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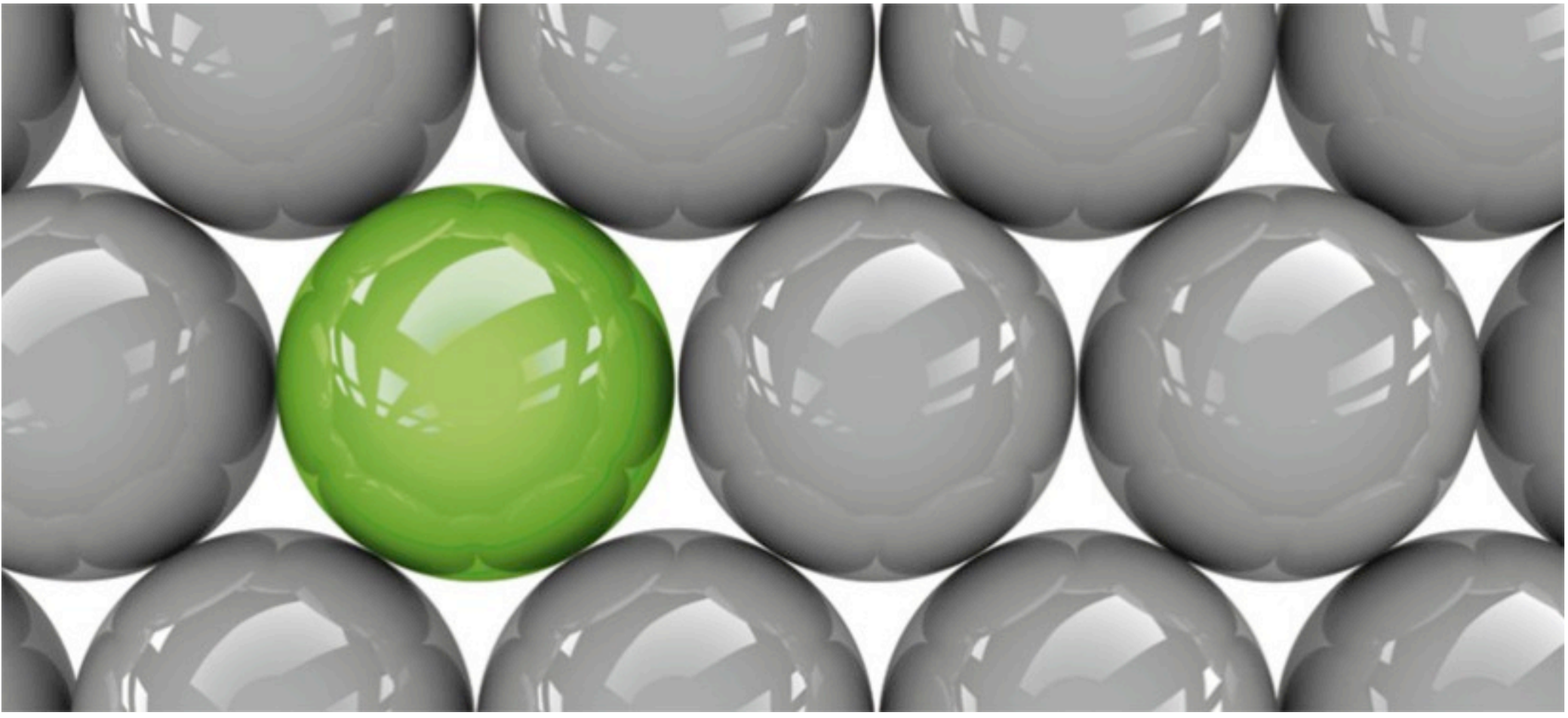

Computational Physics WS15/16

Dr. Götz Lehmann, Inst. f. Theoretische Physik I

Agenda

1. Who is involved?
2. Outline of the lecture
3. Organizational things

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Who is involved?

- Friedrich Schluck
- Stella Glöckner
- Eckhard Suckow

How to reach us

- Email: simu@tp1.uni-duesseldorf.de
- Office: 25.32.01.43
- ...if it concerns your homework, via GitHub

