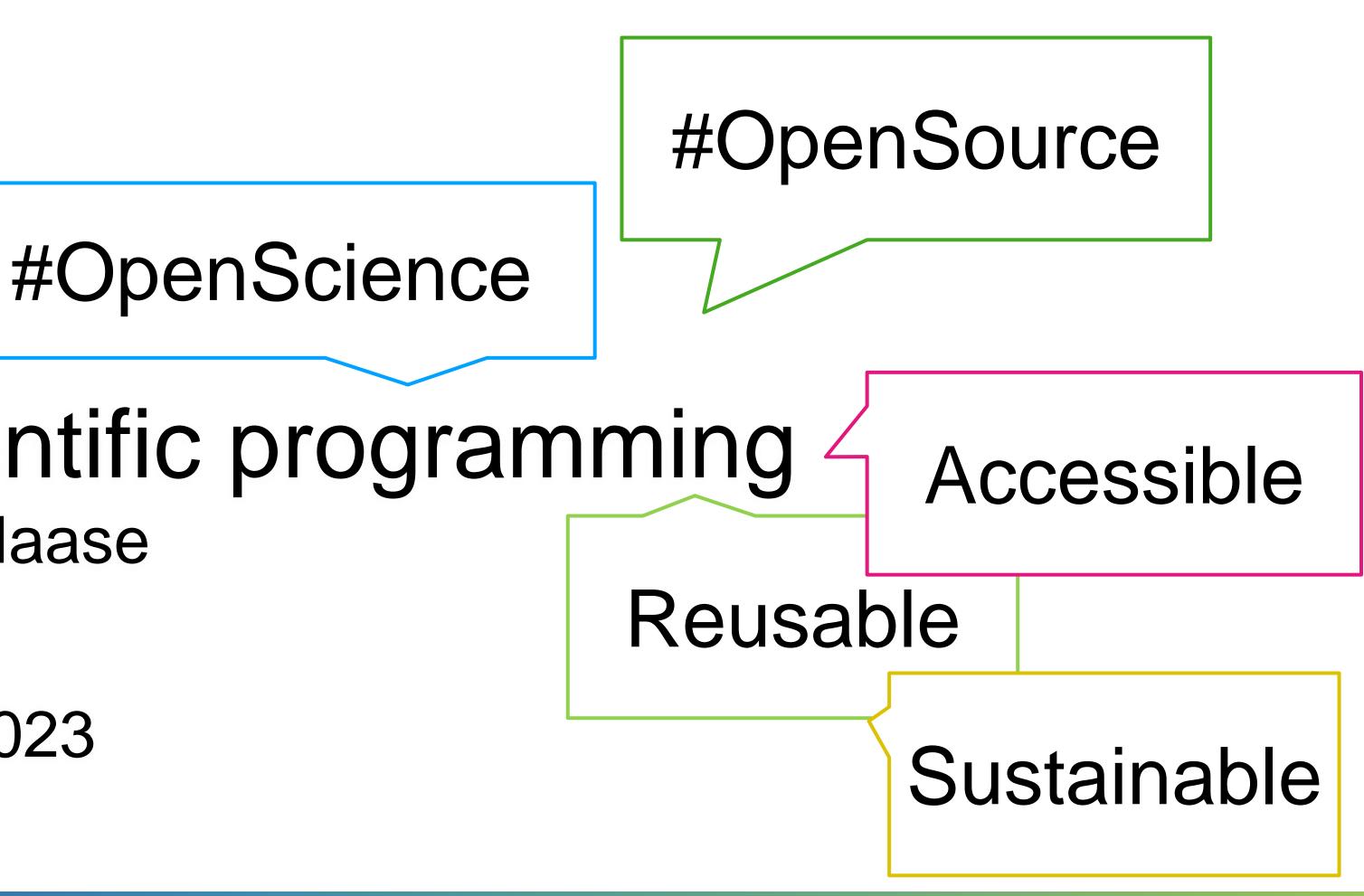
Good practice in scientific programming **Robert Haase**

