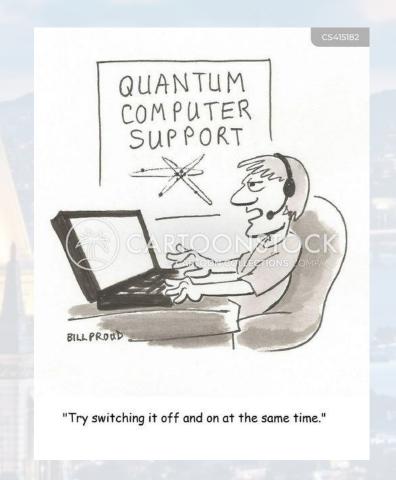


M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics





syllabus:	- Introduction to Unix & Python	(week 1 - 2)
	- Functions, Loops, Lists and Arrays	(week 3 - 4)
	- Visualization	(week 5)
	- Parsing, Data Processing and File I/O	(week 6)
	- Statistics and Probability, Interpreting Measurements	(week 7 - 8)
	- Random Numbers, Simulation	(week 9)
	- Numerical Integration and Differentiation	(week 10)
	- Root Finding, Interpolation	(week 11)
	- Systems of Linear Equations	(week 12)
	- Ordinary Differential Equations	(week 13)
	- Fourier Transformation and Signal Processing	(week 14)
	- Capstone Project Presentations	(week 15)



Week	Dates	Topics	Reading	Lecture Slides	Workshop	Homework
1 - 2	Aug 28th / Sep 4th	Introduction to Unix and Python	K&N Ch. 1			
3 - 4	Sep 11th / Sep 18th	Functions, Loops, Lists, Arrays	K&N Ch.2-3			
5	Sep 25th	Visualization	K&N Ch. 4, K&N Ch. 6.3-6.4			
6	Oct 2nd	Parsing, Data Processing, and File I/O	K&N Ch. 4			
7 - 8	Oct 9th / Oct 16th	Statistics and Probability, Interpreting Measurements	Hughes			



syllabus

Week	Dates	Topics	Reading	Lecture Slides	Workshop	Homework
9 - 10	Oct 23rd / Oct 30th	Random Numbers, Simulation	K&N Ch. 6, Newman Ch. 10			
11 - 12	Nov 6th / Nov 13th	Numerical Integration and Differentiation	K&N Ch. 6 Newman Ch. 5			
13	Nov 20th	Root finding, Interpolation	K&N Ch. 6.5 Newman Ch. 6			
14	Nov 27th	Systems of Linear Equations	Newman Ch. 6 K&N Ch. 6.6			
15	Dec 4th	Ordinary Differential Equations	K&N Ch. 6.8-6.9 Newman Ch. 8			
16	Dec 11th	Fourier Transforms, Signal Processing	Newman Ch. 7			
17	Dec 18th	Capstone Project Presentations				

Lecture: Wednesdays, 2 - 4pm, Dwinelle 88

Workshops: Fridays, 2-4pm (section 1) Social Science, 170 and

Fridays, 4-6pm (section 2) Social Science, 140

Instruction begins: August 28, 2024

Instruction ends: Friday, December 13, 2024

my contact: markus.hohle@berkeley.edu

TA: Krish Desai krish.desai@berkeley.edu

check out: <u>Google Colab</u>

bcourse

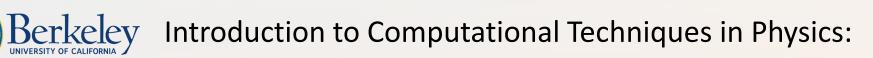
datahub.berkeley



motivation: The good old days:



Salar de Uyuni, Bolivia, Mar 2003



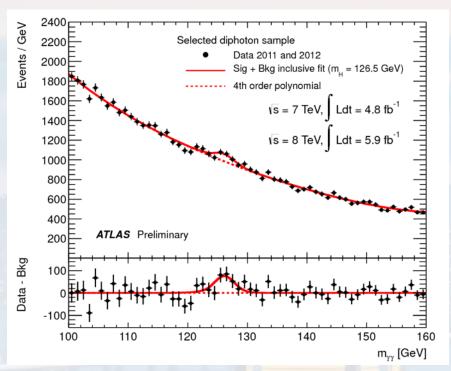


motivation:

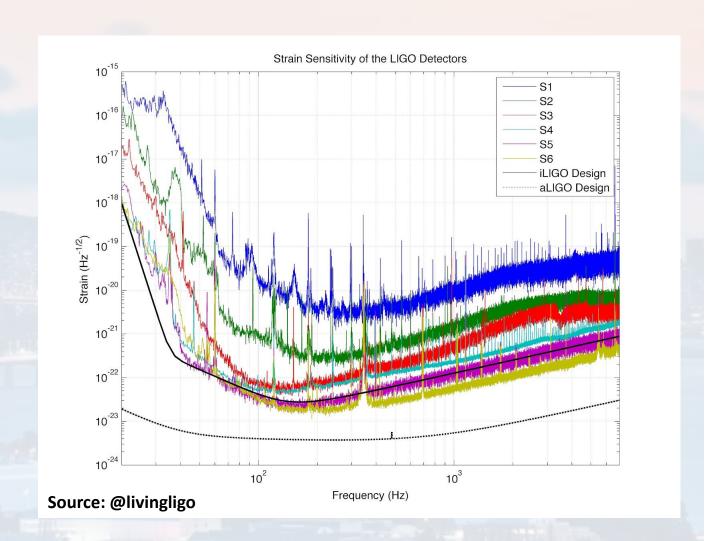




motivation:

