

Computational Sciences Projektseminar

A Python package for solving Poisson's equation



1st group project: Poisson solver

Design/implement a complete Python package

Develop on github

Use a test-driven approach

Discretised Laplacian and successive over-relaxation



Setting up your github account

browser

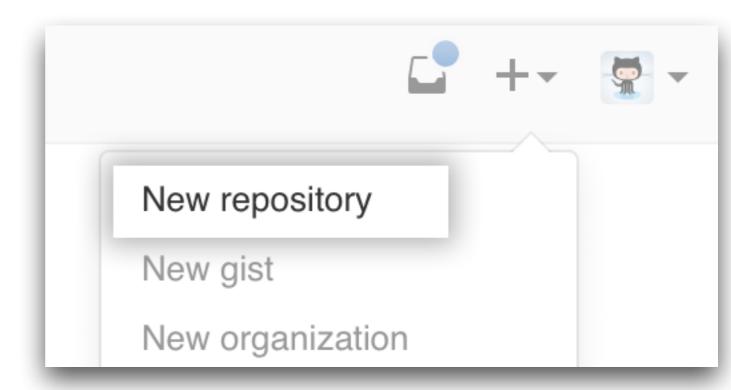
https://github.com/join

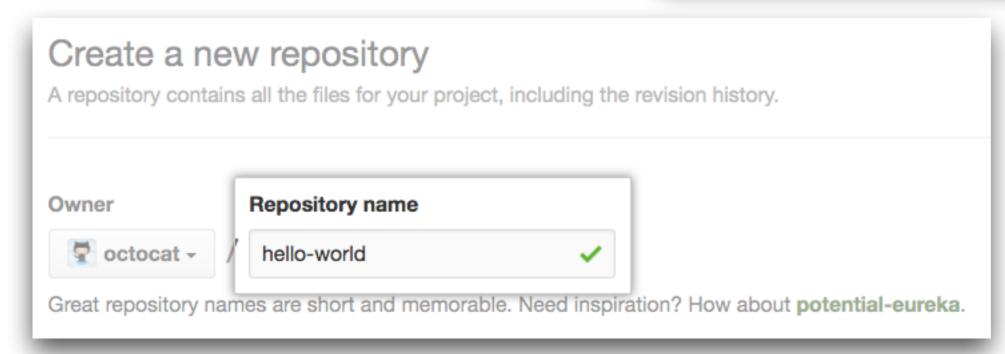
bash

```
git config --global user.name "Mona Lisa"
git config --global user.email "email@example.com"
```



