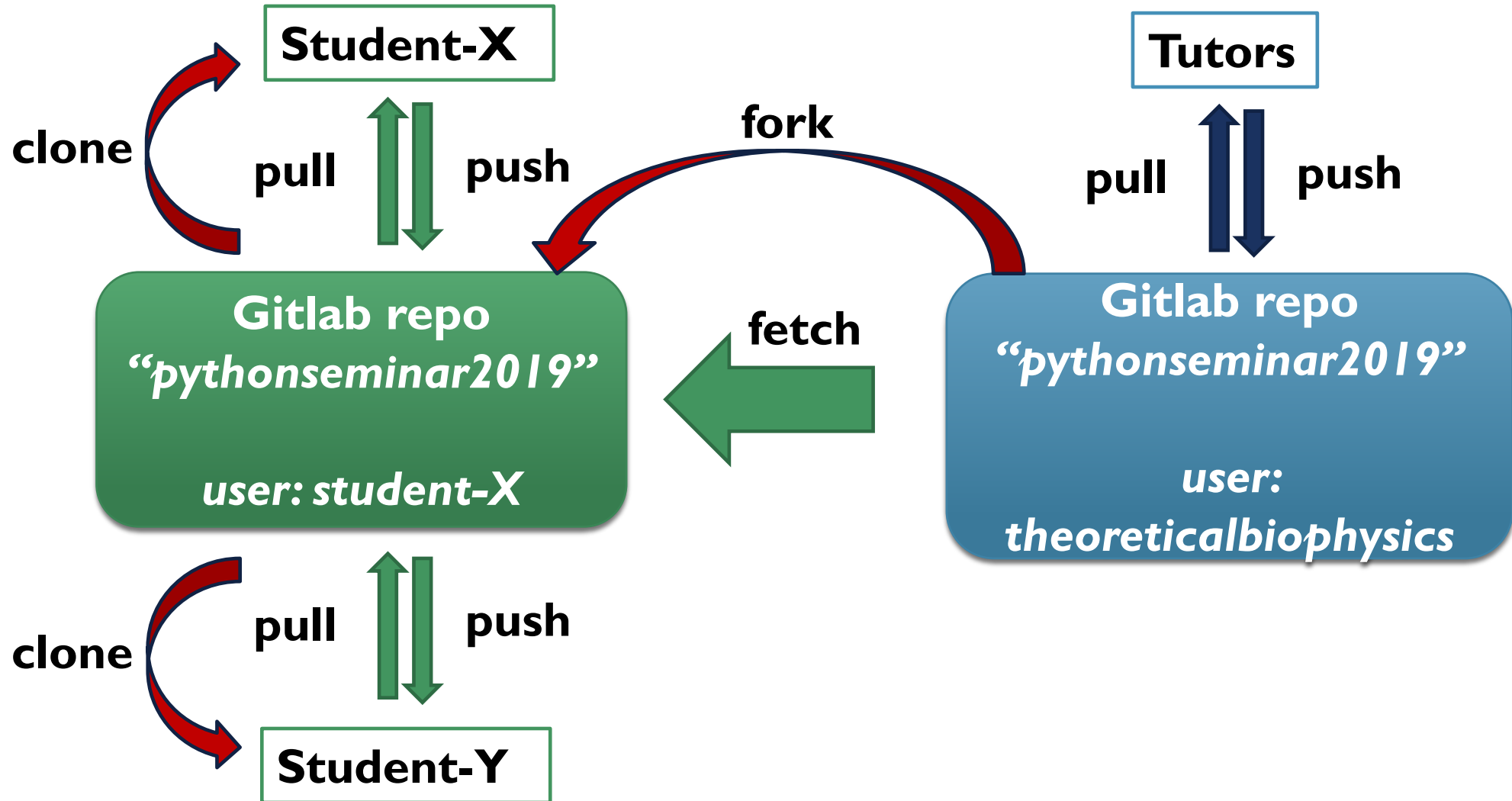
```
git clone https://gitlab.com/username/reponame.git  
git add ./my_file.txt  
git commit -m "I added a file" ./my_file.txt  
git pull  
git push
```

- Check the result online

III.THIS SEMINAR



- Seminar material: https://github.com/tbphu/Python_course.git
- How can you work on course material in your repo??
- FORK IT!!



III. FINAL CONFIGURATION



- Set upstream :

```
git remote add upstream https://github.com/tbphu/Python\_course.git
```

- Configure git:

- `git config --global user.email "meep@meep.com"`
- `git config --global user.name "Jens Hahn"`

III. FURTHER READING

git

- Tutorial (german!)

<https://rogerdudler.github.io/git-guide/index.de.html>

- git webpage

<https://git-scm.com/>

- Codecademy

<https://www.codecademy.com/learn/learn-git>

- gitg

<https://wiki.gnome.org/Apps/Gitg/>

SSH

- SSH tutorial

<https://www.hostinger.com/tutorials/ssh-tutorial-how-does-ssh-work>