Find this document later at GitHub: http://github.com/TP1-HHU

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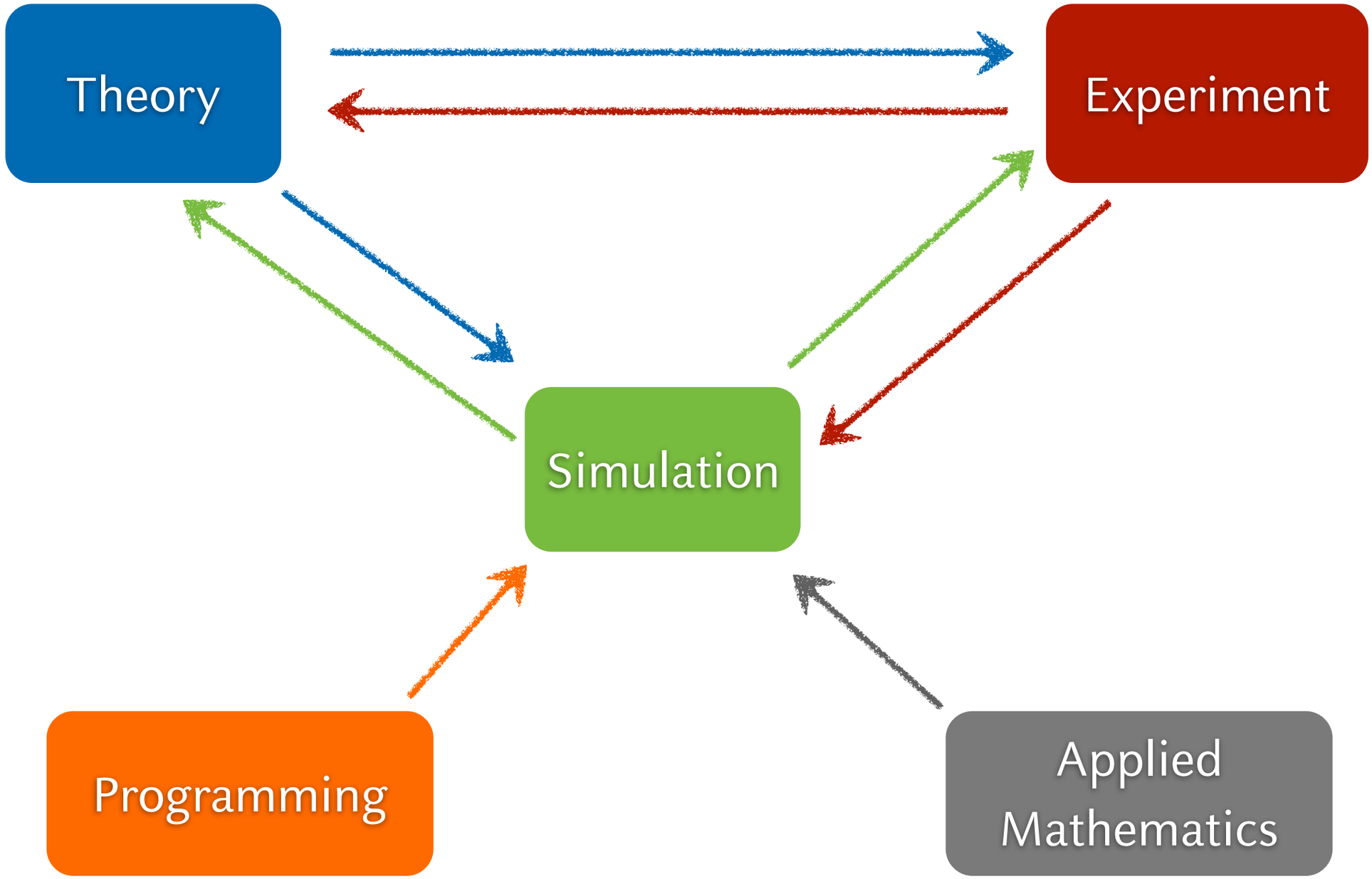
Organization of the class

- 2h lectures + 2h lab/tutorial per week + final exam ➠ 6 CP
- No 3CP rule
- Lecture: Wednesday, 8:30-10:30, HS 5J
- Lab classes: To be decided in a few minutes
- Final exam will (probably) be writing a computer code (problem of organization)
- Attendance at lab classes is mandatory
- Homework: To be handed in via GitHub, 2/3 of problems have to be solved

Computational Physics



Topics of the lecture

- Numerical methods
- Programming

Topics of the lecture

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Numerical methods

- Focus will be on initial value problems for
  - ordinary differential equations (ODEs)
  - partial differential equations (PDEs)
- This will require dealing with
  - finite difference approximations to derivatives
  - systems of linear equations
  - root finding of nonlinear equations
  - discrete Fourier transformation

Topics of the lecture

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Problems to be discussed

ODEs

$$\frac{d\vec{y}}{dt} = f(\vec{y}(t), t)$$

One-step methods: Runge-Kutta
Multi-Step methods: Adams Methods
Verlet Methods

$$\dot{p} = -\frac{\partial H(p,q)}{\partial q}$$
$$\dot{q} = \frac{\partial H(p,q)}{\partial p}$$

Symplectic methods for Hamiltonian systems

Topics of the lecture

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Problems to be discussed

PDEs

$\nabla^2 \phi = -\varrho$ Poisson eq.

$\frac{\partial^2}{\partial t^2} f - \nabla^2 f = 0$ Wave eq.