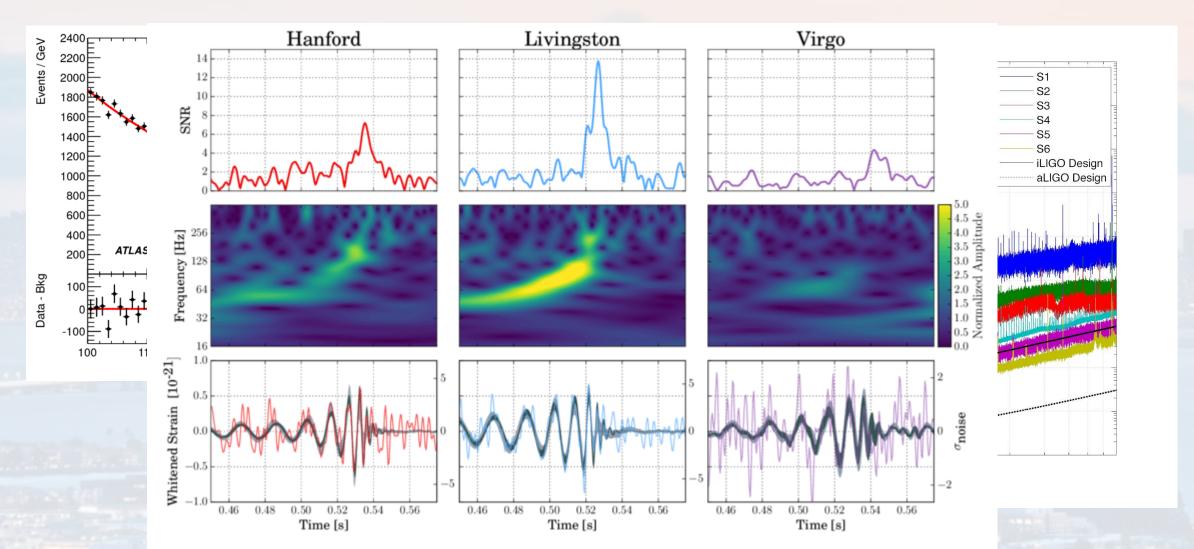


Source: CERN/ATLAS





motivation:

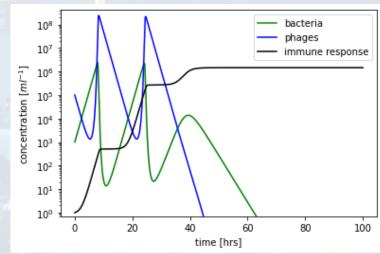


Source: Sergio Gaudio Embry-Riddle Aeronautical University, Prescott, United States · Physics

goal: being able to write code like this...

• • •

...and simulating systems like that



Leung & Weitz 2016



syllabus:	- Introduction to Unix & Python	(week 1 - 2)
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	- Capstone Project Presentations	(week 15)



<u>syllabus:</u>	- Introduction to Unix & Python	(week 1 - 2)
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	- Capstone Project Presentations	(week 15)

Operating System: interface between human and computer

→ **G**raphical **U**ser Interface: Windows, OS X, iOS, Android

→ text based: MS-DOS

→ mixed: Unix

Unix: - Bell Labs, early 70s

- Written in C and Assembly

Linux: - as a an alternative to Unix

- Linus Torvalds (1991)

- Ubuntu, SUSE, ... Scientific Linux

efficient, fast, robust optimized, but...

... not suitable for the *standard* user

Programming Languages: → translate human instructions to a form understandable by a computer

the "style" of programming

procedural: functions/ routines that call each other (Fortran, ALGOL, COBOL, BASIC, Pascal, C)

object oriented (OOP): creating objects/types of different properties (see later) C++, Fortran 2003, Java, MATLAB, Python, Ruby, ...

how a programming language "talks" to your CPU or GPU

compiled language: close to the resulting machine code, **fast**Fortran, C, C++, Java, Cobol, Pascal

interpreted language: an interpreter translates between source code and machine code. Slower, but simpler syntax
Perl, Raku, Python, MATLAB

Bits & Bytes: We need only two states: on and off

How many different states can I create with 8 switches?



smallest memory cell: 8bits = 1byte bit stands for binary digit

For some reason humans use **ten** states a = {0, 1, 2, 3, 4, 5, 6, 7, 8, 9}

$$N_{dec} = \sum_{i=0}^{\infty} a_{ji} 10^i$$

0	00000000
1	0000000 <mark>1</mark>
2	00000010
3	00000011
4	00000100
5	00000101
6	00000110
7	00000111
8	00001000
9	00001001
10	00001010
11	00001011
12	00001100
13	00001101
14	00001110
15	00001111
16	00010000

Bits & Bytes: We need only two states: on and off

For some reason humans use **ten** states $a = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$

$$N_{dec} = \sum_{i=0} a_{ji} 10^i$$

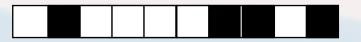
vs **two** states $a = \{0, 1\}$

$$N_{bin} = \sum_{i=0} a_{ji} 2^i$$

Let's write the number 15 in: decimal, binary and to base three:

0	00000000
1	00000001
2	00000010
3	00000011
4	00000100
5	00000101
6	00000110
7	00000111
8	00001000
9	00001001
10	00001010
11	00001011
12	00001100
13	00001101
14	00001110
15	00001111
16	00010000

Bits & Bytes: We need only two states: on and off



So, we are fine with natural numbers...

... what is with negative numbers...

...or fractions...

...or π and e

- → float and double numbers need three *fields*:
 - sign
 - exponent
 - fraction

8 bits	= 1 byte (B)
1 kB	= 1024 B
1 MB	= 1024 kB etc

0	00000000
1	00000001
2	000000 <mark>1</mark> 0
3	00000011
4	00000100
5	00000101
6	00000110
7	00000111
8	00001000
9	00001001
10	00001010
11	00001011
12	00001100
13	00001101
14	00001110
15	00001111
16	00010000
-	

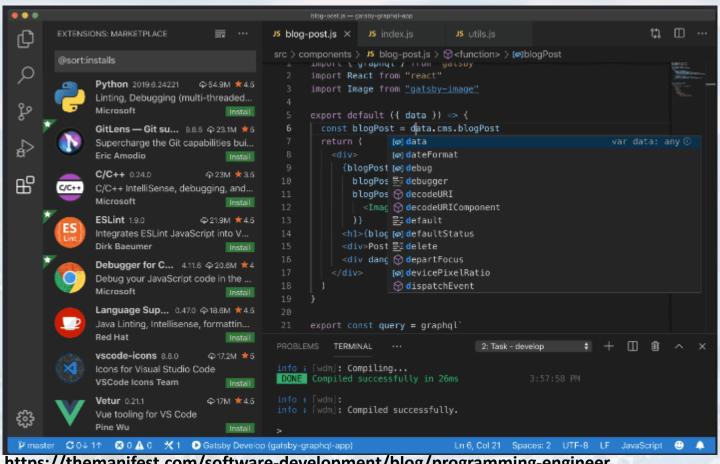
Bits & Bytes:

	rel. approx. error (ϵ)	range
16 bit int		-32768 32767
32 bit int		$\approx -10^9 \dots 10^9$
32 bit float	≈ 10 ⁻⁸	$\approx 10^{-38} \dots 10^{38}$
64 bit double	$\approx 10^{-16}$	$\approx 10^{-308} \dots 10^{308}$

Luckily, Python will tell us when an operation doesn't makes sense based on precision, but still: be cautious!

