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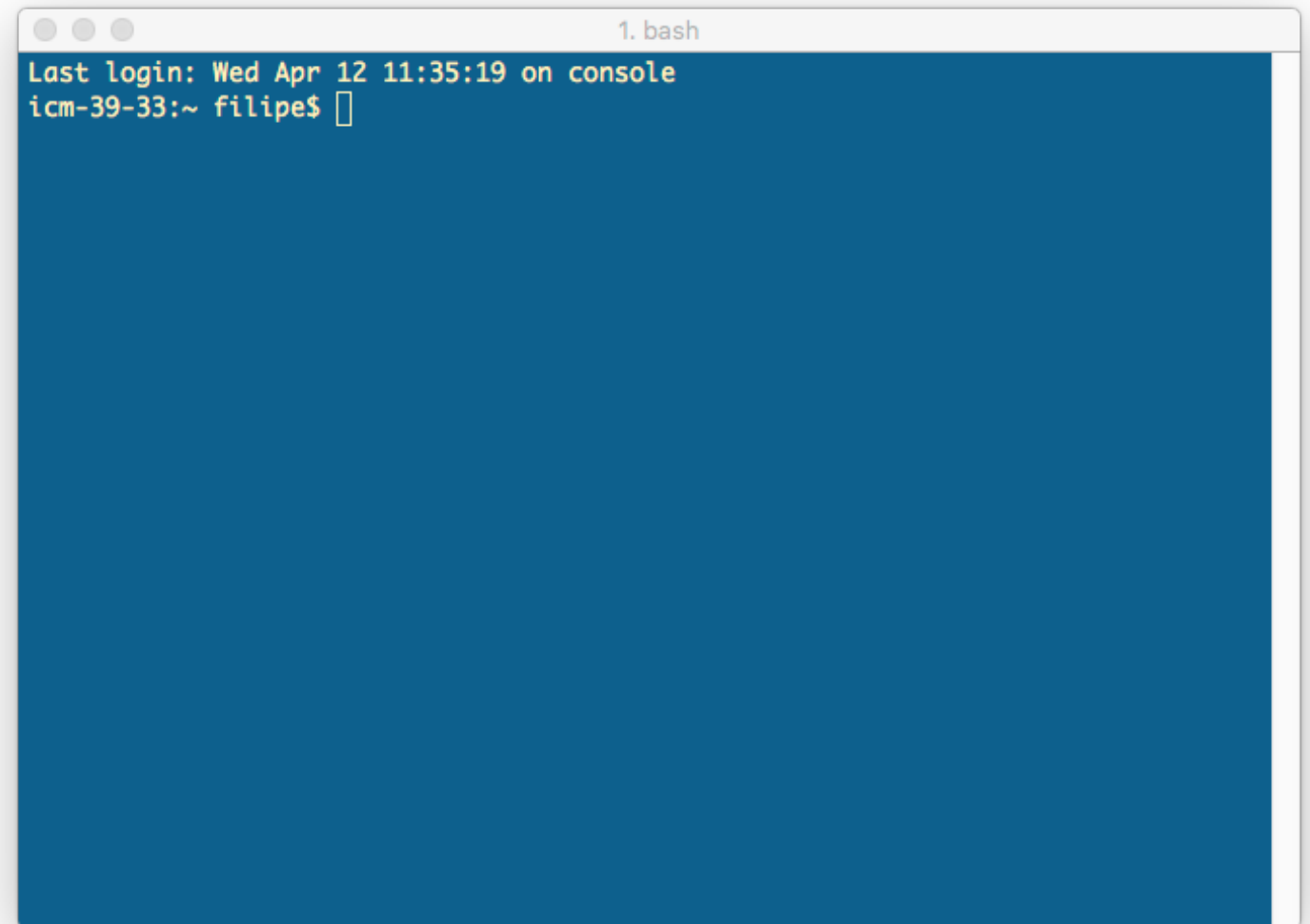
An Introduction To The Unix Shell, Interactive Python And Git Repositories

Day 1 - Shell, Git and Jupyter

Advanced Scientific Programming with Python

The Unix Shell

- Provides a command line interface (CLI) to the operating system
- Large variety of shells: **bash**, **tcsh**, **csch**, **ksh**, **zsh**
- We'll focus on **bash**, the default on most systems
- Documentation can be found by typing **man <command>**, e.g. **man bash**.



```
1. bash
Last login: Wed Apr 12 11:35:19 on console
icm-39-33:~ filipe$
```

A shell on Mac OS X, a Unix system

What shell do you normally use?