$\frac{\partial}{\partial t} f + \nabla \cdot j = 0$ Continuity eq.

$\frac{\partial}{\partial t} f - D \nabla^2 f = 0$ Diffusion eq.

$\frac{\partial}{\partial t} u - u \frac{\partial}{\partial x} u = 0$ Burgers eq.

$\mathrm{i} \frac{\partial}{\partial t} \psi + q \frac{\partial^2}{\partial x^2} \psi + |\psi|^2 \psi = 0$ NLSE

Topics of the lecture

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Programming

- C++, the language
  - as the better C
    - datatypes, functions, pointers, references
  - beyond C: Object oriented programming
    - classes, namespaces
    - external libraries: Avoid *Not invented here* syndrome
    - The basics of multi-core applications
    - You will need a C++ compiler for your homework!
- C++, the eco-system
  - Git as an example for a version control system
  - Makefiles / CMake
  - Valgrind

How to get your hands on C++

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- Windows:
  - MS Visual Studio via www.dreamspark.com
    - ...you‘re on your own
- Linux:
  - Lab class will use Linux
    - proper installation next to Windows (if your advanced, you know what you do)
    - live USB (fairly easy, use Linux Live USB creator to create bootable USB stick)
      - http://www.linuxliveusb.com (choose a “persistant“ capable distribution)
    - virtual machine (medium complexity, best result for the price)
      - Install VirtualBox for Windows https://www.virtualbox.org
      - Download a Linux distribution (Fedora, OpenSUSE, Mint, ...)
      - Install Linux in the virtual machine
- Mac:
  - Install XCode app. Done. Easy as that.

Why Linux?

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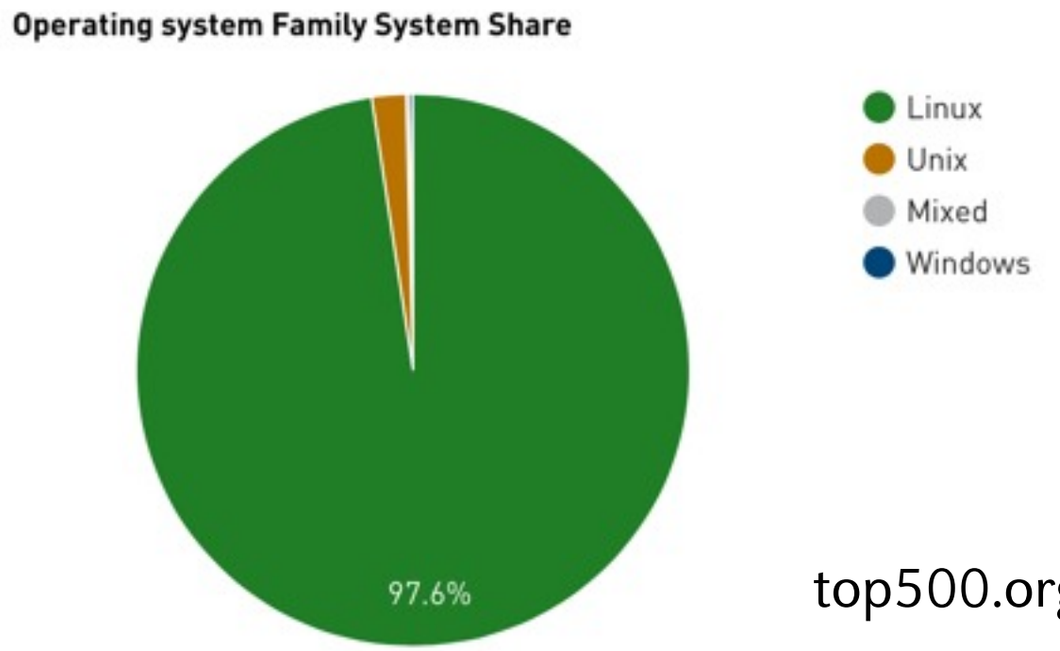
Linux is the backbone of computational science

Virtually all big machines use Linux



top500.org

Everything beyond one computer runs on Linux...