0	00000000
1	00000001
2	00000010
3	00000011
4	00000100
5	00000101
6	00000110
7	00000111
8	0000 1 000
9	00001001
10	00001010
11	00001011
12	00001100
13	00001101
14	0000 111 0
15	00001111
16	00010000

build your environment



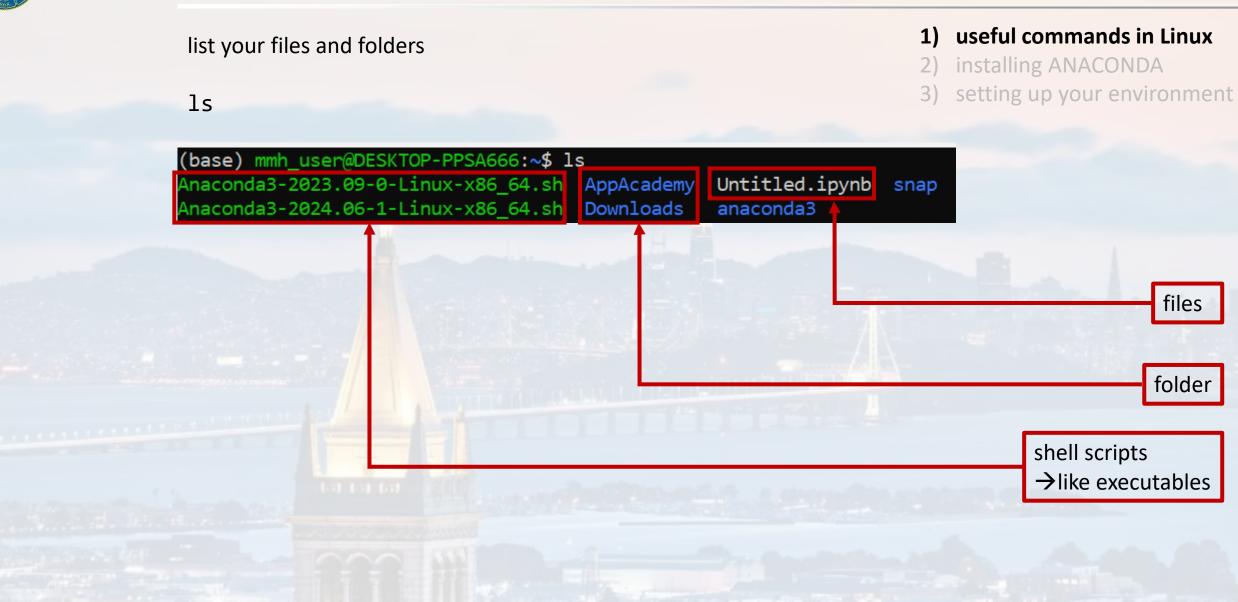
https://themanifest.com/software-development/blog/programming-engineer

- 1) if your OS is Windows
 - → install Windows Subsystem for Linux (WSL)
 - → follow the instructions <u>here</u>



- 2) if your OS is Unix/Linux
 - → we can start right away!
- 3) optional
 - → once you have Linux, there are lot's of <u>useful tools</u> you can install and link together
 - Google Chrome
 - Visual Studio Code (aka VS Code)
 - NodeJS
 - Docker

Unix & Python

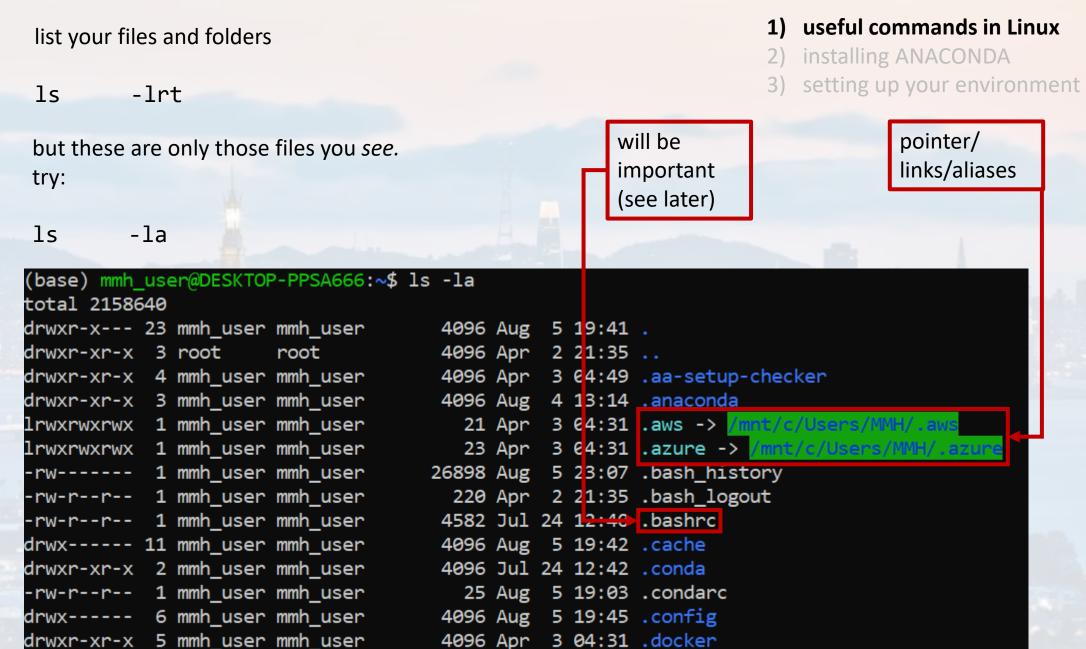




- 1 stands for long: shows a file with all permissions and properties, each per line
- **r** stands for *reverse* (oldest first)
- t stands for the time flag (as criterium for r)

```
(base) mmh_user@DESKTOP-PPSA666:~$ ls -lrt
total 2158464
           2 mmh_user mmh_user
drwx----
                                     4096 Apr 8 20:03 Downloads
           3 mmh_user mmh_user
drwx----
                                     4096 Apr 10 19:16 snap
           5 mmh_user mmh_user
                                     4096 Apr 24 18:29 AppAcademy
drwxr-xr-x
           1 mmh_user mmh_user 1153404010 Jul 24 12:36 Anaconda3-2023.09-0-Linux-x86 64.sh
-rwxr-xr-x
           1 mmh_user mmh_user 1056829859 Aug 5 18:53 Anaconda3-2024.06-1-Linux-x86_64.sh
-rwxr-xr-x
drwxr-xr-x 31 mmh_user mmh_user
                                     4096 Aug 5 19:22 anaconda3
-rw-r--r-- 1 mmh_user mmh_user
                                      616 Aug 5 19:30 Untitled.ipynb
```