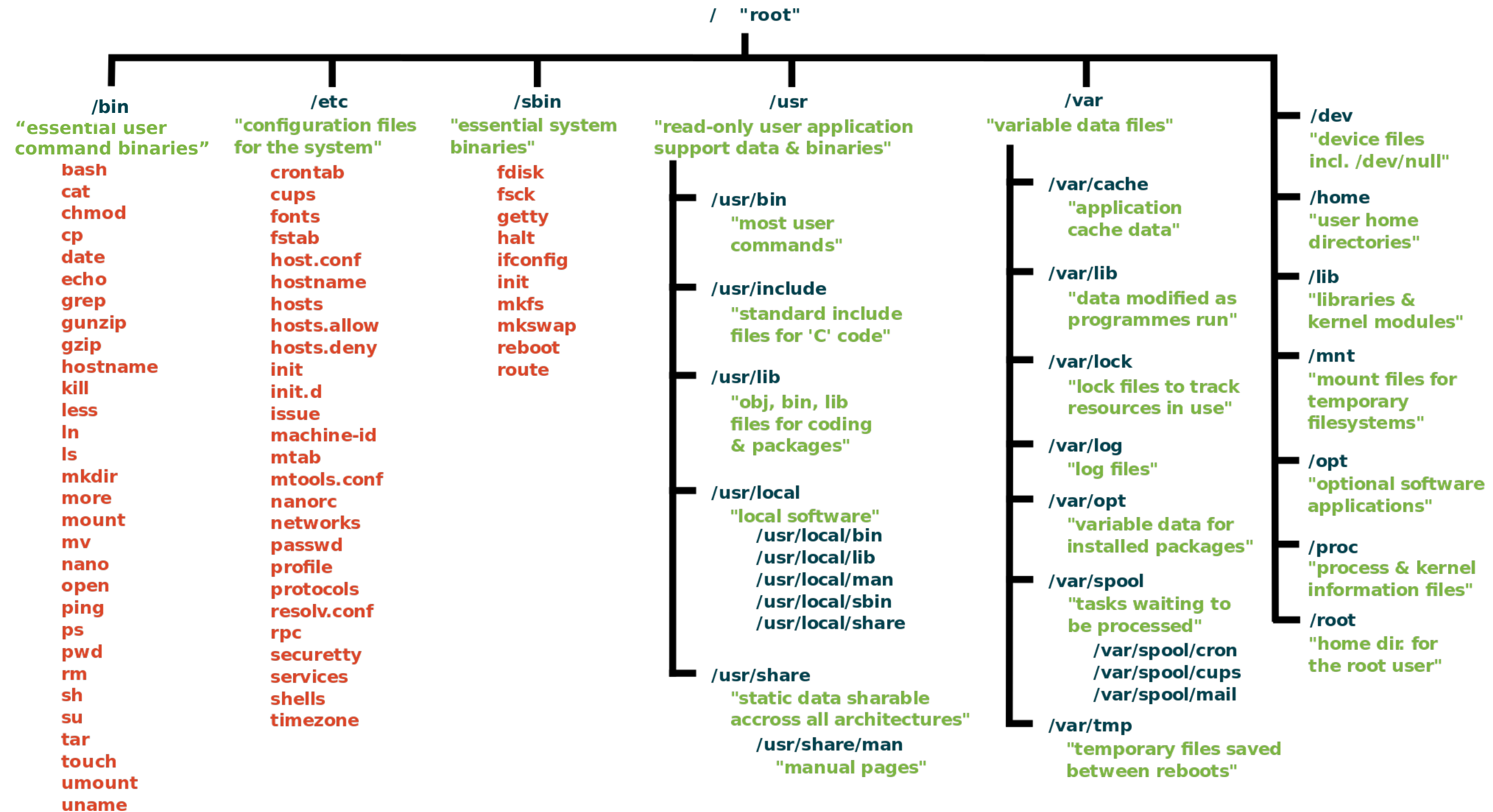
The Unix Shell

- On login the system executes:



- To avoid complications it's recommended to have your `~/.bash_profile` as a symlink to `~/.bashrc`.
- The shell checks the first line of every program and if it finds `#!<interpreter>` it uses the the given interpreter to evaluate the file (e.g. `#!/usr/bin/env python`)
- bash is a very powerful shell that can be used for input redirection (<, >, &, etc...), job control (fg, bg, jobs), file globbing (*, [0-9], ...).
- Check the **man page** for more!

Standard Unix Filesystem



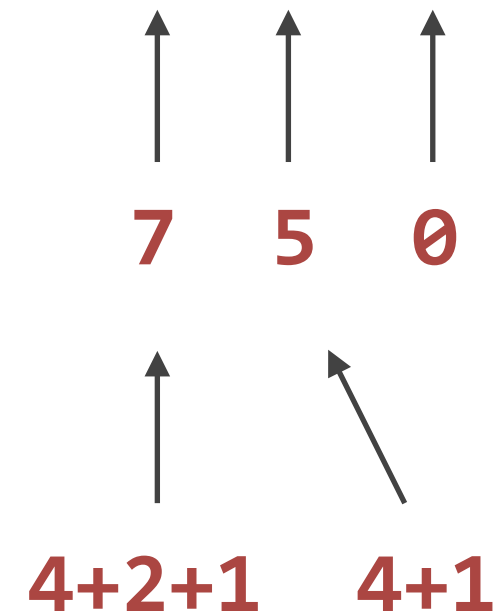
Basic Unix Utilities

- **ls** - list directory contents. Example: **ls -ltr ~**
- **cd** - change working directory. Example: **cd ..**
- **cp** - copy files. Example: **cp -a ~/data/*.h5 /mnt/backup/data**
- **mv** - move files. Example: **mv * package/**
- **rm** - remove files. Example: **rm -rf ~/.***
- **mkdir** - create directories. Example: **mkdir -p ~/data/run1/001/**
- **ln** - create links. Example: **ln -s /long_path_to_data/ data**
- **grep** - text filter. Example: **grep Result ~/data/log.txt**
- **more** - display file contents. Example: **more ~/data/log.txt**

File Permissions

- In Unix systems most things are represented by files.
- All files have owner, group and other permissions.
- The basic 3 permissions are read (4), write(2) and execute(1).
- Permissions can be changed with **chmod**
- Owners can be changed with **chown** and **chgrp**
- Permissions of newly created files are determined by the users' **umask**

drwxr-x--



Examples:

```
$ chmod 760 my_file  
$ chown filipe my_file  
$ chgrp xray my_file
```

File Permissions



- If a file has permissions '-rw-r--r--' and you're neither the owner or part of the group that owns the file, can you execute the file?
- Could you instead copy the file?
- Can you move the file?
- What about creating another file in the same directory?

File Globbing

Wildcards can specify sets of files. For example:

```
$ ls molecules
```

```
cubane.pdb  ethane.pdb  methane.pdb
```

```
cubane.txt  ethane.txt  methane.txt
```

```
$ rm molecules/*.txt
```

```
$ ls
```

```
cubane.pdb  ethane.pdb  methane.pdb
```

* matches 0 or more characters

? matches exactly 1 character

[abc] matches 1 character in the set

[a-z] matches 1 character in the range

For more details check **man 7 glob**

Demo: Files And Permissions

Pipes And Filters

- You can use **>** to redirect the output of a command to a file, e.g.:

```
$ wc -l *.pdb
12  cubane.pdb
20  ethane.pdb
9   methane.pdb
41  total
```

```
$ wc -l *.pdb > lengths.txt
$ cat lengths.txt
12  cubane.pdb
20  ethane.pdb
9   methane.pdb
41  total
```

- **>>** works similarly, but the output is appended to the file instead of replacing it.

Pipes And Filters

- You can use **|** (called a pipe) to make the output of a command the input of the next, e.g.:

```
$ sort -n lengths.txt  
9  methane.pdb  
12 cubane.pdb  
20 ethane.pdb  
41 total
```

```
$ wc -l *.pdb | sort -n  
9  methane.pdb  
12 cubane.pdb  
20 ethane.pdb  
41 total
```

Pipes And Filters

- You can use `<` to make the content of a file the input of a command, e.g.:

```
$ wc -l methane.pdb
9  methane.pdb
```

is the same as:

```
$ wc -l < methane.pdb
9  methane.pdb
```

- Most commands that read from standard input also accept files as arguments so this is not as useful.

Standard File Descriptors

- Every process opens 3 numbered standard file descriptors, **stdin** (0), **stdout** (1), **stderr** (2).
- They correspond to the input (**stdin**), output (**stdout**) and error messages (**stderr**).
- You redirect the streams independently, e.g.:

```
$ ls /bin/foo /bin/ls > /dev/null  
ls: /bin/foo: No such file or directory
```