April 2023



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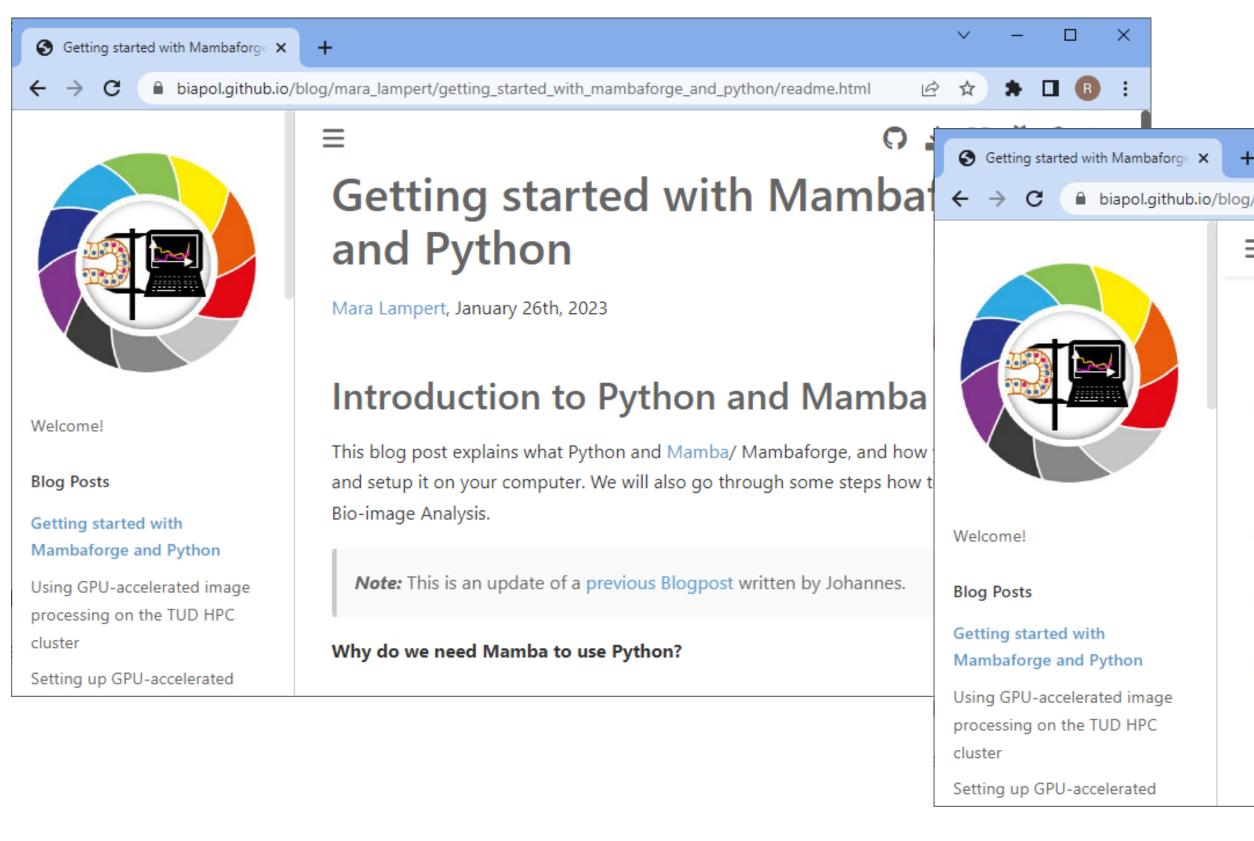






Document what you use

- Installation instructions enable reproducible science
- Not necessary as detailed as a blog-post





https://biapol.github.io/blog/mara_lampert/getting_started_with_ma mbaforge_and_python/readme.html



 \sim _ C biapol.github.io/blog/mara_lampert/getting_started_with_mambaforge_and_python/readme.html 6 \$ 0 🛣 🖸 \equiv You should at any time be able to Creating a new environment You can create a new environment typing the following command into the Comman rebuild the mamba create -n my_first_env devbio-napari python=3.9 -c conda-forge environment you're This will create a new environment with the name my first env and with Python working with. installed. Furthermore, the latest version of devbio-napari will be installed in this er too. Devbio-napari is a collection of Python libraries and Napari plugins maintained BiAPoL team, that are useful for processing fluorescent microscopy image data. Conyou about your permission to download the needed packages with Proceed [y]/n Enter you confirm this and mamba will download and install the necessary packages. Recommendation: Create one conda environment for every project you are working on. This allows you to keep an overview on the needed packages for the project, maintaining