1) useful commands in Linux

3) setting up your environment

installing ANACONDA

Berkeley Introduction to Computational Techniques in Physics:

list your files and folders

ls -lrt

ls -la

You can search for files/folders with particular substrings using a "wildcard"

ls *.py ls *py*

```
(base) mmh_user@DESKTOP-PPSA666:~$ ls -lrt *A*
-rwxr-xr-x 1 mmh_user mmh_user 1153404010 Jul 24 12:36 Anaconda3-2023.09-0-Linux-x86_64.sh
-rwxr-xr-x 1 mmh_user mmh_user 1056829859 Aug 5 18:53 Anaconda3-2024.06-1-Linux-x86_64.sh

AppAcademy:
total 12
drwxr-xr-x 13 mmh_user mmh_user 4096 Apr 17 18:34 HTMLExercises
drwxr-xr-x 4 mmh_user mmh_user 4096 Apr 23 21:13 GitExercises
drwxr-xr-x 7 mmh_user mmh_user 4096 May 3 23:36 JavaExercises
```



changing your directory		 useful commands in Linux installing ANACONDA
cd	always leads back to the home directory	3) setting up your environment
cd/	one level up	
cd/my_dir	one level up, down to my_dir	
cd another/dir	one level down to dir	
mkdir test	creating the new directory test	
rm -r test	removing the directory using the flag r (he	ere: recursively)
rm any_file	when removing a file, no flag is needed	

Danger: Be careful with rm! There is no undelete command in Unix!

copying files and folders

- 1) useful commands in Linux
-) installing ANACONDA
- 3) setting up your environment

```
cp my_file ../somewhere/else
```

cp -r /entireDirectory somewhere/else/to/new_destination

note: the flag *r* is needed to copy the directory with all the sub directories

note: there are way more commands and flags we will be learning soon :)



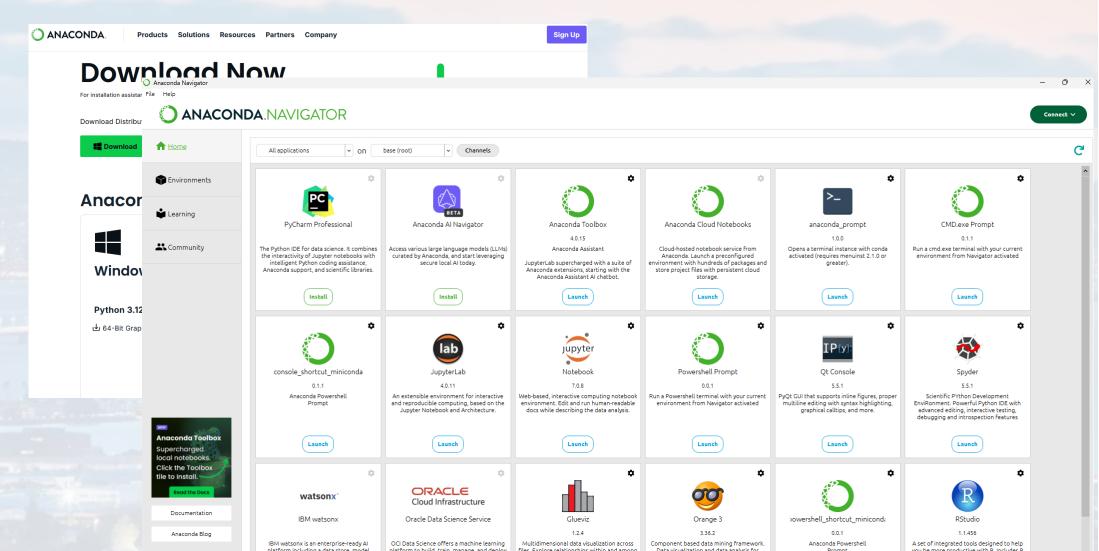
You can install ANACONDA Navigator for Windows

useful commands in Linux

installing ANACONDA

setting up your environment





- 1) we move into the home directory (cd) and run the curl (Client URL) command in order to download the ANACONDA installer from here
- 1) useful commands in Linux
- 2) installing ANACONDA
- 3) setting up your environment

```
curl -0 https://repo.anaconda.com/archive/Anaconda3-2024.06-1-Linux-x86_64.sh
```

2) running the installer

```
bash ~/Downloads/Anaconda3-2024.06-1-Linux-x86_64.sh
```

3) it might give us an error message "permission denied"

→ turning the installer shell script into an "executable" using chmod

```
chmod +x Anaconda3-2024.06-1-Linux-x86_64.sh
```

- 4) run the installer manually
- ./Anaconda3-2024.06-1-Linux-x86_64.sh



- 3) it might give us an error message "permission denied"
- chmod +x Anaconda3-2024.06-1-Linux-x86_64.sh
- 4) run the installer manually
- ./Anaconda3-2024.06-1-Linux-x86_64.sh
- 5) confirm license terms by typing yes and press enter
- 6) you might need to refresh your terminal by running source ~/.bashrc

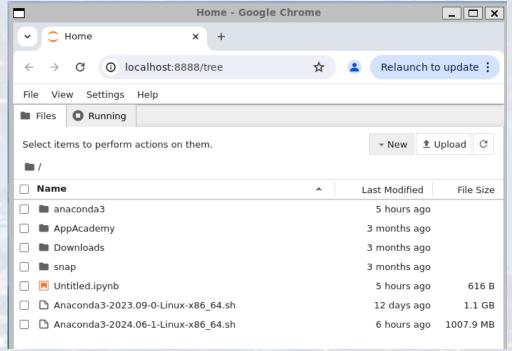
Now Anaconda should be working. Type

conda install python

finally, run

jupyter-notebook &

- 1) useful commands in Linux
- 2) installing ANACONDA
- 3) setting up your environment