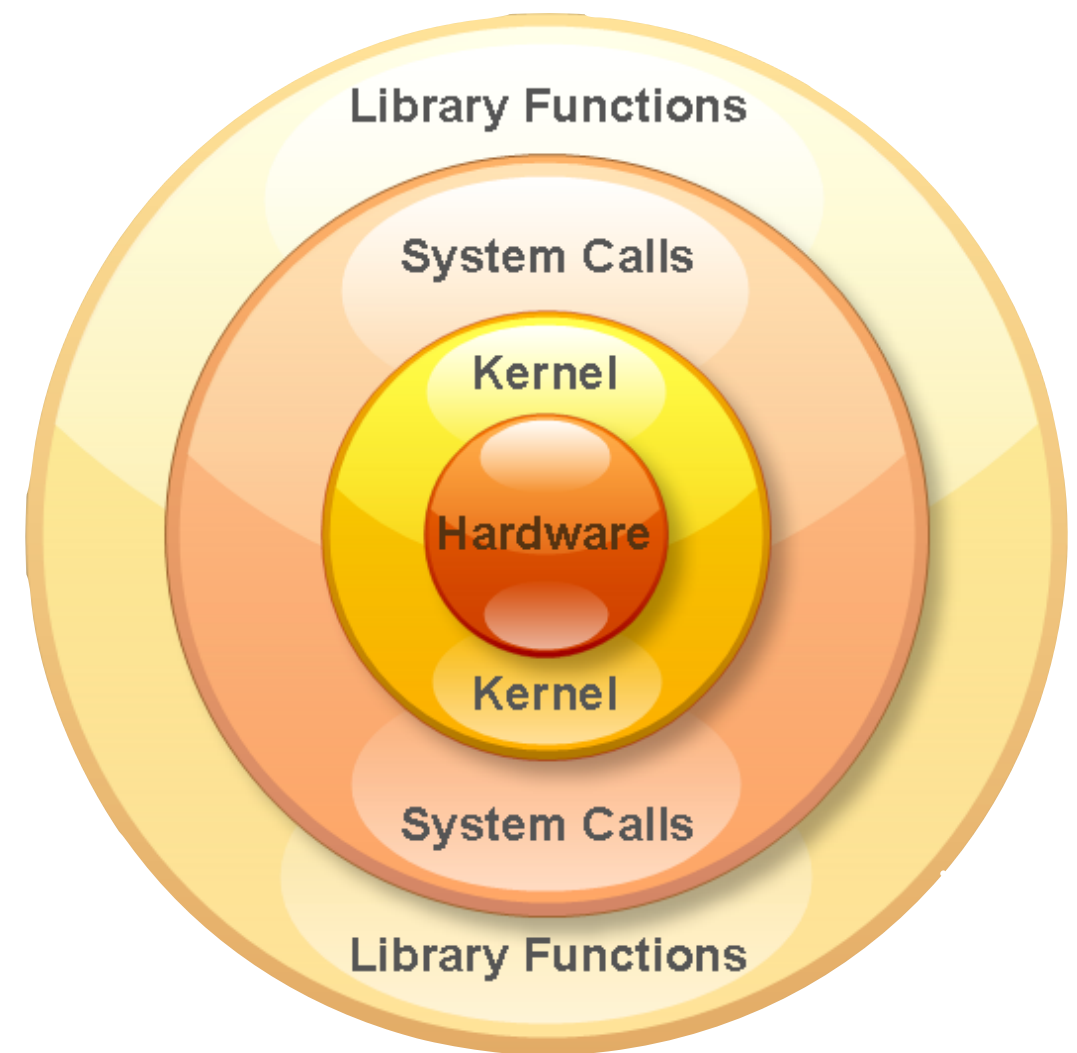


```
$ ls /bin/foo /bin/ls 2> /dev/null  
/bin/ls
```
- You can combine streams, e.g.:

```
$ ls /bin/foo /bin/ls > /dev/null 2>&1  
$ ls /bin/ls /bin/foo 2>&1 |wc -l  
2
```

Unix Processes

- A **process** is a running program and has a unique **pid** (process id).
- Each process has a parent. It inherits its **environment** from the parent.
- You can use **pstree** to check the process tree.
- Each process has its own memory address.
- Processes can have one or more **threads**.
- All threads in a process share the same memory space.



Process Environment

- Each process has a parent process from which it inherits the environment.
- **PATH** is an environment variables used to search for executables. You can display it with **echo \$PATH**.
- You can change variables using **export**, e.g. **export PATH=/bin**.
- You can use **which** to find out the full path of an executable (e.g. **which cp** returns **/bin/cp**).
- **LD_LIBRARY_PATH** is another, which lets the program know where to find dynamic libraries.
- You can use **ldd** to print out the libraries found by the system:

```
[root@login ~]# ldd /bin/cat  
linux-vdso.so.1 => (0x00007ffc4b73c000)  
libc.so.6 => /lib64/libc.so.6 (0x00007f8e0a978000)  
/lib64/ld-linux-x86-64.so.2 (0x00007f8e0ad28000)
```
- As usual, **man 7 environ** for more information.

Job Control

- Signals can be used to control a process.
- **Ctrl+C (SIGINT)** asks the process to terminate.
- **Ctrl+Z (SIGSTP)** suspends the process. You can use **fg** to continue the process.
- You can also use the **kill** command to send signals.
- **kill 9 <pid>** sends the **SIGKILL** signal to the process causing it to terminate immediately.
- Certain processes (stuck inside kernel calls) cannot be killed.
- You can also use **nice** to control the priority of execution of the process.
- Check **man 7 signal** for more information.

Demo: Pipes And Job Control

If you need to refresh your knowledge check:
<https://swcarpentry.github.io/shell-novice/>

Some More Useful Programs

SSH Tips And Tricks

- You can use ssh to login to a remote system:

```
ssh filipe@davinci.icm.uu.se
```

username host domain

- You can edit your ~/.ssh/config to save you some typing:

```
Host login
```

```
    Hostname davinci.icm.uu.se
```

```
    User filipe
```

```
Host *
```

```
    ForwardAgent yes
```

```
    ForwardX11 yes
```

```
    UseKeychain yes
```

- Using ssh keys one does not need to retype your password

```
$ ssh-keygen
```

 (this creates the key pair. Use a password!)

- This will create a ~/.ssh/id_rsa (this is the secret!) and

```
~/.ssh/id_rsa.pub
```

 (the public key).

- You can copy your public key to remote systems using **ssh-copy-id** to be able to login without using a password. It will copy it to ~/.ssh/authorized_keys

Remote File Copy

- You can use **scp** to copy files:
scp -r my_dir davinci:
- For larger transfers you can use **rsync**.
- It can be used to continue transfers and to synchronise two directories.

rsync -av my_images davinci:data

copies my_images inside the data directory

rsync -av my_images/ davinci:data

copies the files inside my_images inside the data directory

- Be careful with it as it can easily delete files in your own computer!
Test with -n first!
- For very large transfers it's best to use Globus Online (globus.org).

Working Remotely

- **screen** allows you to maintain a remote session even without a permanent connection. Example:

```
localhost$ ssh big_machine
big_machine$ screen
screen_session$ ./my_slow_script.py
```

- Now you can detach from the session (usually with **Ctrl+A+D**)

```
[detached]
big_machine$ exit
localhost$
```

- To return to your session just login to **big_machine** again and do:

```
big_machine$ screen -r
screen_session$ ./my_slow_script.py
Result: 42
screen_session$ exit
[screen is terminating]
big_machine$
```

