Computational Sciences Projektseminar

Introduction

Objective

- **apply the contents of the lecture**

- **develop code in a team**

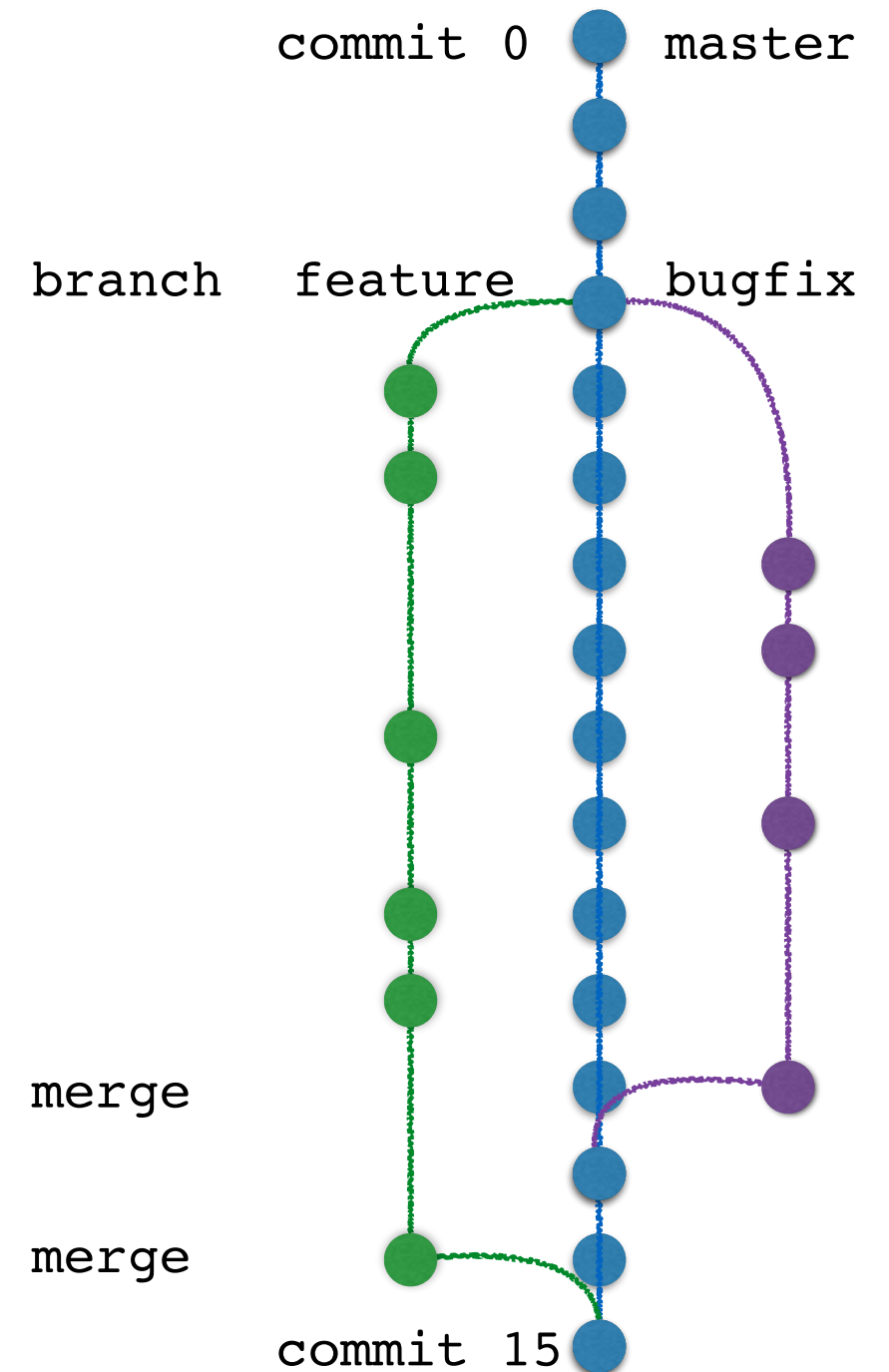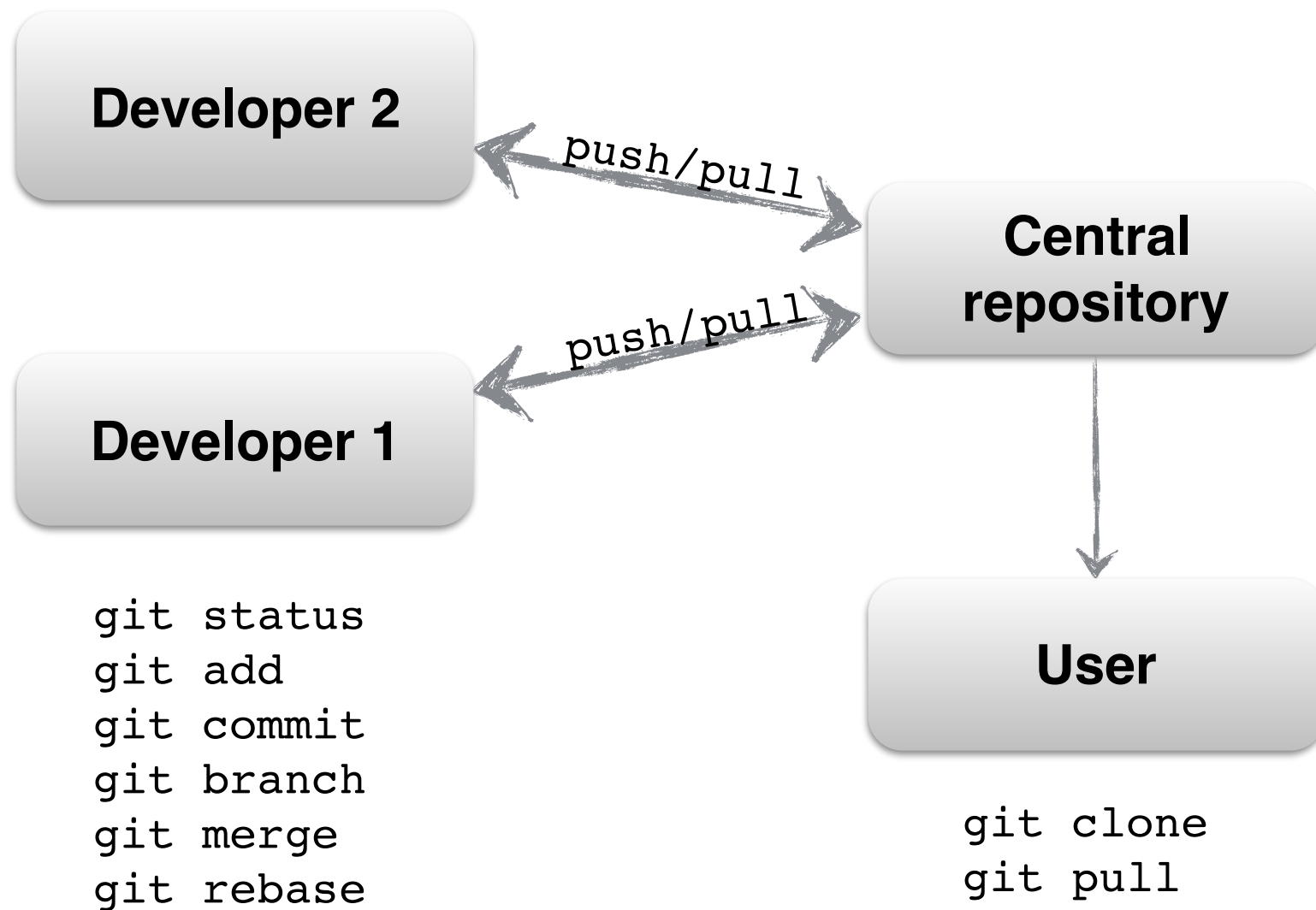- **usage of tools and programming techniques**