Note: conda on unix doesn't work well with Spyder

- 1) useful commands in Linux
- 2) installing ANACONDA
- 3) setting up your environment

```
(base) mmh_user@DESKTOP-PPSA666:~$ spyder &
[1] 52032
(base) mmh_user@DESKTOP-PPSA666:~$ Could not load the Qt platform plugin "xcb" in "" even though it was found.
This application failed to start because no Qt platform plugin could be initialized. Reinstalling the application may fix this problem.

Available platform plugins are: eglfs, minimal, minimalegl, offscreen, vnc, webgl, xcb.

[1]+ Aborted spyder
(base) mmh_user@DESKTOP-PPSA666:~$
```

creating a conda environment for the Spyder IDE:

conda create -n spyder-env -c conda-forge python=3.11 spyder

activating the environment:

conda activate spyder-env

Note: conda on unix doesn't work well with Spyder

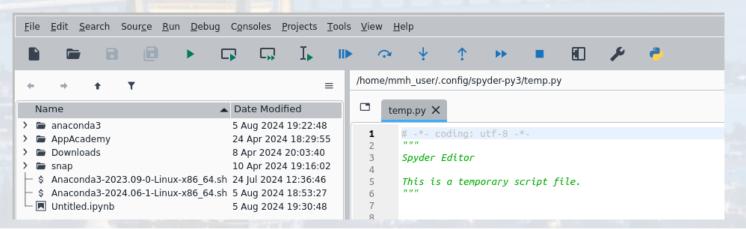
creating a conda environment for the Spyder IDE:

- 1) useful commands in Linux
- 2) installing ANACONDA
- 3) setting up your environment

conda create -n spyder-env -c conda-forge python=3.11 spyder activating the environment:

conda activate spyder-env

```
(base) mmh_user@DESKTOP-PPSA666:~$ conda activate spyder-env
(spyder-env) mmh_user@DESKTOP-PPSA666:~$ spyder &
[1] 53245
(spyder-env) mmh_user@DESKTOP-PPSA666:~$ fromIccProfile: failed minimal tag size sanity
```



depending on your project, you can create many different conda environments

```
conda create -n <MyEnv> python=3.10 scipy=0.17.3
```

showing all libraries:

conda list

showing all environments

conda info --envs

```
(base) mmh_user@DESKTOP-PPSA666:~$ conda info --envs
# conda environments:
#
base * /home/mmh_user/anaconda3
spyder-env /home/mmh_user/anaconda3/envs/spyder-env
```

- 1) useful commands in Linux
- 2) installing ANACONDA
- 3) setting up your environment

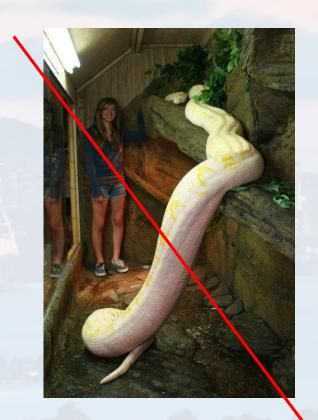
Now it is time for python!