For more info check **man screen**
Also do create your own **.screenrc**

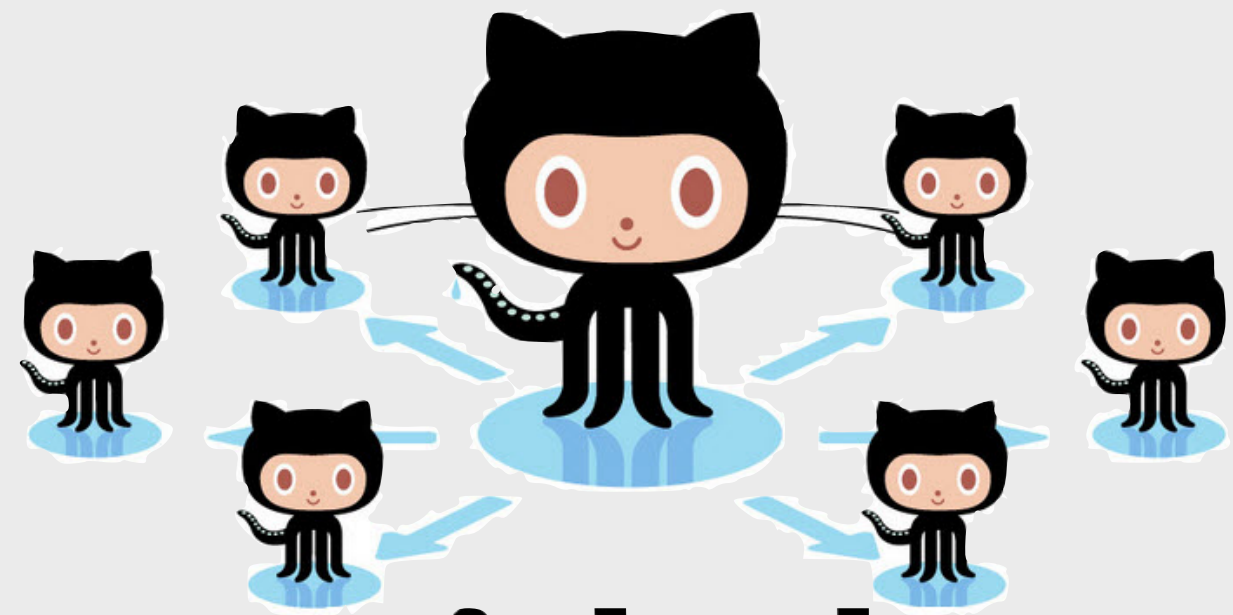
- Is it safe to give someone you don't know your id_rsa.pub file?
- What about your id_rsa file?

An Introduction To Git

THIS IS GIT. IT TRACKS COLLABORATIVE WORK
ON PROJECTS THROUGH A BEAUTIFUL
DISTRIBUTED GRAPH THEORY TREE MODEL.

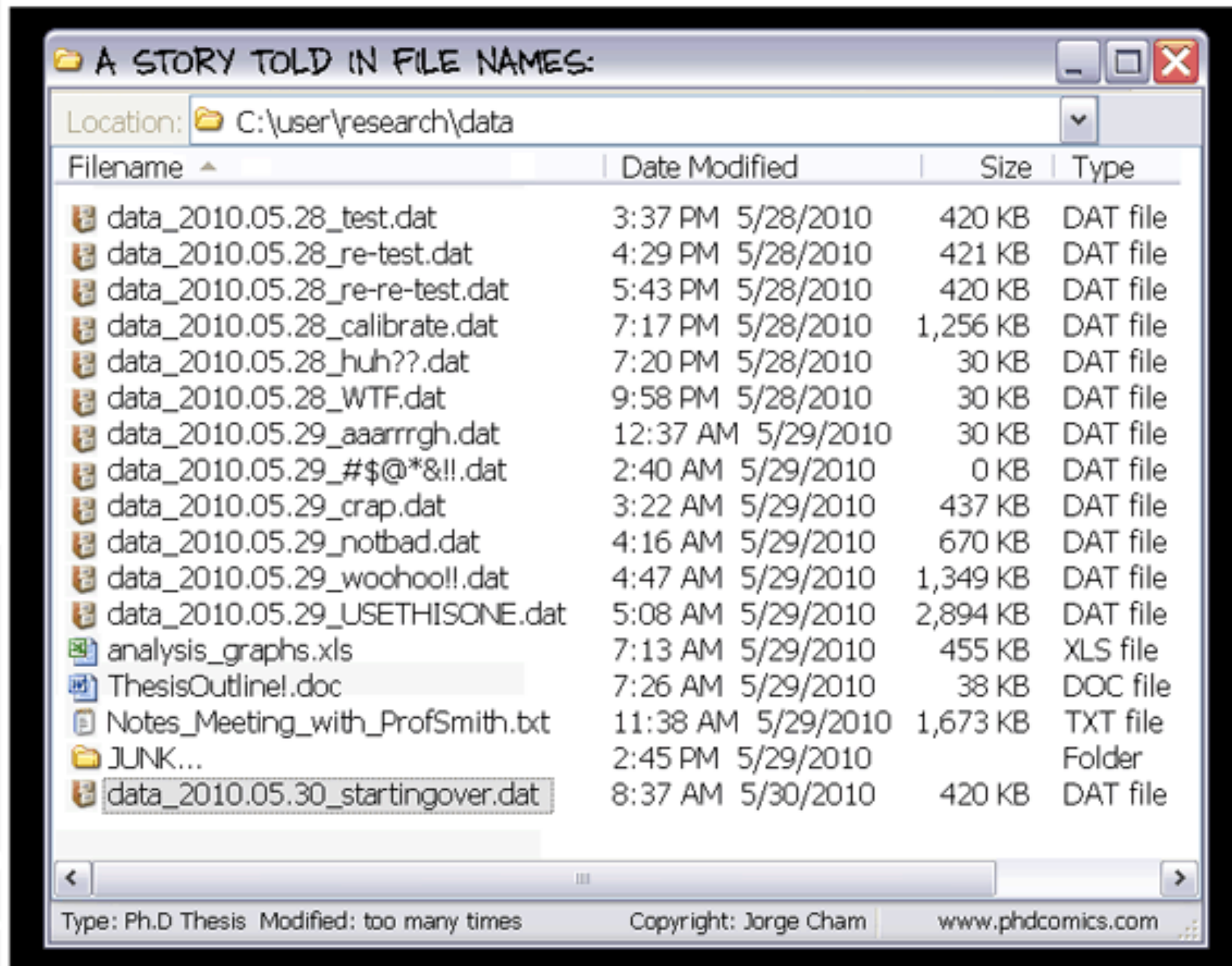
COOL. HOW DO WE USE IT?

NO IDEA. JUST MEMORIZE THESE SHELL
COMMANDS AND TYPE THEM TO SYNC UP.
IF YOU GET ERRORS, SAVE YOUR WORK
ELSEWHERE, DELETE THE PROJECT,
AND DOWNLOAD A FRESH COPY.