SGI UV2000, 512 Cores, ZIM

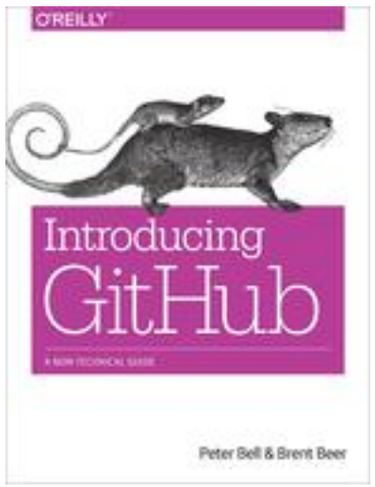
Managing sources

Git & GitHub

- Git is software that allows you to organize your source-code

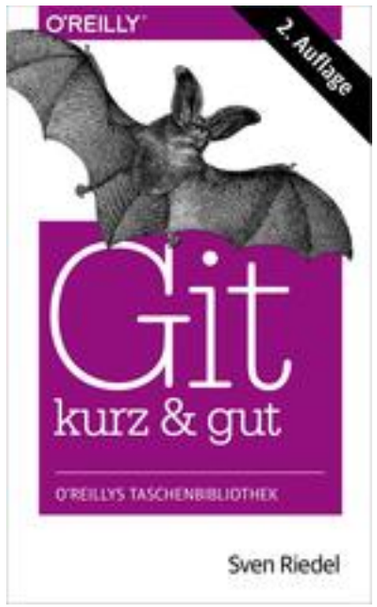
- We will use GitHub to *hand out & collect* sources for lab classes and homework

- First homework & first lab class will deal with GitHub & Git



Introducing GitHub
Bell & Beer

Preißel, Stachmann



Riedel

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Single User Git scenario - Using Git as a log book

repository

A repository contains a set of files
May reside on a local disk or somewhere on the internet

local work directory

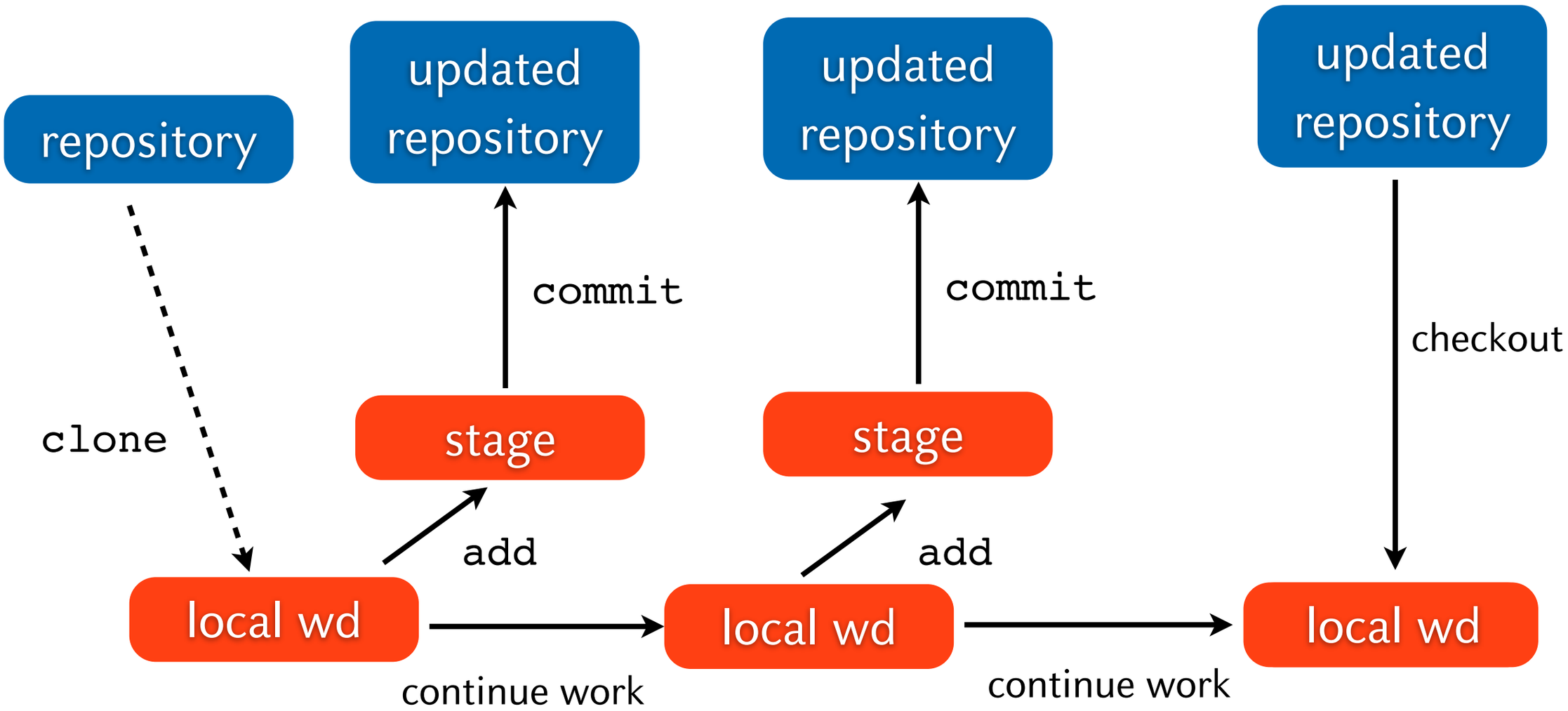
A directory on your hard disk

By `cloning` the repository into your local working directory, you create a local copy of the files contained in the repository.

