TU/e – March 2021 Software Carpentry Workshop – online

March 16, 17, 23 and 24, 2021

Links

Workshop webpage (schedule, lessons, survey, installation instructions, etc): https://4turesearchdata-carpentries.github.io/2021-03-16-tudelft-online

Videoconference (BigBlueButton) https://bbb.tbm.tudelft.nl/b/pau-owe-dgp-vjp

Passcode access: 128223

Host

- Paula Martinez Lavanchy
- Sil van Lieshout

Instructors

- Iñigo Aldazabal Mensa
- Rohit Goswami
- Raphaela Heil
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Helpers

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Schedule (all times CET)

Day 1 – Tue. March. 16th – The UNIX Shell

09:15 Welcome and introdution *(PML)*
09:30 Introduction to the Unix shell *(SO)*
10:30 Coffee break
10:45 Automating tasks with the Unix Shell *(SO)*
11:45 Coffee break
12:00 Introduction to the Unix shell (continued) *(SO)*
13:00 Wrap Up *(SO)*

Day 2 – Wed. March 17th – Version Control with Git

09:15 Welcome and instructions of the day *(PML)*
09:30 Version control with Git *(IAM)*
10:30 Coffee break
10:45 Version control with Git *(IAM)*
11:45 Coffee break
12:00 Version control with Git *(IAM)*
13:00 Wrap Up *(IAM)*

Day 3 – Tue. March 23rd Introduction to Python

09:15 Welcome and instructions of the day *(PML)*
09:30 Programming with Python *(RG)*
10:30 Coffee break
10:45 Programming with Python *(RG)*
11:45 Coffee break
12:00 Programming with Python *(RG)*
13:00 Wrap Up *(SO)*

Day 4 – Tue. March 24th – Introduction to Python (II)

09:15 Welcome and instructions of the day *(PML)*
09:30 Programming with Python *(RH)*
10:30 Coffee break
10:45 Programming with Python *(RH)*
11:45 Coffee break
12:00 Programming with Python *(RH)*
13:00 Post-workshop Survey, final wrap up. End *(PML)*

Shell basic commands

```
$ pwd
$ ls
$ cd <PATH>

$ mkdir  <DIRECTORY>
$ nano <FILE>
$ cat <FILE>
$ rm <FILE|DIRECTORY>
$ mv <ORIG> <DEST>
$ cp <ORIG> <DEST>

$ wc <FILE(s)>
$ wc -l *.pdb > lenghts.txt  # > redirection operator
$ sort -n lenghts.txt
$ head <FILE>
$ wc -l *pdb | sort -n  # | pipe operator
$ wc -l *pdb | sort -n | head -n 1

$ for filename in *.dat
  do
     echo $filename
  done

# Text commmands
$ find   # find by filename / type
$ grep   # find by file content
$ sed    # substitute text inside files
$ awk    # kind of excel for the command line
```

Git basic commands

```
$ git init
$ git status
$ git diff
$ git add <FILE(s)>
$ git commit

$ git clone <REPO>
$ git pull
$ git push
```

Python importing conventions

```
$ import numpy as np
$ import scipy as sp
$ import pandas as pd
$ import matplotlib.pyplot as plt

$ from scipy import optimize as opt
```

jupyter notebook quick reference

Shortcut (mode)	Action
ESC (any)	Go into command mode
ENTER (any)	Go into cell edit mode
SHIFT+ENTER (any)	Run the current cell and *select* the one below
ALT+ENTER (any)	Run the current cell and *insert* a new one below
CTRL+ENTER (any)	Run the current cell and *enter command mode* in current cell.
A (command)	Insert cell Above
B (command)	Insert cell Below
H (command)	Keyboard shortcut reference
Command/Ctrl Shift C	Command palette
object_name.<TAB> (edit)	Tab autocompletion
object_name.<SHIFT+TAB> (edit)	Object help (twice for full help)
object_name.<SHIFT+TAB+TAB> (edit)	Full object help
object_name.<SHIFT+TAB+TAB+TAB+TAB> (edit)	Full object help in a new frame