github
SOCIAL CODING

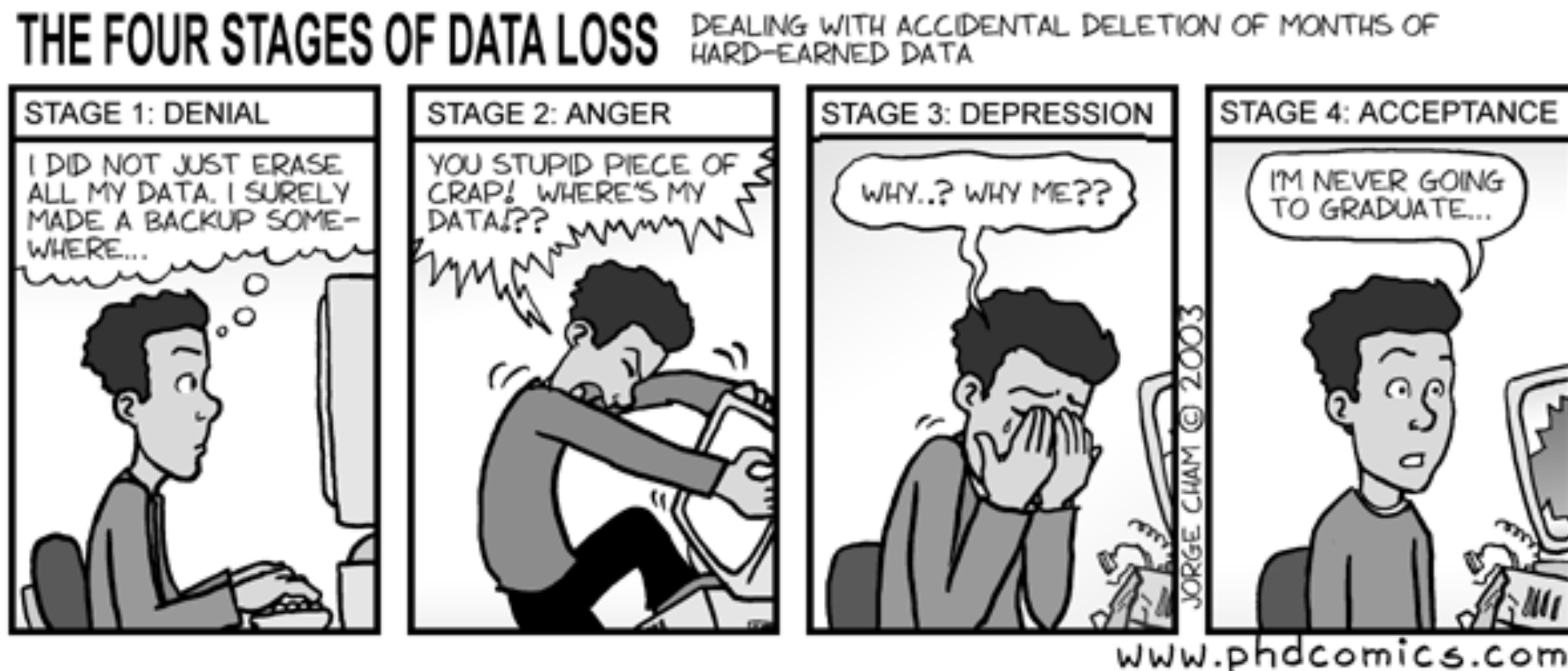
Why Do I Need Version Control?



by Jorge Cham
www.phdcomics.com

Why Do I Need Version Control?

- Your files are better organised
- You keep a history of all previous versions
- Your research is faster, more efficient and more reproducible
- Version control benefits collaborative work
- You always have a backup



How Do I Use Git?



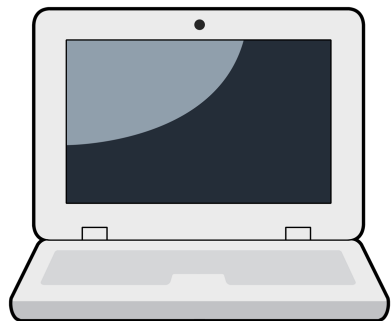
<http://github.com>



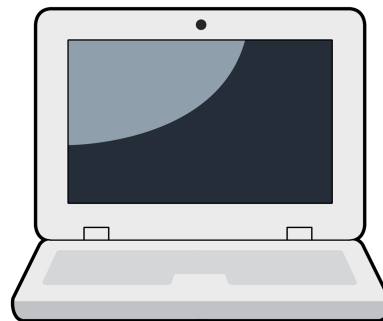
<http://bitbucket.org>

Remote

pull/push



**Collaborator A
Local**



**Collaborator B
Local**

Creating a new project

```
$ git init
```

Cloning an existing project

```
$ git clone
```

```
https://github.com/.../project.git
```

Adding new files to be committed

```
$ git add README.md
```

Commit all new files

```
$ git commit -m "Useful message"
```

Updating the local copy ("pulling")

```
$ git pull
```

Updating the remote ("pushing")

```
$ git push
```

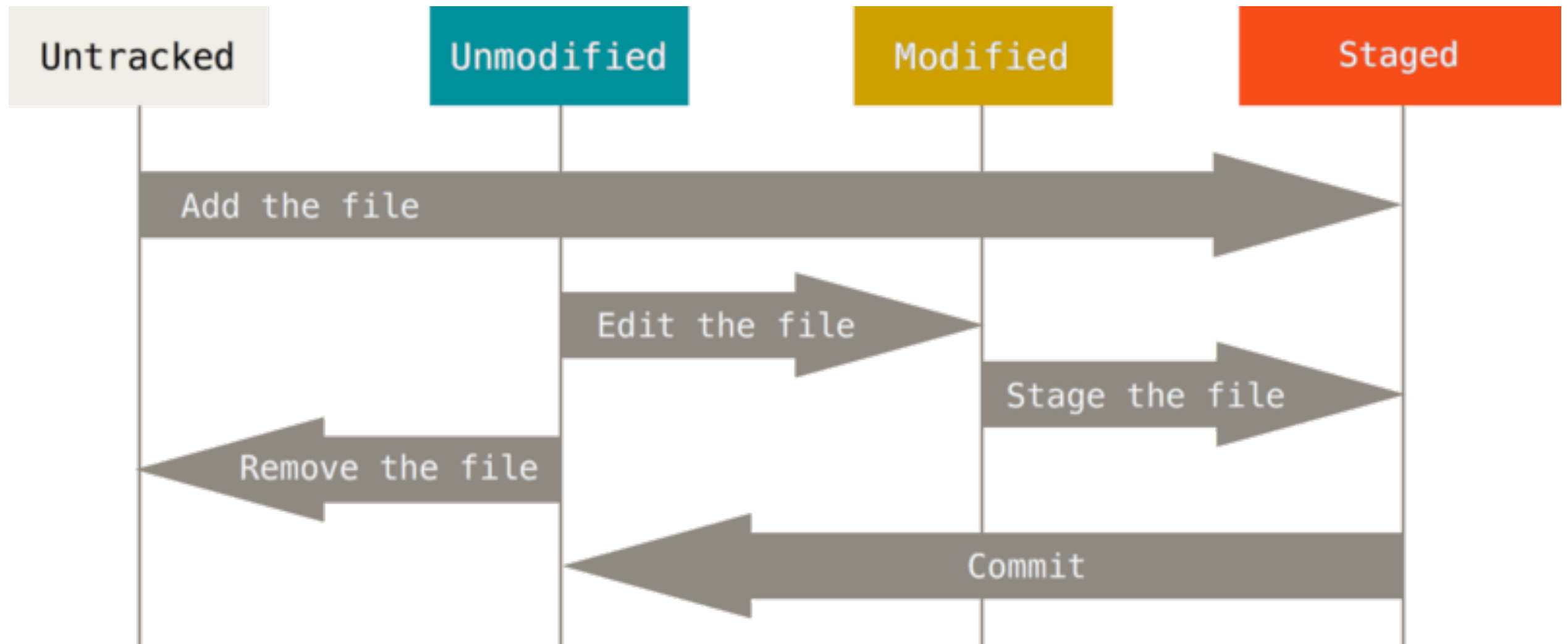
Current status of all files of repository

```
$ git status
```

Show the history (commit log)

```
$ git log
```

The Lifecycle Of The Status Of Your Files



Pro Git Boot, by Scott Chacon: <http://git-scm.com/book>

Setting Up Git

- Local configurations (only the current repository is affected)
`$ git config [options]`
- Global configurations (only the user's configuration is modified)
`$ git config --global [options]`
- System configurations (all users are affected)
`$ git config --system [options]`
- Change your identity
`$ git config --global user.name "Benedikt J. Daurer"`
`$ git config --global user.email "benedikt.daurer@icm.uu.se"`
- Set your favourite editor (e.g. emacs or vim)
`$ git config --global core.editor emacs`
- Check your current settings
`$ git config --list`