After editing the files, you `add` the changes to the staging area. This is an intermediate step before sending them actually to the repository by `comitting` them.

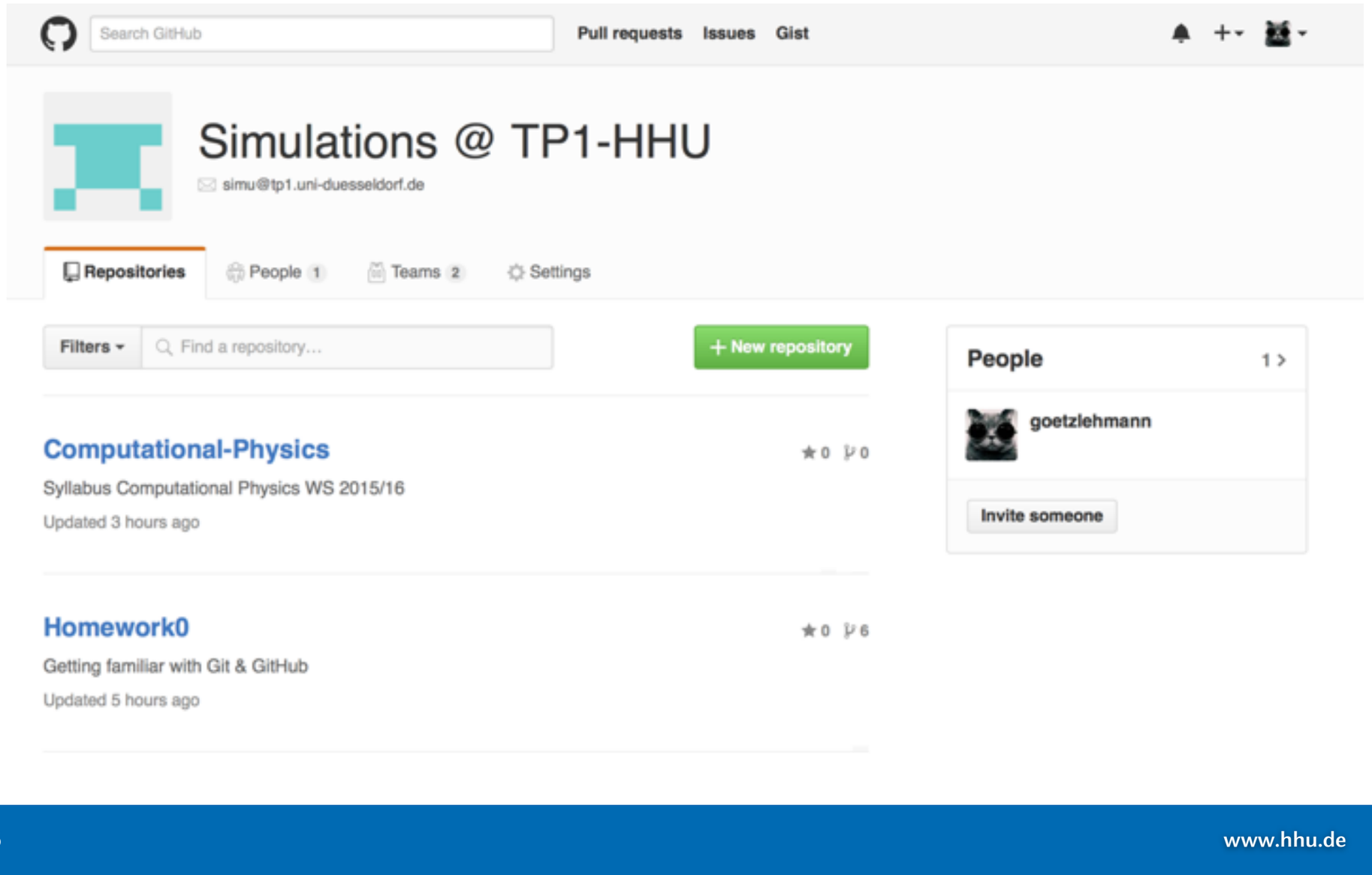
The repository keeps track of all older versions of all files. You can easily compare changes between between different `commits`.