- 1990, von Guido van Rossum



 named after "Monty Python", not the serpent



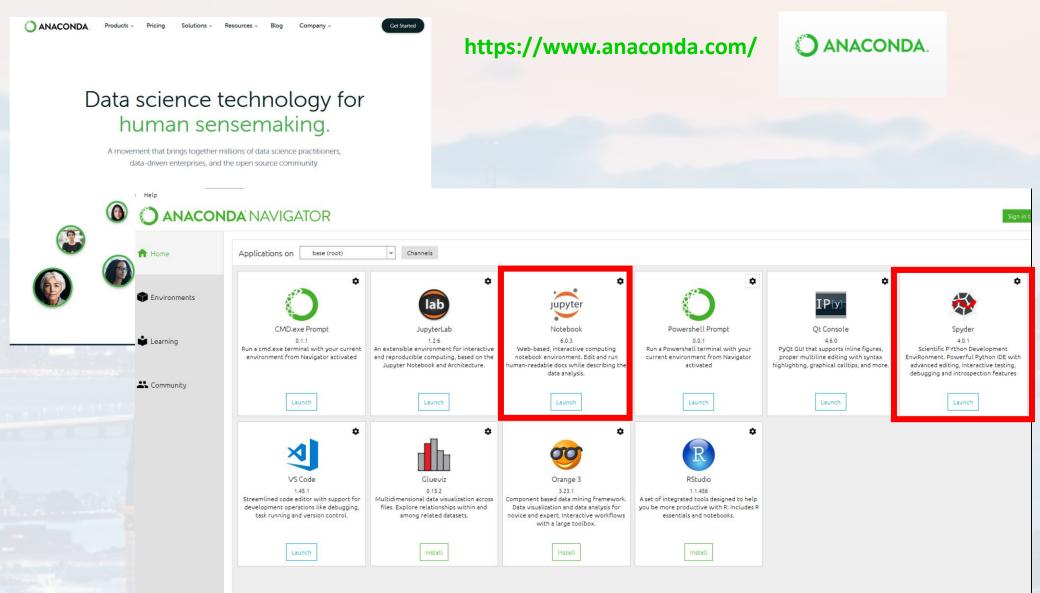


- idea: flexible, simple and compact syntax, extendable

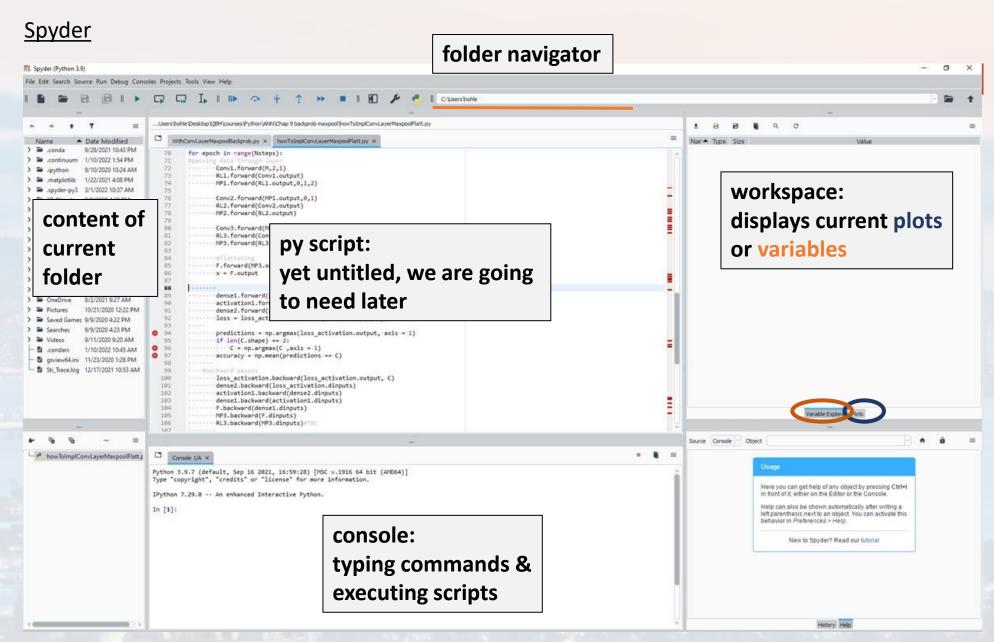
TIOBE index July 2024

Jul 2024	Jul 2023	Change	Prograr	nming Language	Ratings	Change
1	1		•	Python	16.12%	+2.70%
2	3	^	G	C++	10.34%	-0.46%
3	2	•	9	С	9.48%	-2.08%
4	4		<u>«</u> ,	Java	8.59%	-1.91%
5	5		<u>@</u>	C#	6.72%	-0.15%
6	6		JS	JavaScript	3.79%	+0.68%
7	13	*	-GC	Go	2.19%	+1.12%
8	7	~	VB	Visual Basic	2.08%	-0.82%
9	11	^	B	Fortran	2.05%	+0.80%
10	8	~	SQL	SQL	2.04%	+0.57%
11	15	*	(3)	Delphi/Object Pascal	1.89%	+0.91%
12	10	•		MATLAB	1.34%	+0.08%
13	17	*	®	Rust	1.18%	+0.29%
14	16	^	4	Ruby	1.16%	+0.25%
15	12	•	(23.22)	Scratch	1.15%	+0.08%
16	9	*	php	PHP	1.15%	-0.27%



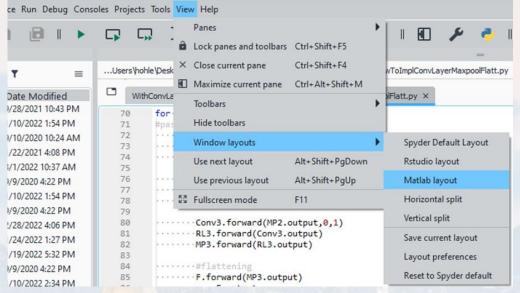








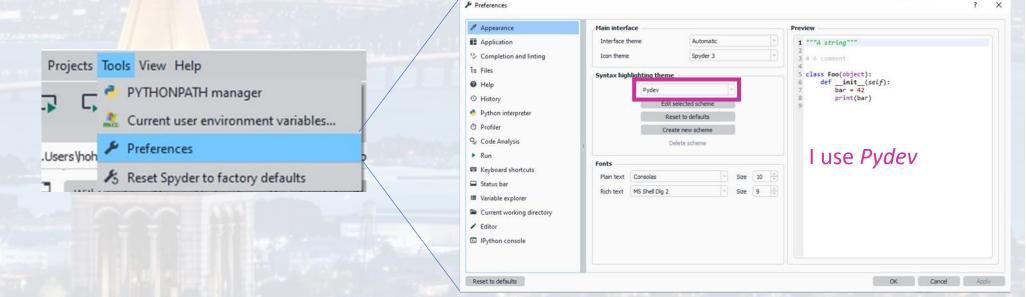




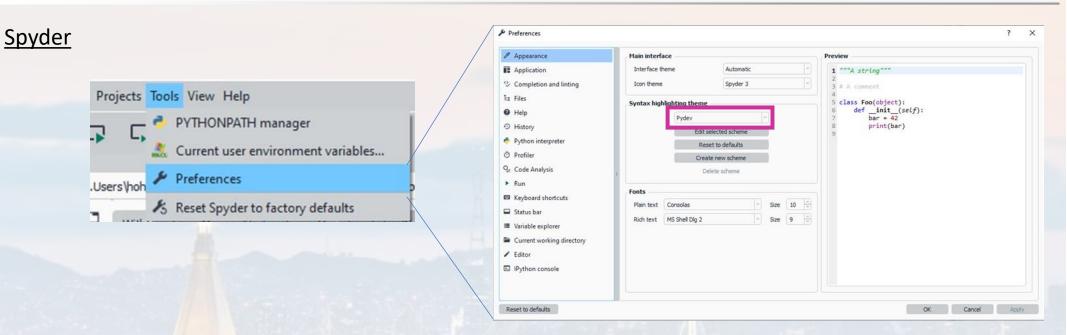
settings:

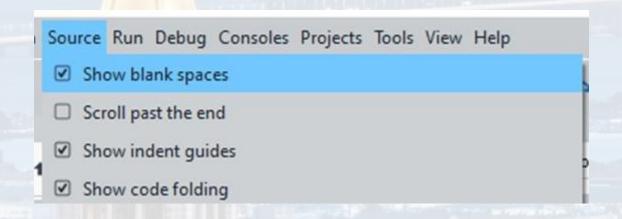
toolbar: *View* → *Window layouts*

e. g. Matlab





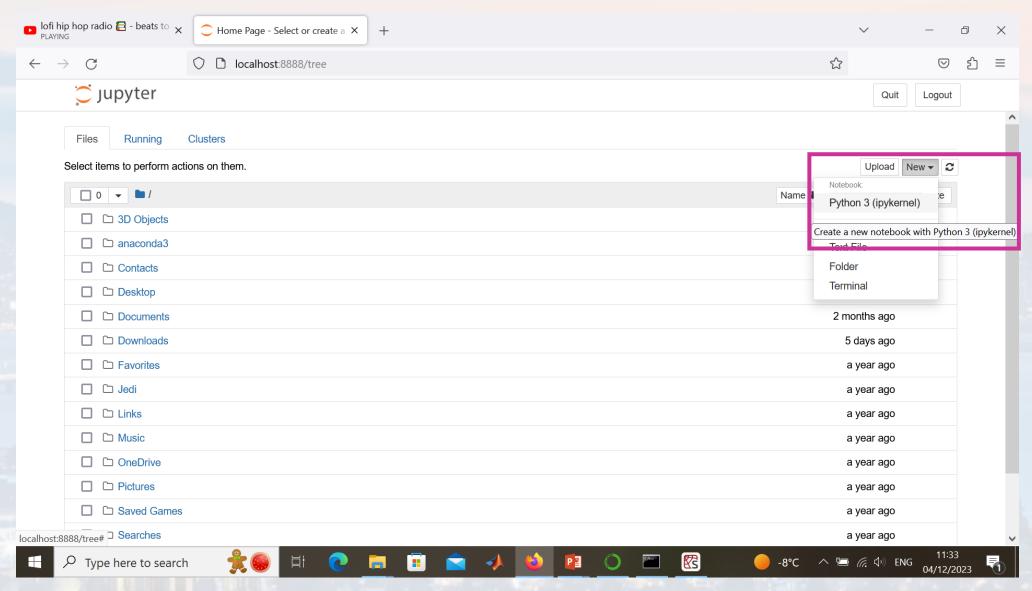




blanks are relevant for synthax!