Demo: Basic Git Commands

Getting Familiar With Basic Commands

1. Create a local copy (clone) of the following project:

<https://github.com/uu-python/participants>

```
$ git clone https://github.com/uu-python/participants.git
```

2. Create a new file YOURNAME.md

```
$ $EDITOR filipe.md
```

3. Write something about yourself and add your file to the files tracked by git

4. Commit your changes and give a meaningful log message

```
$ git add filipe.md
```

```
$ git commit -m "Create new file"
```

5. Update your local repository by pulling from the remote

```
$ git pull
```

6. Update the remote repository by pushing your local changes

```
$ git push
```


Deleting, Moving, Cancelling, Resetting

- Deleting a tracked file
\$ git rm FILE
- Deleting a tracked file (but keeping an untracked copy)
\$ git rm --cached FILE
- Moving a file (renaming)
\$ git mv FILE TARGET
- Unstaging a file
\$ git reset HEAD FILE
- Undo modifications of unstaged files
\$ git checkout -- FILE1 FILE2
- Checkout a previous version
\$ git checkout HASH

Branching And Merging

Check the history of the branch

```
benedikt@icm-241-135:~/participants$ git log
```

```
commit 776e7c4f19493d88a85832dcef44ff2e569586bb
Author: Benedikt Daurer <benedikt.daurer@icm.uu.se>
Date:   Mon Nov 21 15:59:00 2016 +0100
```

Fixed typo

```
commit 6acb9e49d9de91a8aa1536a659f3003f477e9c7d
Author: Benedikt Daurer <benedikt.daurer@icm.uu.se>
Date:   Mon Nov 21 15:57:53 2016 +0100
```

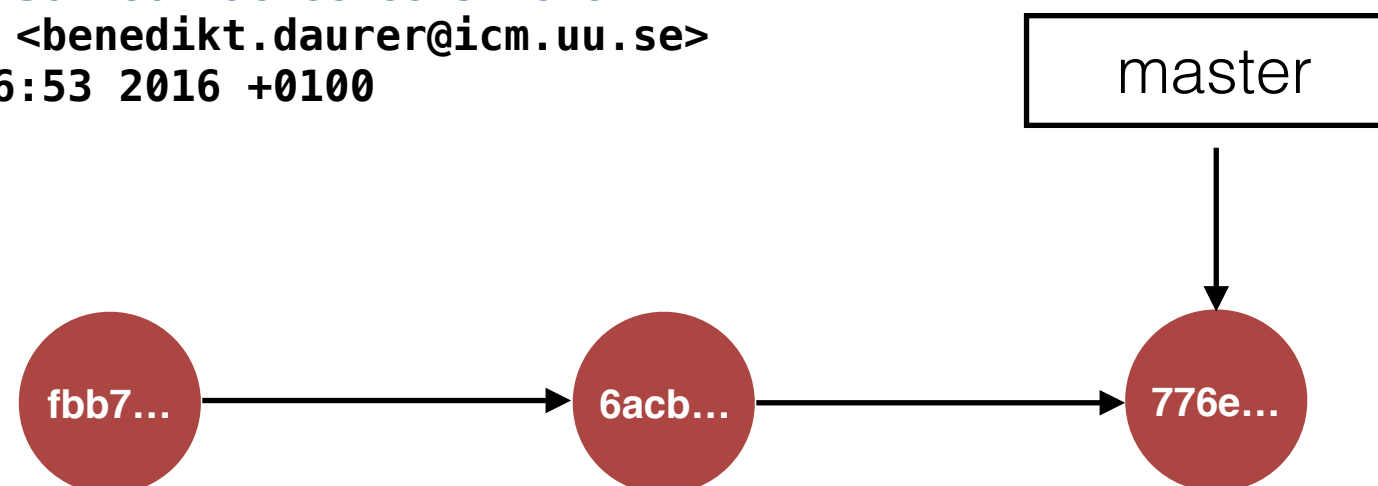
Fixed link

```
commit fbb7ef51497d8aa77304280419c7cc4c67511626
Author: Benedikt Daurer <benedikt.daurer@icm.uu.se>
Date:   Mon Nov 21 15:56:53 2016 +0100
```

Initial commit

Check on the status of the branch

```
benedikt@icm-241-135:~/participants$ git status
On branch master
Your branch is up-to-date with 'origin/master'.
nothing to commit, working directory clean
```



Branching And Merging

Create a new branch "testing"

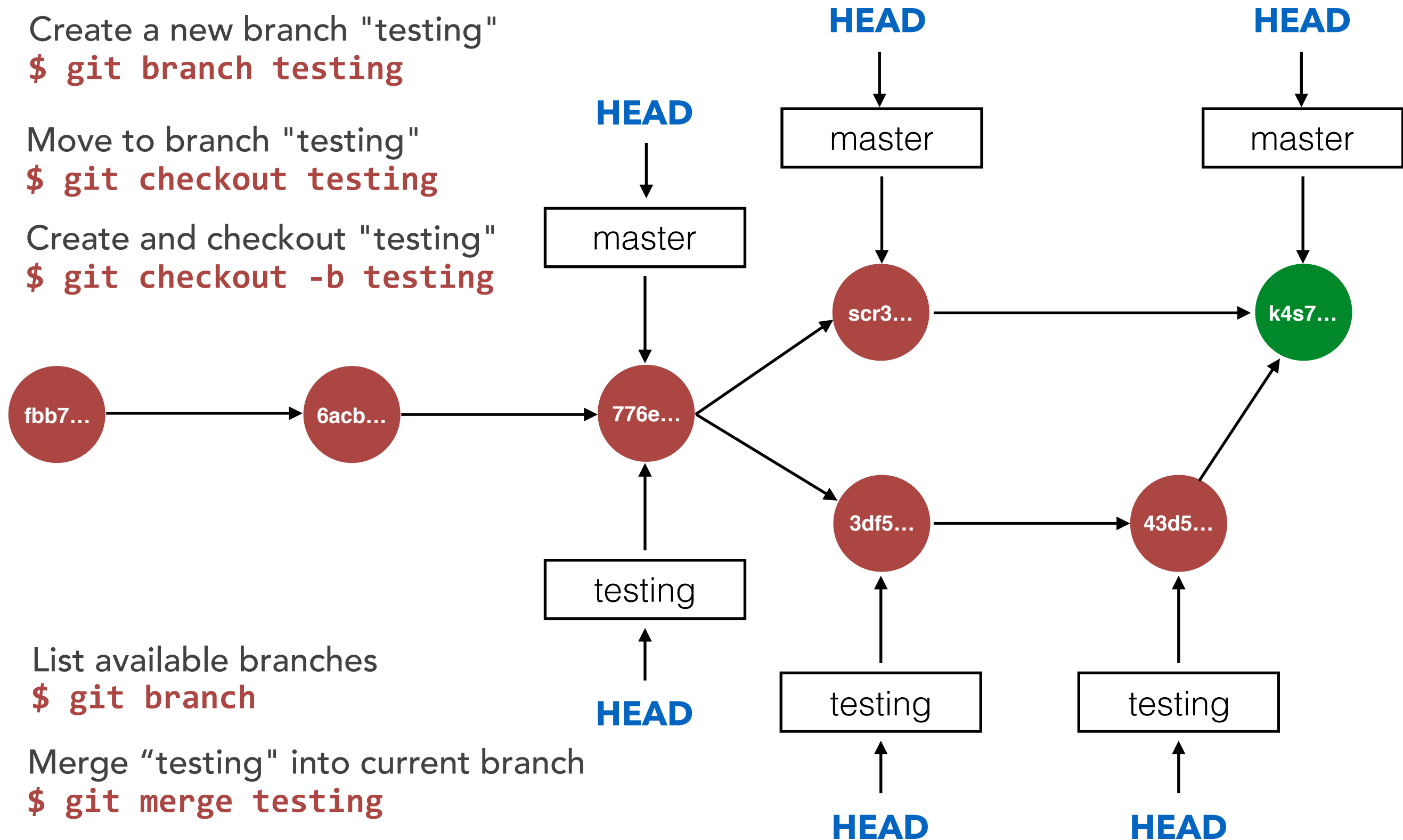
\$ git branch testing

Move to branch "testing"