Single User Git scenario - Using Git as a log book



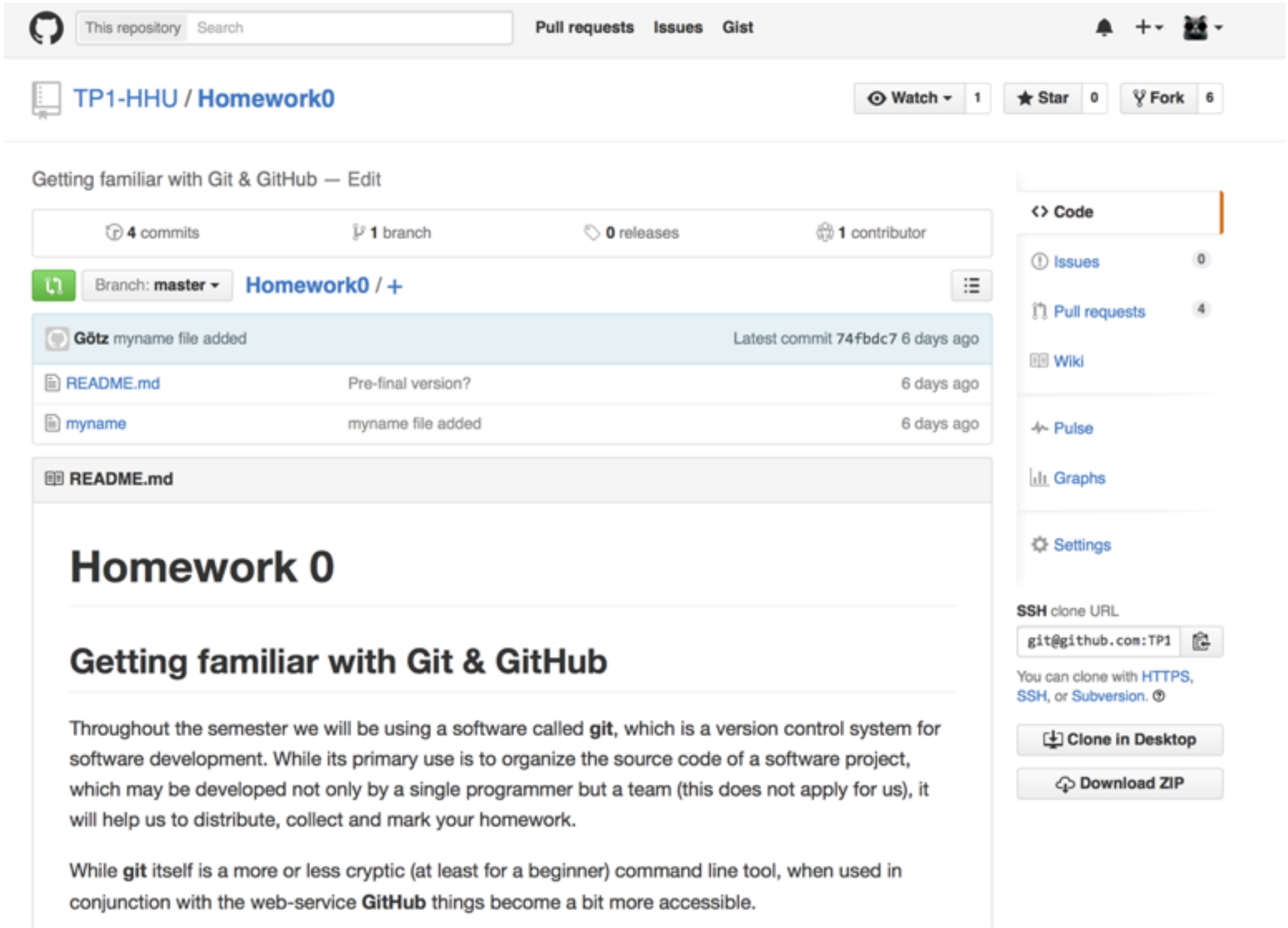
GitHub

- GitHub is a platform which allows to host repositories online
- Accounts are free, you will have to create one
- Our account is named TP1-HHU, thus our address is
  http://github.com/TP1-HHU