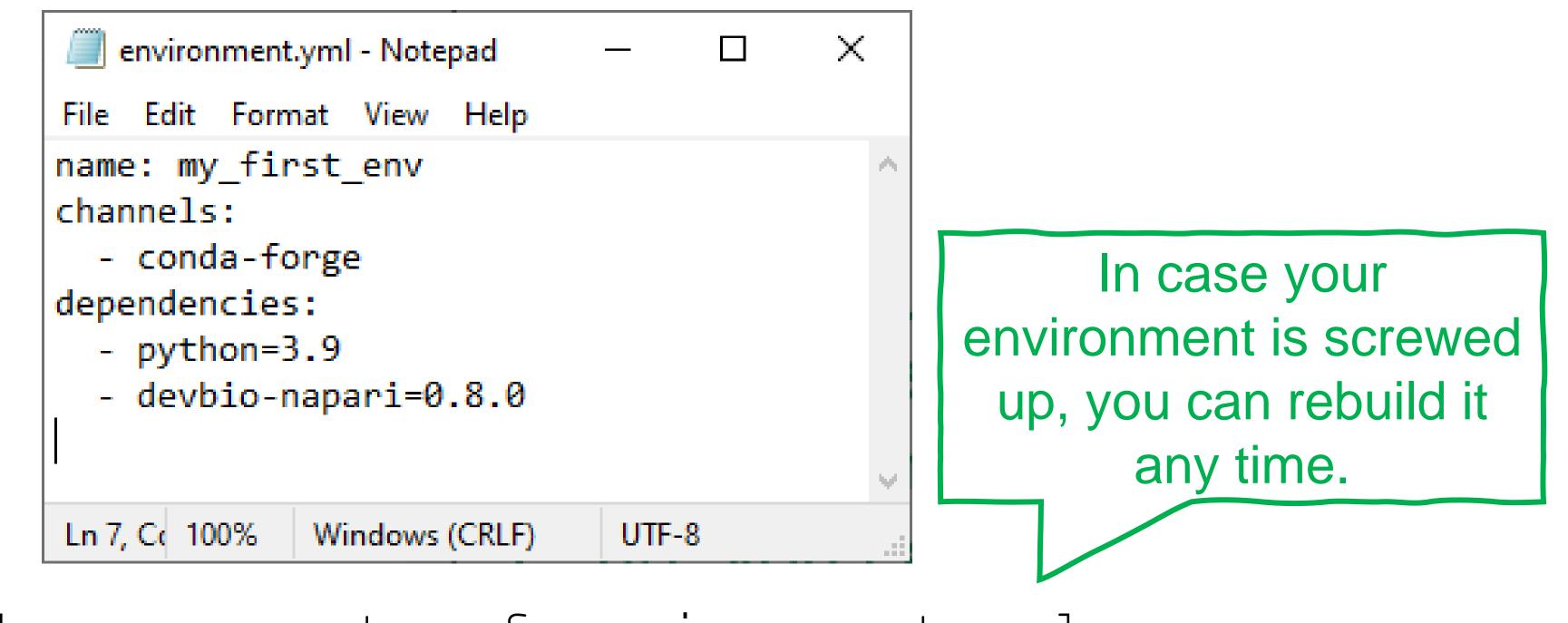


DRESDEN concept





Document what you use



conda env create -f environment.yml

https://conda.io/projects/conda/en/latest/user-guide/tasks/manageenvironments.html#creating-an-environment-from-an-environment-yml-file https://pip.pypa.io/en/stable/cli/pip_install/#examples





Maintain a document with the dependencies (and versions) you need in your project!