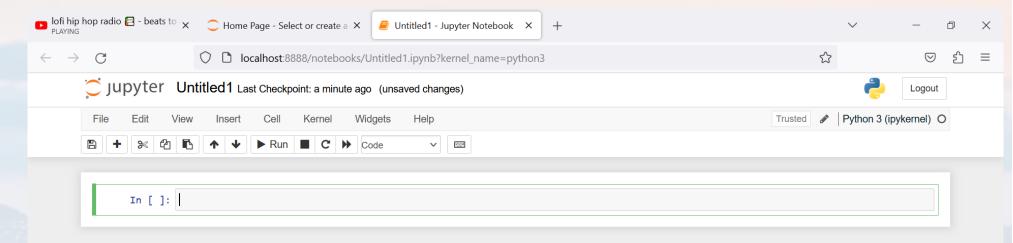


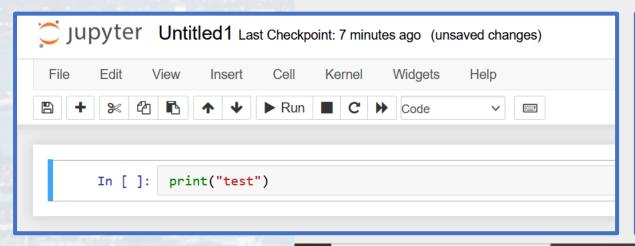
<u>Jupyter</u>

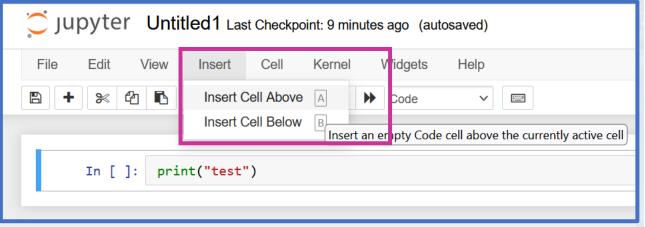




<u>Jupyter</u>

























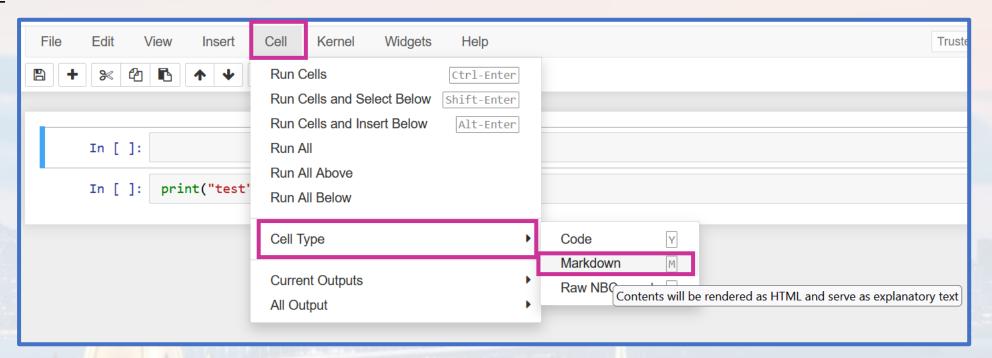




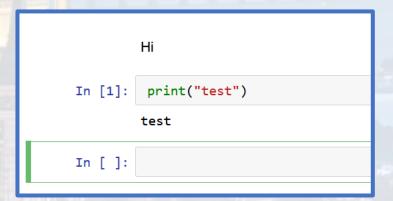




<u>Jupyter</u>



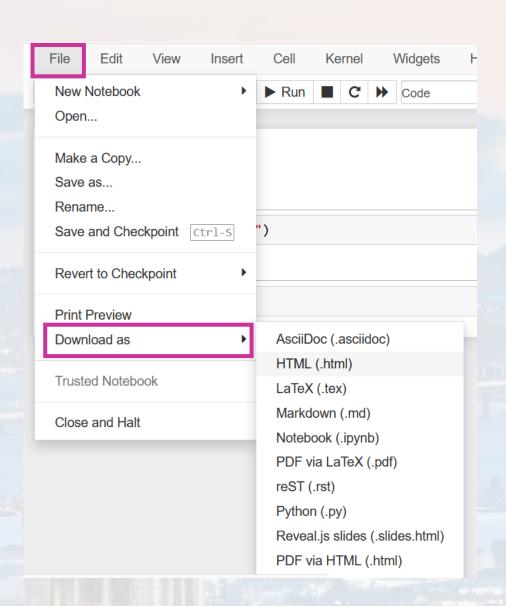
type something → click **run**



web: Jupyter → markdown styles (including LaTeX)



<u>Jupyter</u>



```
basic types: String = 'Hello ' + ''World''

List = [1, 2, 3, 5, ''World''] #default

Tuble = (1, 2)

Dict = {'A': 1, 'B': 2}

Array = np.array([1, 2, 3, 5])

pd.DataFrame
```

other objects:

class

def #function/method



- labels and titles of plots
- paths and file names

slices:

error messages

```
string1 = 'Hello Students'
string2 = ', how are you'
string12 = string1 + string2
Out[1]: 'Hello Students, how are you'
S = 'abc'
3*5
Out[2]: 'abcabcabc'
string12[2:6]
```

[1, 5, 0, -3]

```
String = 'Hello ' + ''World''
List = [1, 2, 3, 5, ''World'']
Tuble = (1, 2)
Dict = {'A': 1, 'B': 2}
Array = np.array([1, 2, 3, 5])
pd.DataFrame
```

concatenating is incredibly easy!

slicing



- labels and titles of plots
- paths and file names
- error messages

string12[2:6]

index: -4 -3 -2 -1

string12[-1]

string12[1:]

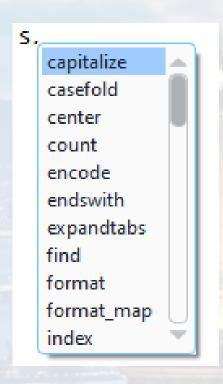
string12[:-1]

```
String = 'Hello ' + ''World''
List = [1, 2, 3, 5, ''World'']
Tuble = (1, 2)
Dict = {'A': 1, 'B': 2}
Array = np.array([1, 2, 3, 5])
pd.DataFrame
```

indexing

slicing

- labels and titles of plots
- paths and file names
- error messages



```
String = 'Hello ' + ''World''
List = [1, 2, 3, 5, ''World'']
Tuble = (1, 2)
Dict = {'A': 1, 'B': 2}
Array = np.array([1, 2, 3, 5])
pd.DataFrame
```

try some of the functions like

```
S.count()
S.find()
```

```
default type in python
```

$$L = [1, 2, 3, -2]$$

2*L

Out[3]: [1, 2, 3, -2, 1, 2, 3, -2]

type(L)