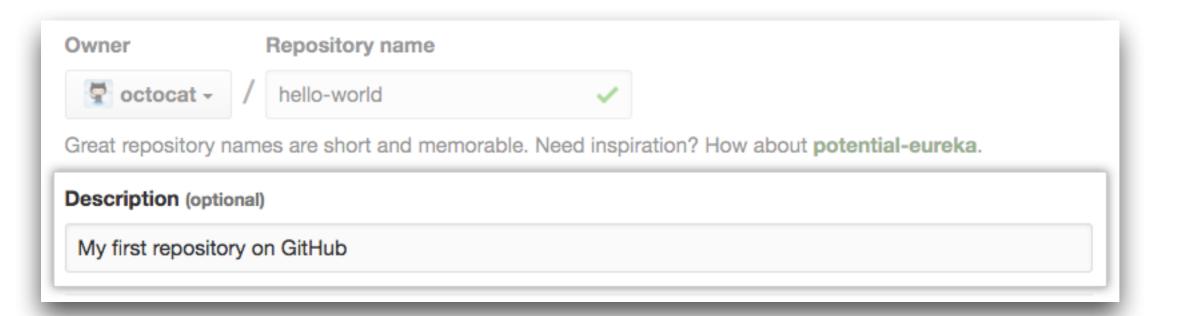
Creating a github repository

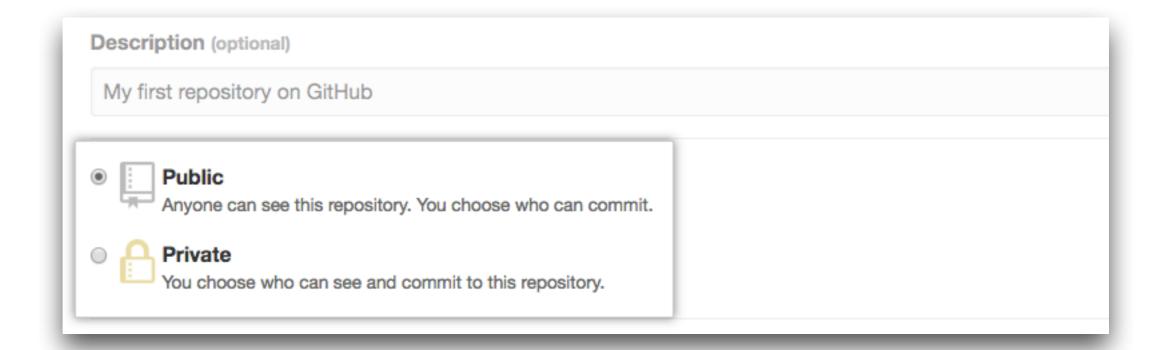






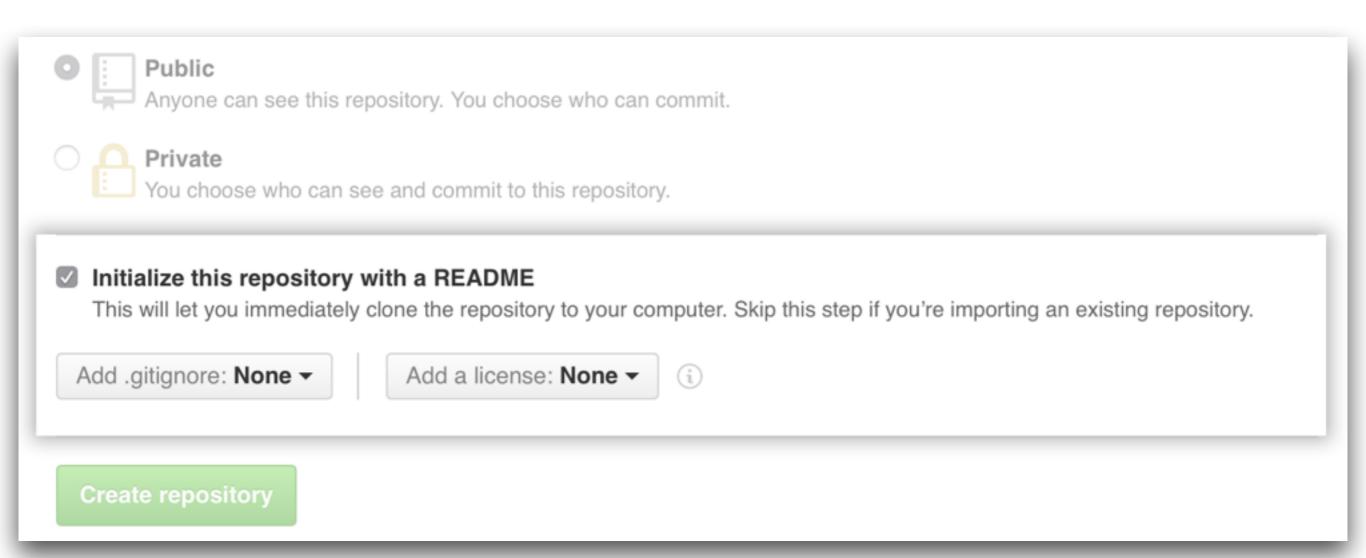
Creating a github repository





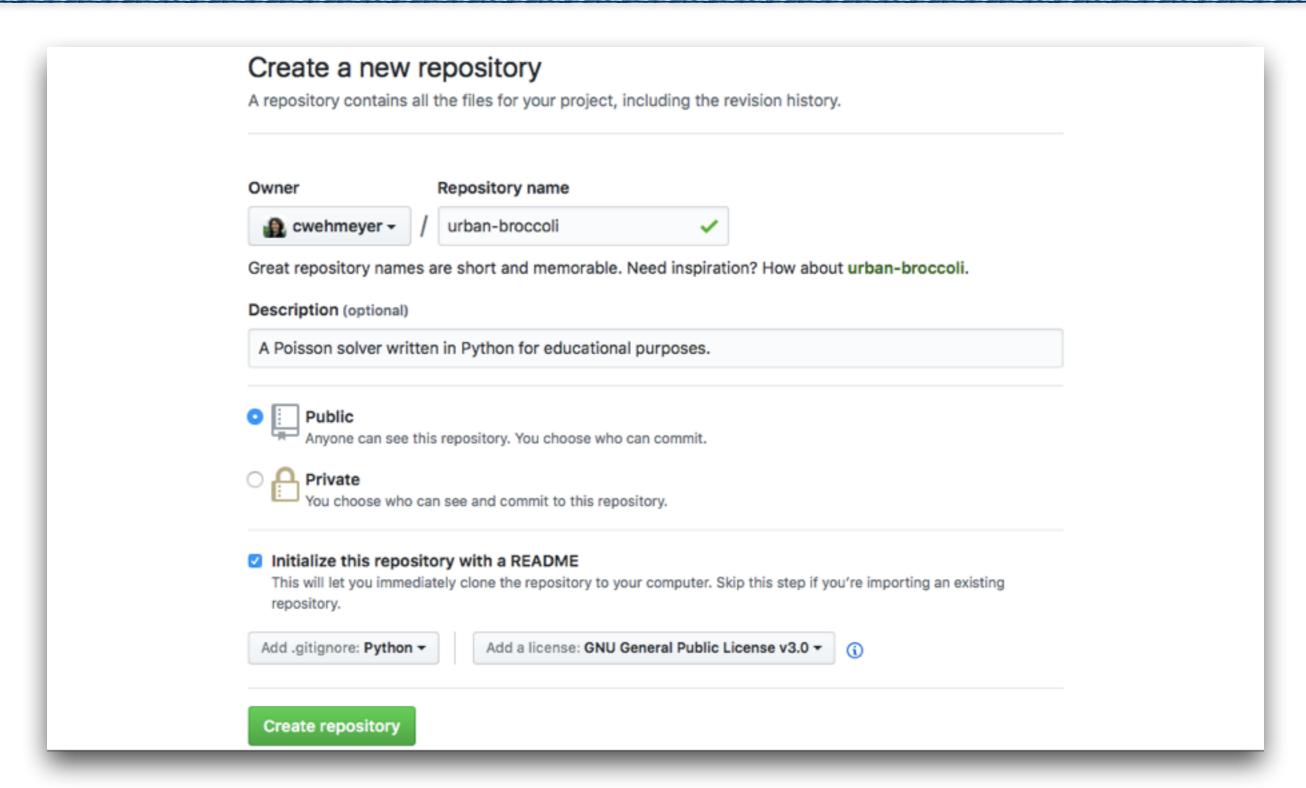


Creating a github repository



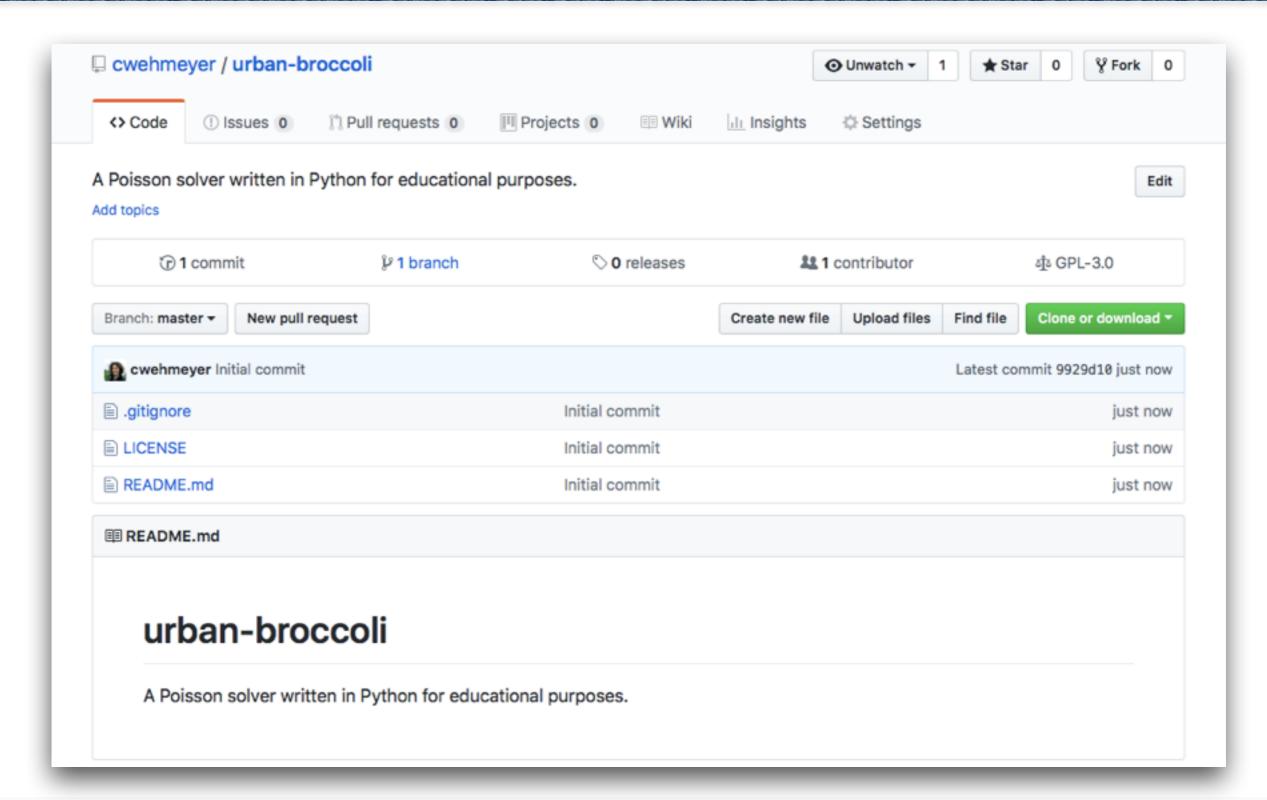


Example





Example





Package layout

```
module.py
import module
package/
      init .py
    module1.py
    module2.py
import package
```

```
package/
    mypck/
          init .py
        module1.py
        module2.py
        test/
              init .py
            test module1.py
            test module2.py
    setup.py
    README.md
cd /path/to/package
python setup.py test
python setup.py install
import mypck
```

http://docs.python-guide.org/en/latest/writing/structure/



Interface

```
import numpy as np
from PACKAGE NAME import solve, create laplacian
rho = np.random.rand(100, 50)
rho -= np.mean(rho)
phi = solve(rho, epsilon=1.0, h=[0.1, 0.2])
laplacian = create laplacian(phi.shape, h=[0.1, 0.2])
phi = phi.reshape(-1, 1)
rho = np.dot(laplacian, phi )
rho = rho .reshape(rho.shape)
np.testing.assert_allclose(rho_, rho)
\frac{\partial^2 \phi}{\partial x^2} \approx \frac{\partial}{\partial x} \frac{\phi(x + \frac{h}{2}) - \phi(x - \frac{h}{2})}{h} \approx \frac{\phi(x + h) + \phi(x - h) - 2\phi(x)}{h^2}
```