Document what you use

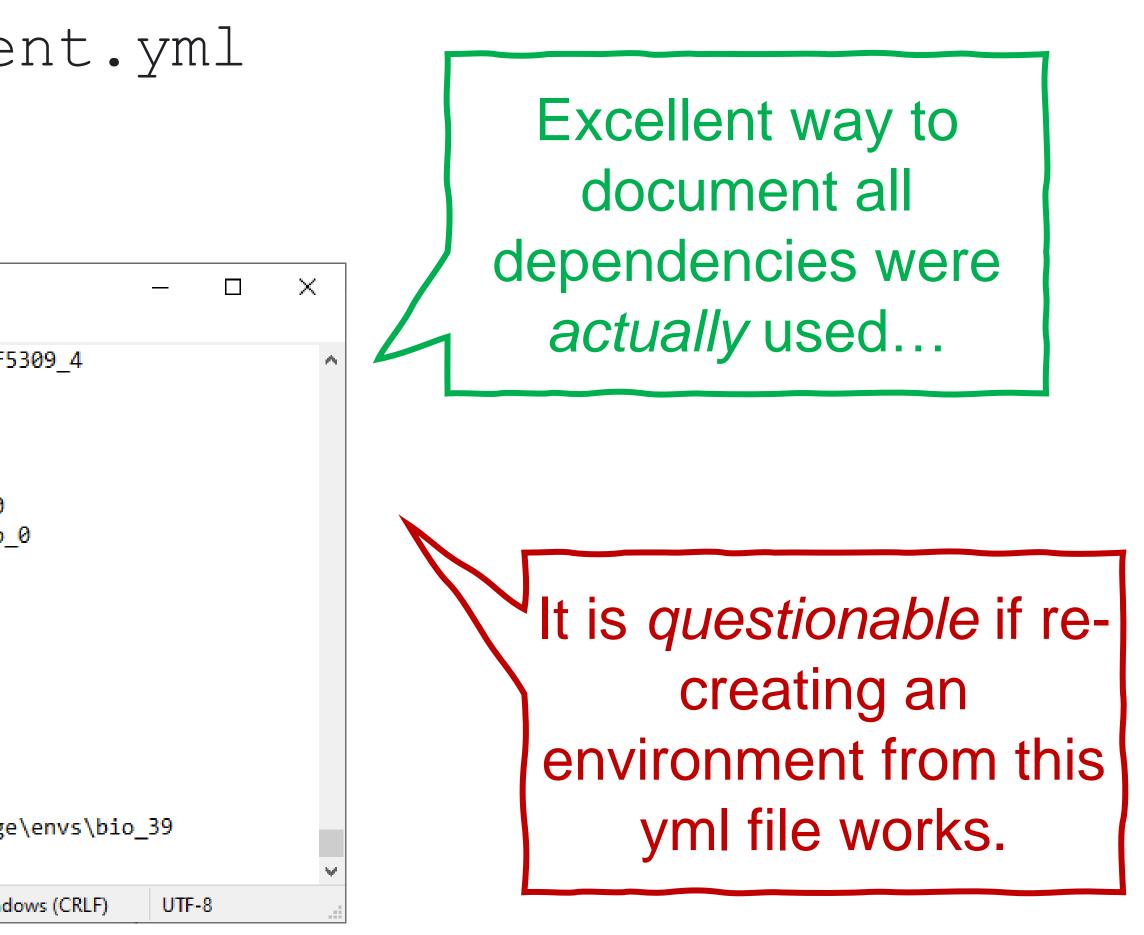
... the complete way.

conda env export > environment.yml

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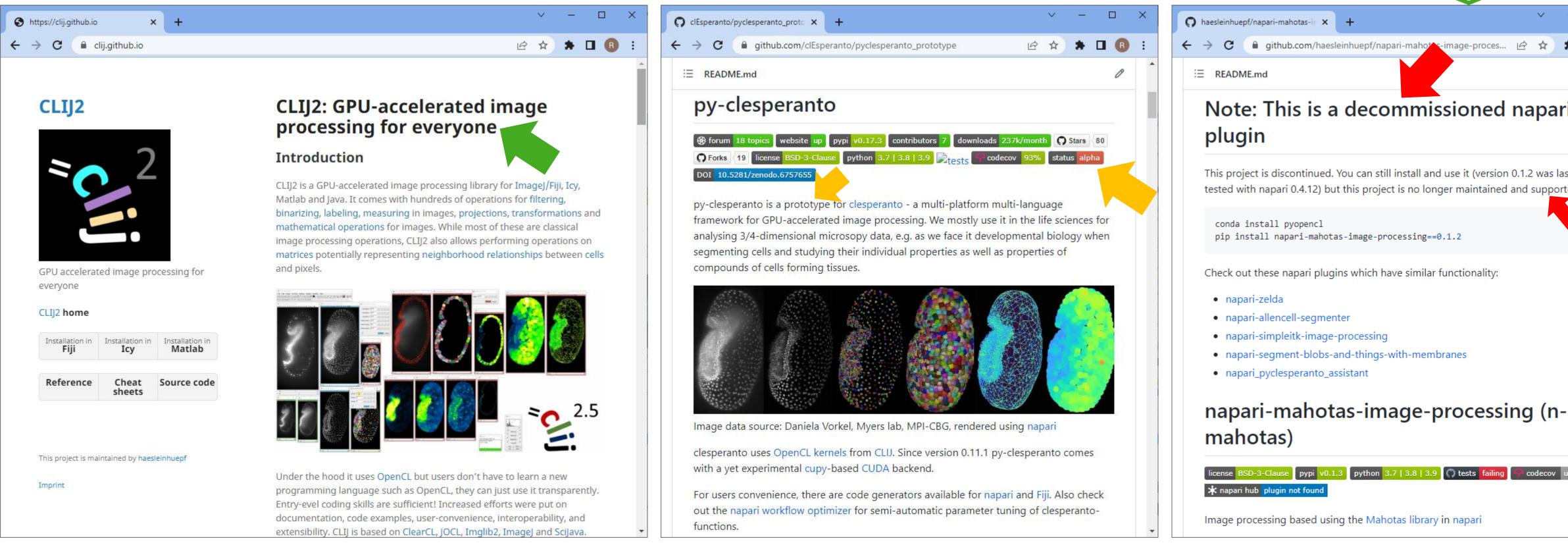
Software quality indicators ... to differentiate the good stuff from the bad.