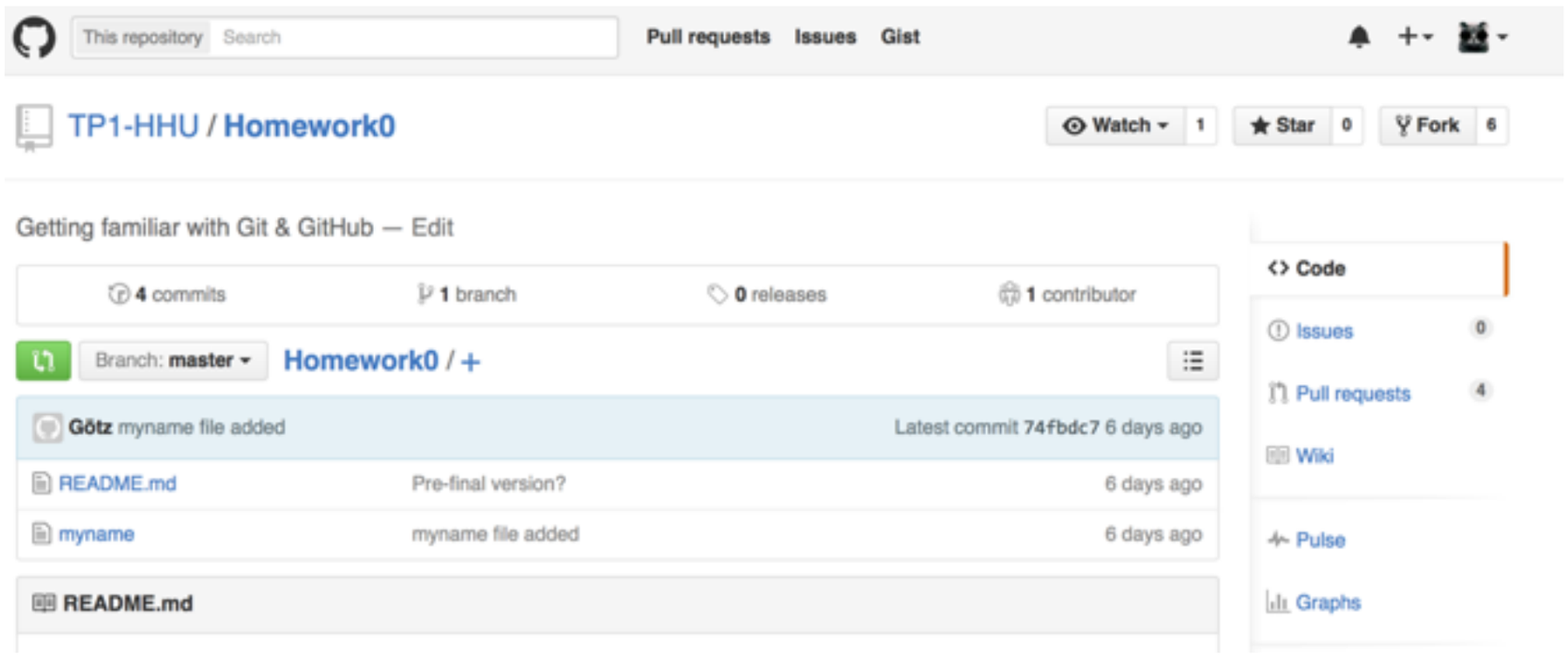
Repositories

GitHub


This repository Search
Pull requests
Issues
Gist
TP1-HHU / Homework0
Watch 1
Star 0
Fork 6
Getting familiar with Git & GitHub — Edit
4 commits
1 branch
0 releases
1 contributor
Branch: master
Homework0 / +
Götz myname file added
Latest commit 74fbdc7 6 days ago
README.md
Pre-final version?
6 days ago
myname
myname file added
6 days ago
Code
Issues 0
Pull requests 4
Wiki
Pulse
Graphs
Settings
SSH clone URL
git@github.com:TP1
You can clone with HTTPS, SSH, or Subversion.
Clone in Desktop
Download ZIP
README.md
Homework 0
Getting familiar with Git & GitHub
Throughout the semester we will be using a software called git, which is a version control system for software development. While its primary use is to organize the source code of a software project, which may be developed not only by a single programmer but a team (this does not apply for us), it will help us to distribute, collect and mark your homework.
While git itself is a more or less cryptic (at least for a beginner) command line tool, when used in conjunction with the web-service GitHub things become a bit more accessible.