\$ git checkout testing

Create and checkout "testing"

\$ git checkout -b testing



List available branches

\$ git branch

Merge "testing" into current branch

\$ git merge testing

Demo: Branching And Merging

Contribute To A Collaborative Project

1. Create a local copy (clone) of the following project:

<https://github.com/uu-python/participants>

```
$ git clone https://github.com/uu-python/participants
```

2. Create a new branch "yourname"

```
$ git checkout -b filipe
```

3. Edit the file of your neighbour or someone else (e.g. describe the person, write a message, ...)

4. Commit your changes and give a meaningful log message

```
$ git commit -m "Edited benedikt's file."
```

5. Push your local to remote branch with the same name

```
$ git push --set-upstream origin filipe
```

6. Switch to the master branch and merge the branch "yourname" into master

```
$ git checkout master
```

```
$ git merge filipe
```

7. Update local master branch (pull)

```
$ git pull
```

8. Update remote master branch (push)

```
$ git push
```

Take Home Messages

- Version control using git helps you better organize your work (e.g. code, documentation, manuscripts, thesis, webpages, ...)
- **git** (together with **github** or **bitbucket**) enables collaborative coding/writing
- You always have a backup and you can easily go back to previous versions

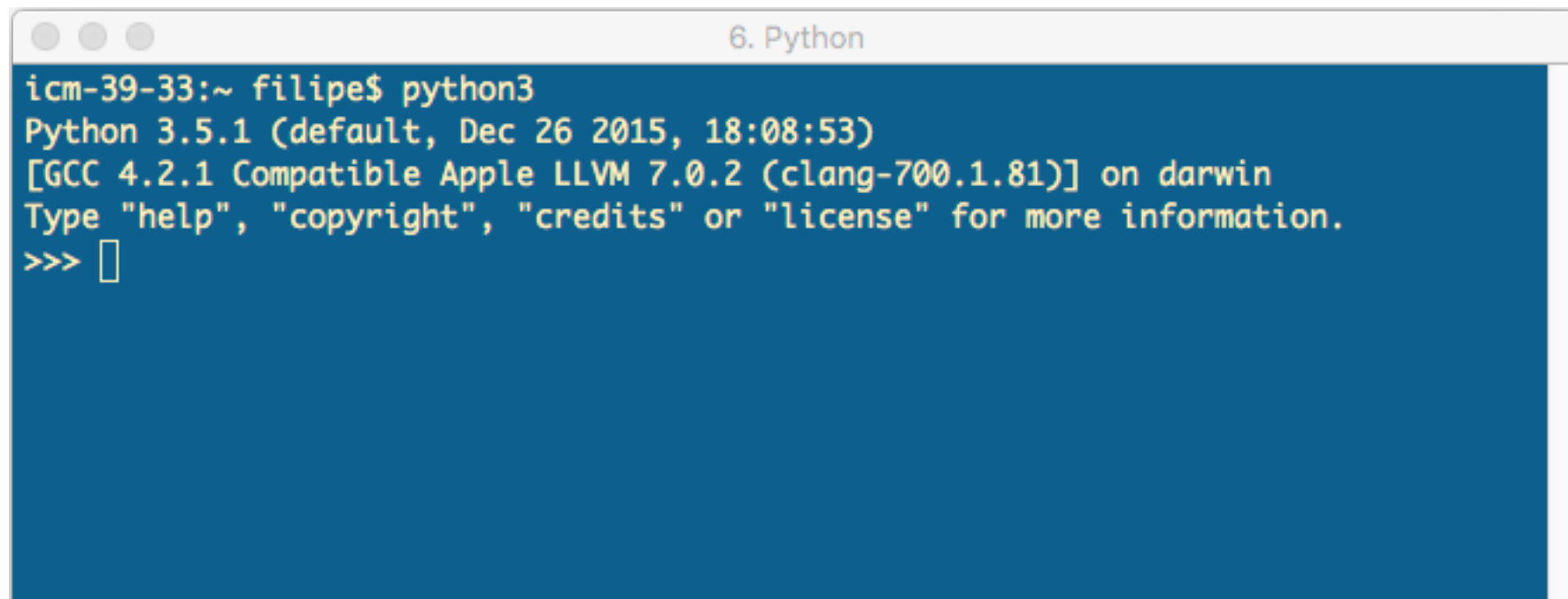
Further Reading And Playing

- The Pro Git Book (<https://git-scm.com/book/en/v2>)
- Githug - a game for learning git (<https://github.com/Gazler/githug>)

Interactive Python

Standard Python Interpreter

- The standard Python interpreter is **python**.
- For example, to run a script **my-program.py**:
\$ python my-program.py
- We can also start the interpreter by simply typing python at the command line, and interactively type Python code into the interpreter.