Out[4]: list

```
String = 'Hello ' + ''World''
List = [1, 2, 3, 5, ''World'']
Tuble = (1, 2)
Dict = {'A': 1, 'B': 2}
Array = np.array([1, 2, 3, 5])
pd.DataFrame
```

default type in python

be careful:

L1[0] = 5 print(L2[0])

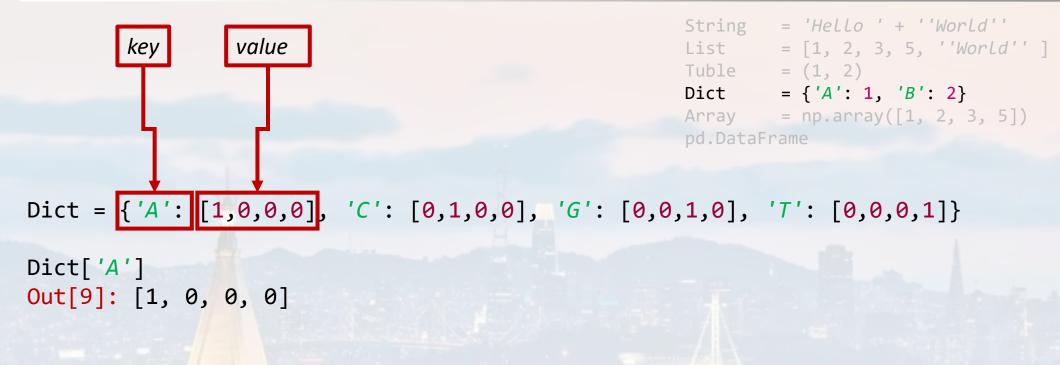
```
String = 'Hello ' + ''World''
List = [1, 2, 3, 5, ''World'']
Tuble = (1, 2)
Dict = {'A': 1, 'B': 2}
Array = np.array([1, 2, 3, 5])
pd.DataFrame
```

What is the result? What happens if you do the same with an int?

lists, dictionaries, sets and bytearrays are **mutable**.

```
L1 = [1,2,4]
L2 = ['a', 'b', 'c']
T = (L1, L2)
len(T)
Out[5]: 2
T[1]
Out[6]: ['a', 'b', 'c']
type(T)
Out[7]: tuple
(out1, out2) = T
out1
Out[8]: [1, 2, 4]
```

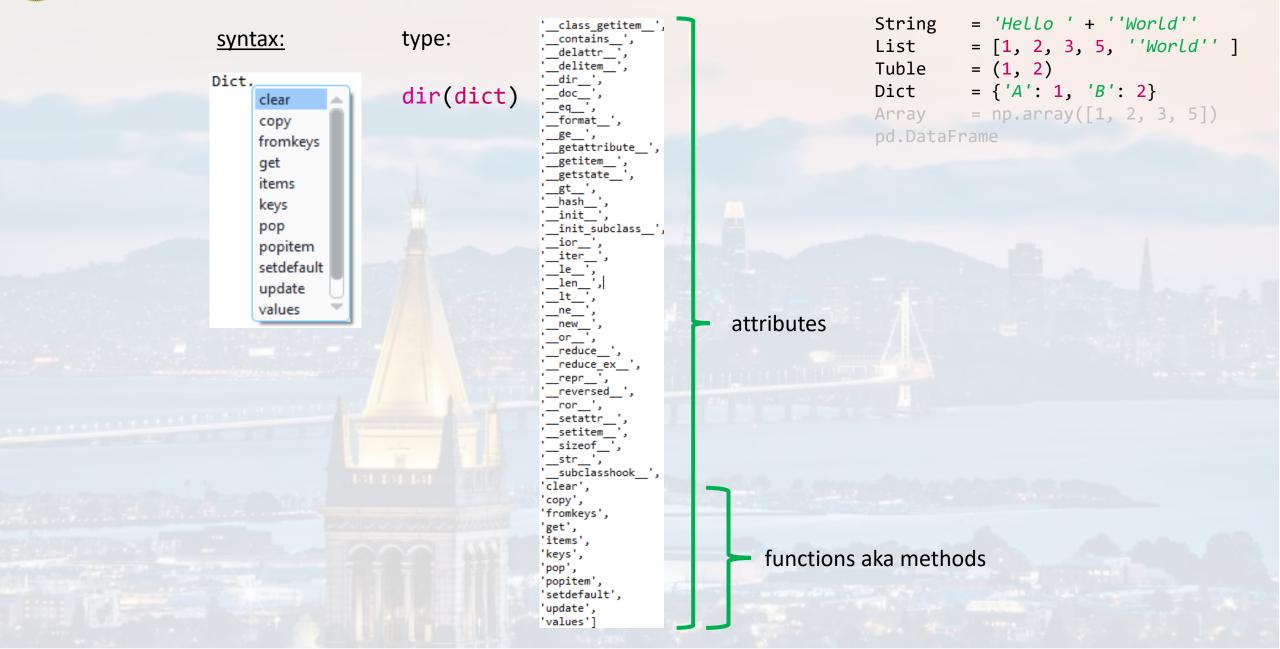
```
String = 'Hello ' + ''World''
List = [1, 2, 3, 5, ''World'']
Tuble = (1, 2)
Dict = {'A': 1, 'B': 2}
Array = np.array([1, 2, 3, 5])
pd.DataFrame
```



type(Dict)
Out[21]: dict

String = 'Hello ' + ''World'' check out List = [1, 2, 3, 5, ''World''] Tuble = (1, 2) $= \{ 'A': 1, 'B': 2 \}$ Dict Array = np.array([1, 2, 3, 5])Dict. clear pd.DataFrame copy fromkeys get items keys pop popitem setdefault try some of the functions like update values Dict.values() Dict.pop('A') Dict.update({'U': [2, 0, 0, 0]})

```
= 'Hello ' + ''World''
                                                           String
syntax:
                                                           List
                                                                   = [1, 2, 3, 5, ''World'']
                                                           Tuble
                                                                   = (1, 2)
                                                           Dict
                                                                   = \{ 'A': 1, 'B': 2 \}
        → arrays (lists, np.array, data frames → see next week)
                                                                   = np.array([1, 2, 3, 5])
                                                           Array
                                                           pd.DataFrame
()
        → functions or tupel
        T = (a, v)
        (a_new, v_new) = T
{}
        → Dictionaries
        Dict = {'A': [1,0,0,0], 'C': [0,1,0,0], 'G': [0,0,1,0], 'T': [0,0,0,1]}
```



Introduction to Unix & Python



Thank you for your attention!