Target audience

 Documentation should tell who is the target audience and how far it is developed





https://clij.github.io/ https://github.com/clEsperanto/pyclesperanto_prototype https://github.com/haesleinhuepf/napari-mahotas-image-processing









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Visit the project's github or gitlab page and review indicators.

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	binder	Drop python 3.7 (#4063)	5 months ago	napari
	docs	Add NAP-3: Spaces (#4684)	8 days ago	🛄 Readme
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	napari	Allow pandas.Series as propert	16 hours ago	🔀 Cite this repository 🗸
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	tools	More updates to the ignored t	22 days ago	 ⊙ 45 watching ♀ 290 forks
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Ľ	README.md	Add CZI as an Institutional and	2 months ago	🙉 🙉 🗊 🕞 🖓 🚳
Ľ	Singularity	singularity and docker contain	2 months ago	
Ľ	asv.conf.json	add ci for asv benchmark suite	23 days ago	V 🕂 🛨 🖤 🖤

- **Stars**: People like software, similarly to tweets on Twitter
- **Watching**: People receive updates for new releases
- Forks: People made a copy of the code, e.g. to contribute to the project
- **Contributors**: People who contributed to the code
- **Commits**: Changes to the code











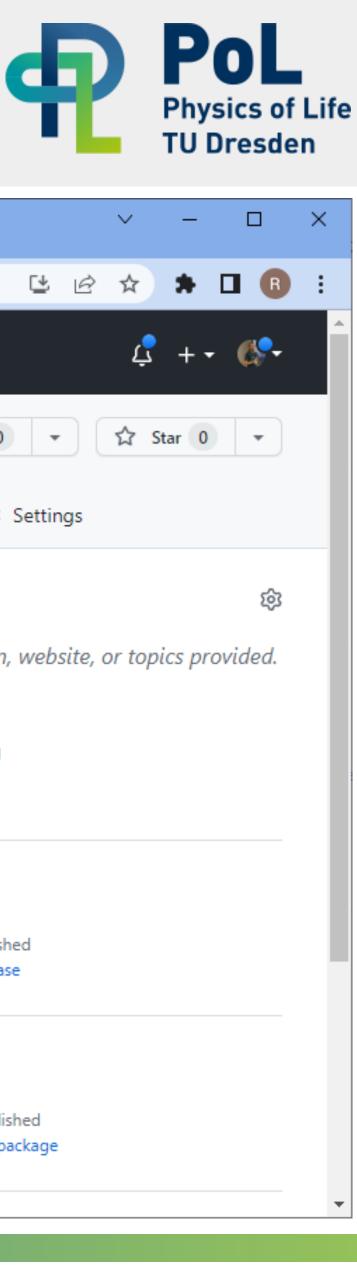
Bad example

- No readme / documentation
- No license / copyright statement
- No stars / users (?)
- Not maintained (last update 4 years ago)
- bus factor = 1

haesleinhuepf/napari_playgroun	< × +		~ -
\leftrightarrow \rightarrow C \cong github.com,	/haesleinhuepf/napari_playground		단 년 ☆ 🛸
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🗋 nap.py	bugfix: create QT Application before viewing	4 years ago	Releases
test_vispy.py	initial version	4 years ago	No releases published Create a new release
Help people interested in t README.	his repository understand your project by adding a	Add a README	Packages No packages published Publish your first package



https://github.com/haesleinhuepf/napari_playground









Visit the project's github or gitlab page and review indicators.