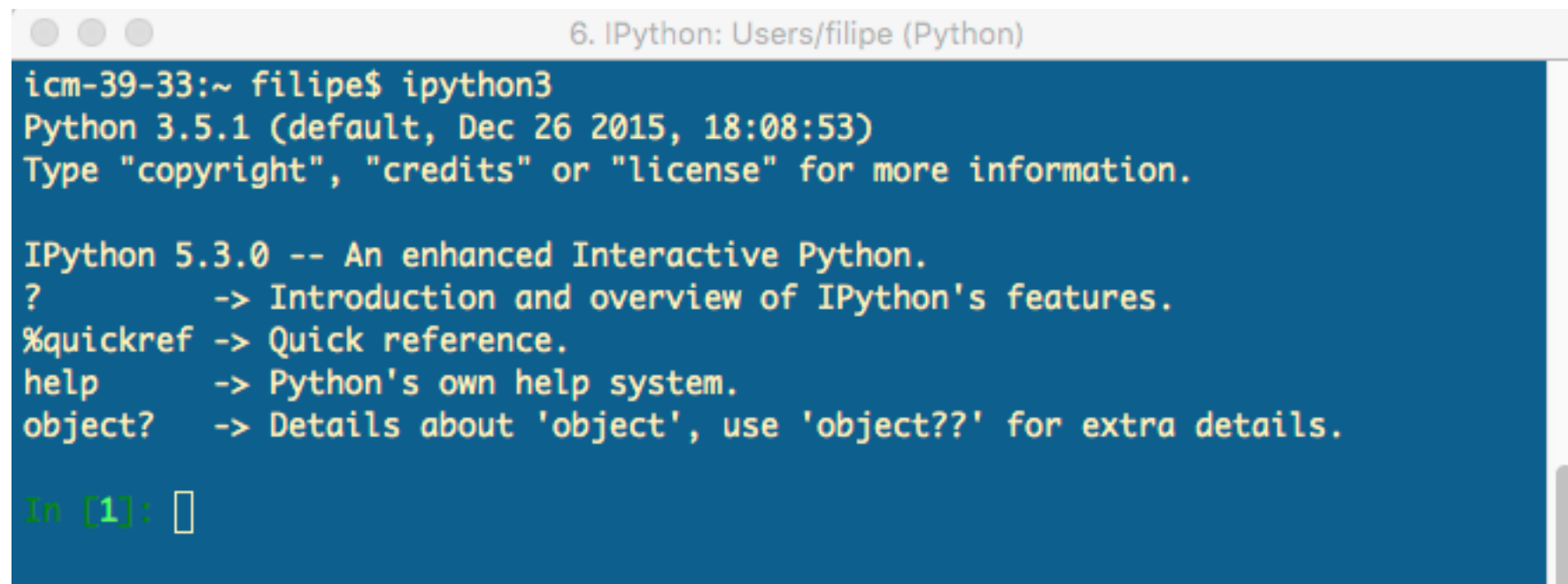


```
icm-39-33:~ filipe$ python3
Python 3.5.1 (default, Dec 26 2015, 18:08:53)
[GCC 4.2.1 Compatible Apple LLVM 7.0.2 (clang-700.1.81)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> 
```

- The standard Python interpreter is not very convenient due to a number of limitations.

IPython

- IPython addresses the limitation of the standard python interpreter
- A work-horse for scientific use of python. It provides an interactive prompt to the python interpreter with a greatly improved user-friendliness.



```
6. IPython: Users/filipe (Python)
icm-39-33:~ filipe$ ipython3
Python 3.5.1 (default, Dec 26 2015, 18:08:53)
Type "copyright", "credits" or "license" for more information.

IPython 5.3.0 -- An enhanced Interactive Python.
?          -> Introduction and overview of IPython's features.
%quickref  -> Quick reference.
help       -> Python's own help system.
object?    -> Details about 'object', use 'object??' for extra details.

In [1]:
```

- It includes:
 - Command history, using the up and down arrows.
 - Tab auto-completion.
 - In-line editing of code.
 - Object introspection, and docstring extraction.
 - Good interaction with operating system shell.

Jupyter Notebook

- Open-source web application
- Allows you to create and share documents that contain live code, equations, visualisations and explanatory text
- Based on the IPython shell, but provides a cell-based environment with great interactivity
- Similar interface capabilities to Matlab.
- Calculations can be organised and documented in a structured way.
- Jupyter notebooks are usually run locally, from the same computer that run the browser.
- To start a new Jupiter notebook session, run the following command:
\$ jupyter-notebook

```
In [7]: output = mesolve(H, psi0, tlist, c_ops, [a.dag() * a, sm.dag() * sm])
```

Visualize the results

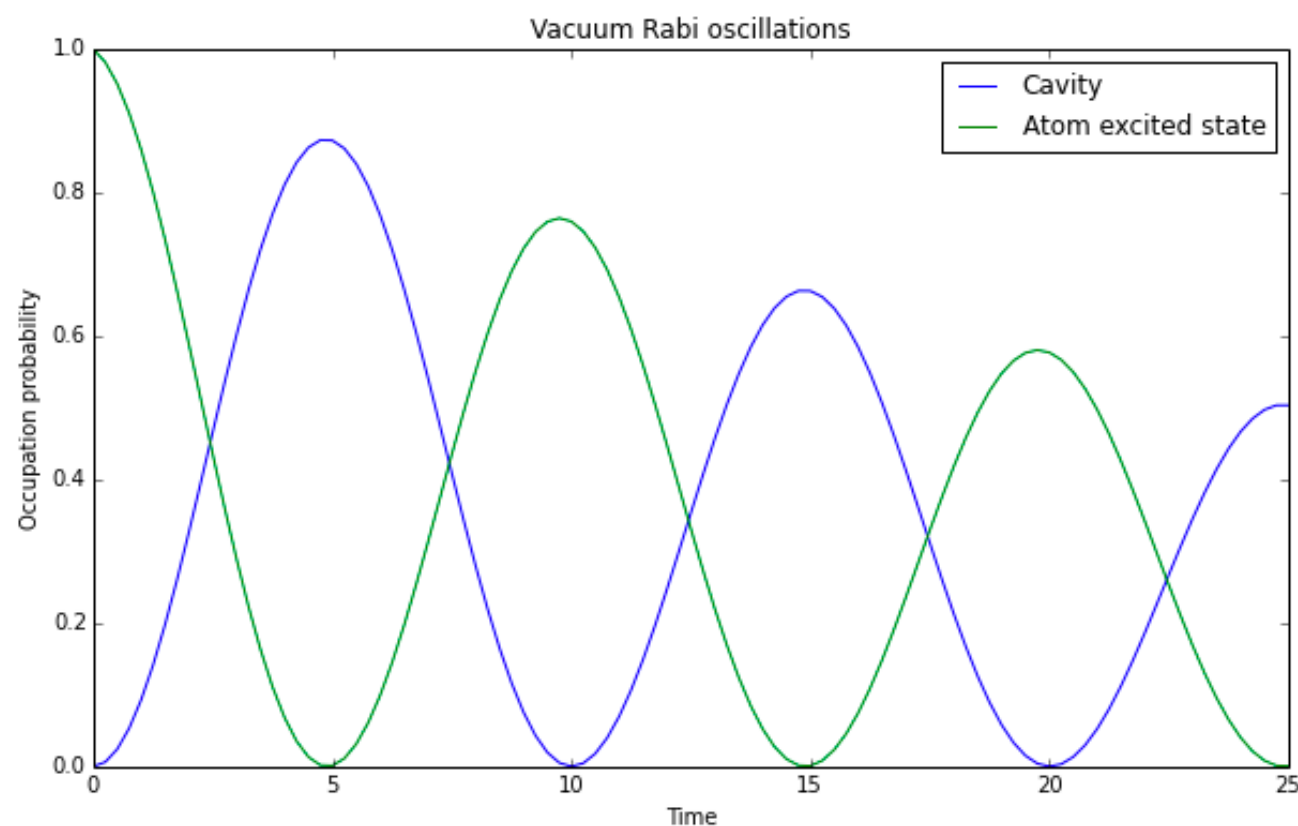
Here we plot the excitation probabilities of the cavity and the atom (these expectation values were calculated by the `mesolve` above). We can clearly see how energy is being coherently transferred back and forth between the cavity and the atom.

```
In [8]: n_c = output.expect[0]
n_a = output.expect[1]

fig, axes = plt.subplots(1, 1, figsize=(10,6))

axes.plot(tlist, n_c, label="Cavity")
axes.plot(tlist, n_a, label="Atom excited state")
axes.legend(loc=0)
axes.set_xlabel('Time')
axes.set_ylabel('Occupation probability')
axes.set_title('Vacuum Rabi oscillations')
```

```
Out[8]: <matplotlib.text.Text at 0x7f8f0b8c3908>
```



Demo: Jupyter Notebook