Tasks

- **individual and group exercises**

- **development of a large project**

- **presentation and application**

Schedule

- **Tuesdays, 8:15–9:45, room 017/A6
  15 meetings for general discussion and lectures**

- **group-based extra meetings for specific problems**

- **email support**

git (version control) & github (social coding)

https://github.com

commit 0 ● master

●
●

branch feature ● bugfix

Developer 2

push/pull

Central repository

push/pull

Developer 1

```
git status
git add
git commit
git branch
git merge
git rebase
```

User

```
git clone
git pull
```

merge

merge

commit 15 ●

Language

```
https://www.python.org
```

- **Python (anaconda) and C/C++**

- **useful libraries: numpy, scipy, cython, numba, …**

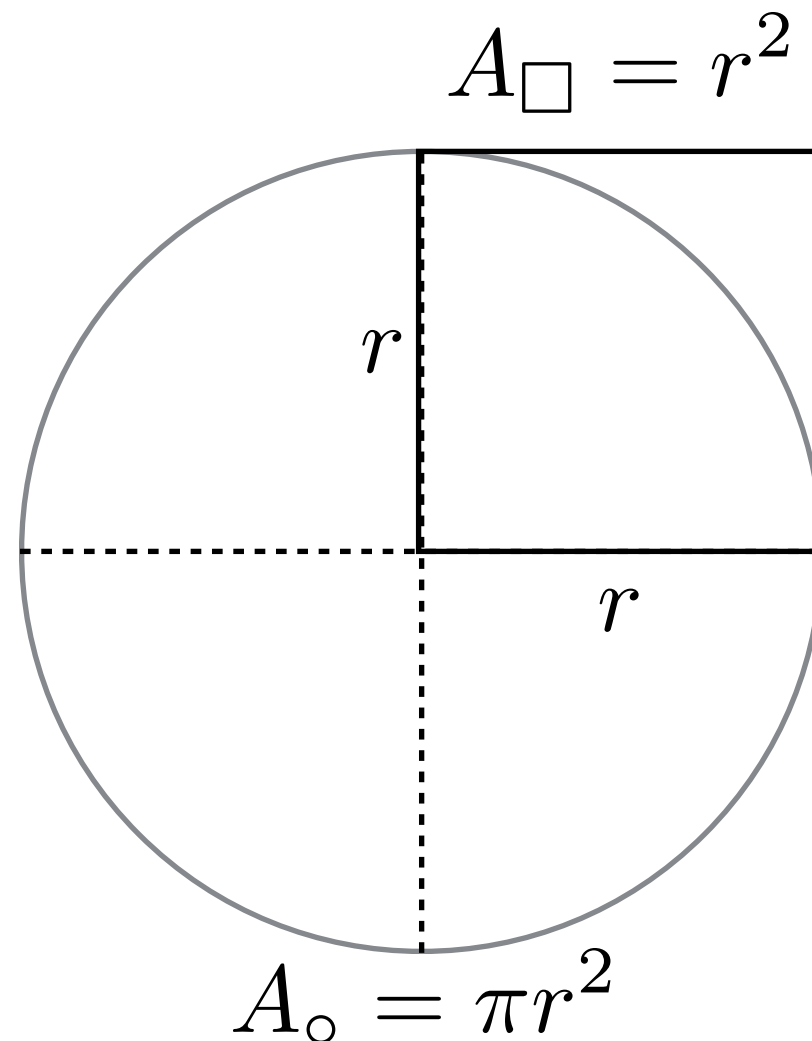- **easy to distribute (packaging, user base)**

```
http://conda.pydata.org/miniconda.html
```

Jupyter notebook (IPython)

`http://jupyter.org`

- **live code + equations + visualisations + explanatory text**

- **fast prototyping**

- **applications, tutorials, examples**

Exercise: approximate π

$$A_\square = r^2$$

$$\chi(x,y) = \begin{cases} 1, & x^2 + y^2 \leq r^2 \\ 0, & else \end{cases}$$

$$A_\circ = \pi r^2$$

$$\frac{\frac{1}{4}A_\circ}{A_\square} \approx \frac{1}{N}\sum_{n=0}^{N-1}\chi(x_n,y_n)$$

$$(x_n, y_n) \in [0,r]^2 \ \forall n$$

$$\frac{\frac{1}{4}A_\circ}{A_\square} = \frac{\frac{1}{4}\pi r^2}{r^2} = \frac{\pi}{4}$$

Exercise: approximate π

- **choose** $r = 1$

- **generate N=10^6 random tuples** $(x_n, y_n) \in [0, 1]^2$

- **compute** $\pi_{\text{sampled}} = \dfrac{4}{N} \displaystyle\sum_{n=0}^{N-1} \chi(x_n, y_n)$

```
numpy.random.rand(), numpy.sum()
```

Exercise: approximate π