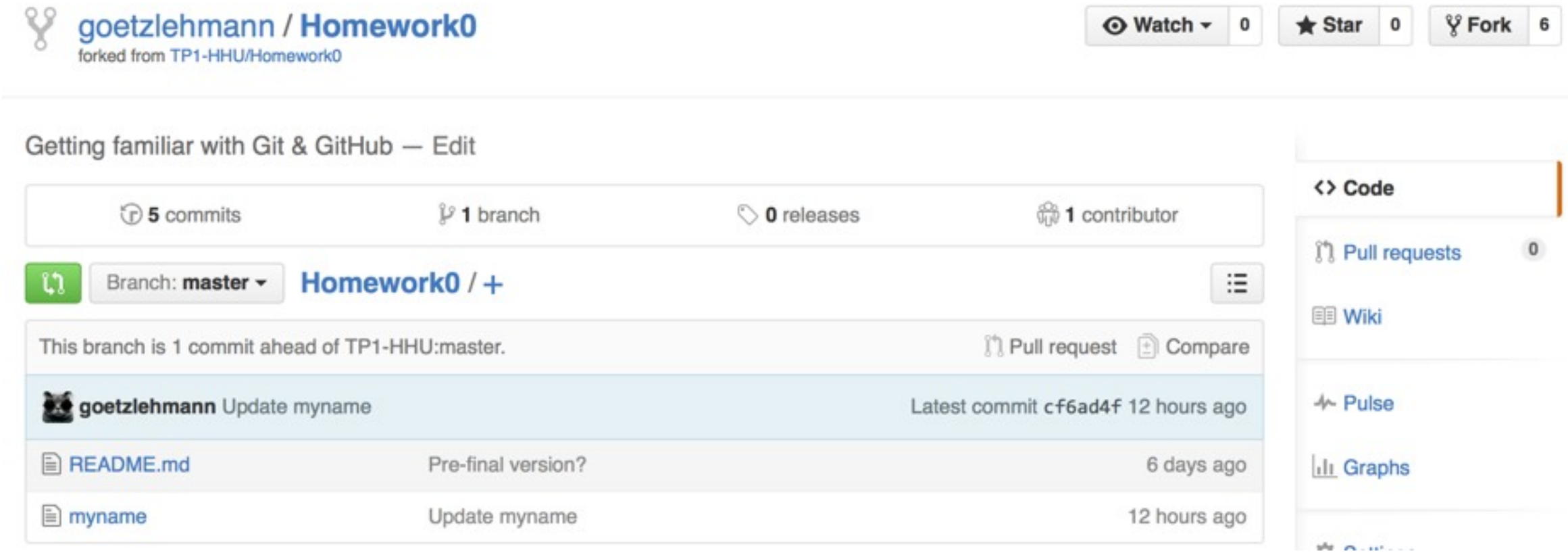
GitHub Homework

- Create a GitHub account for yourself
  - choose any nickname you want
  - the goal of this homework is to associate you to your nick
- Navigate to the Homework0 repository on our account and fork the repository by pressing the **fork** button on the top right



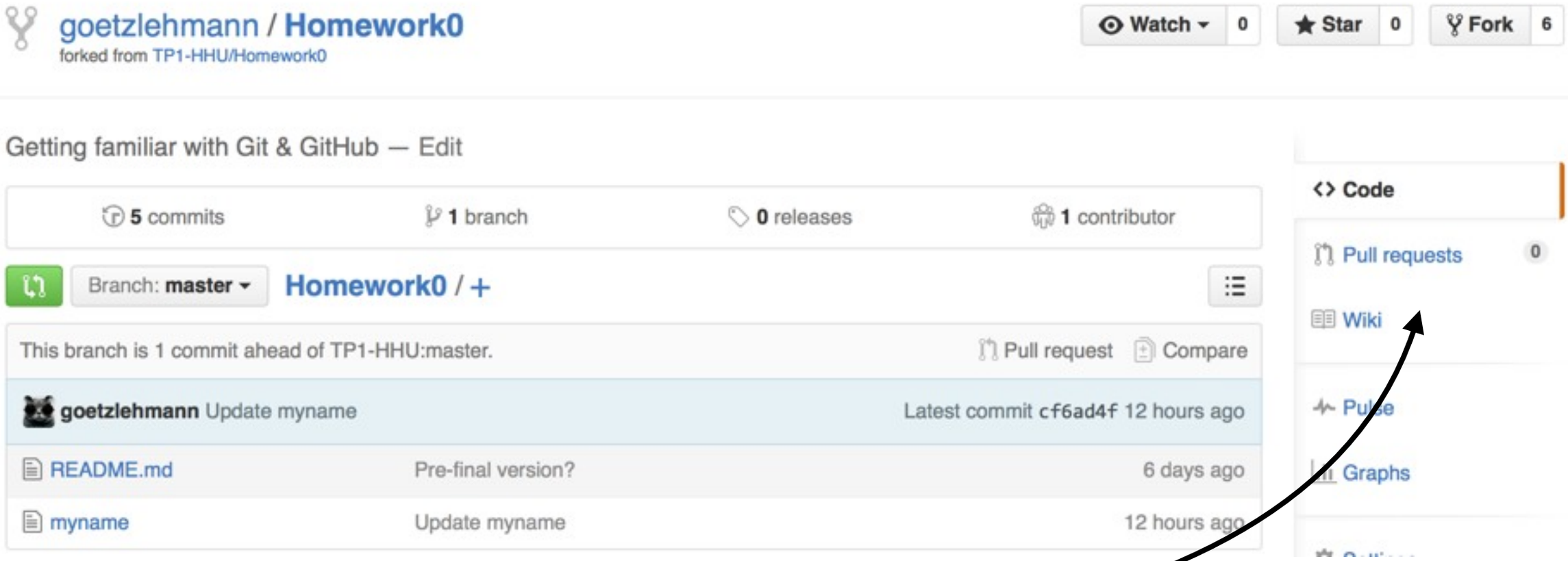
GitHub Homework

- Now a fork of the repository has been created in your own account
- The files in your account belong to you - you can change them



GitHub Homework

- Edit the file myname and write your name into it
- Upon saving the changed file,
  leave Commit directly to the `master` branch unchanged



- Create a pull request

GitHub Homework

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Creating the pull request:

- Green button „new pull request“
- Green button „view pull request“
- Leave your real name in the comment field for the Pull request
- done