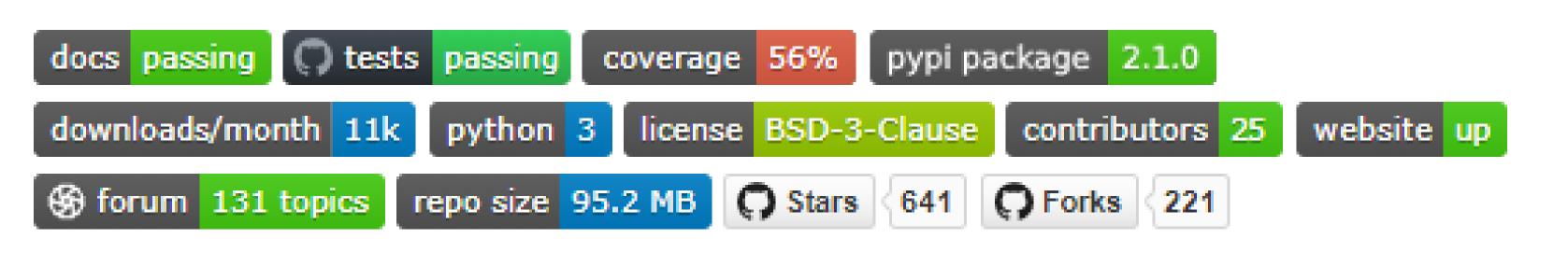




Image source: Adapted from https://www.pexels.com/photo/shallow-focus-photo-of-twopersons-wearing-military-uniform-2859046/



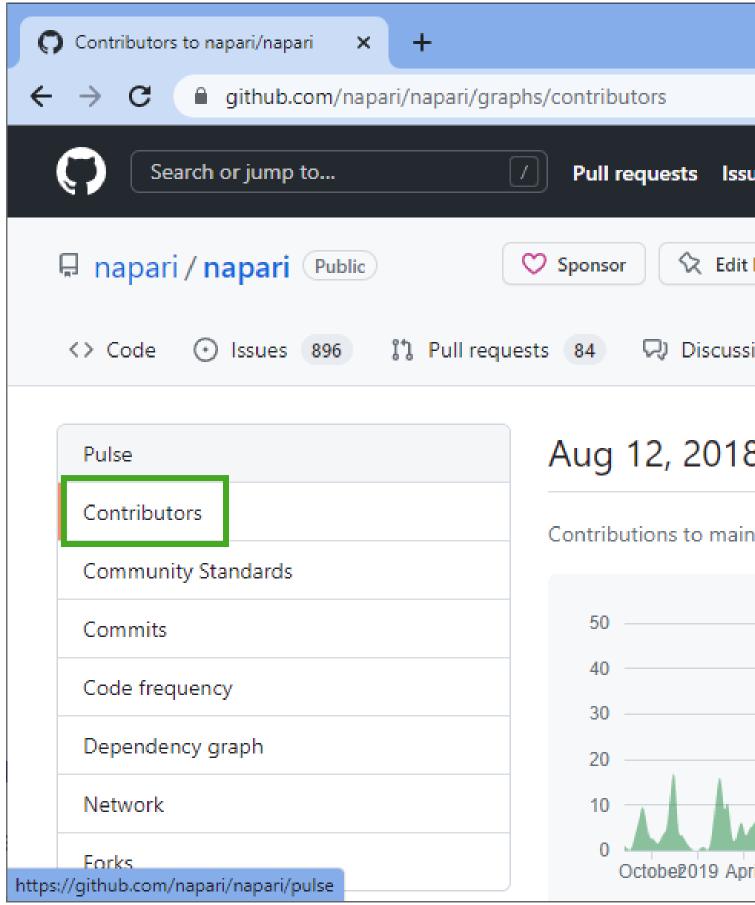
Note, github badges cannot be deserved. Developers put them there







Visit the project's github or gitlab page and review indicators.





https://github.com/napari/napari/graphs/contributors

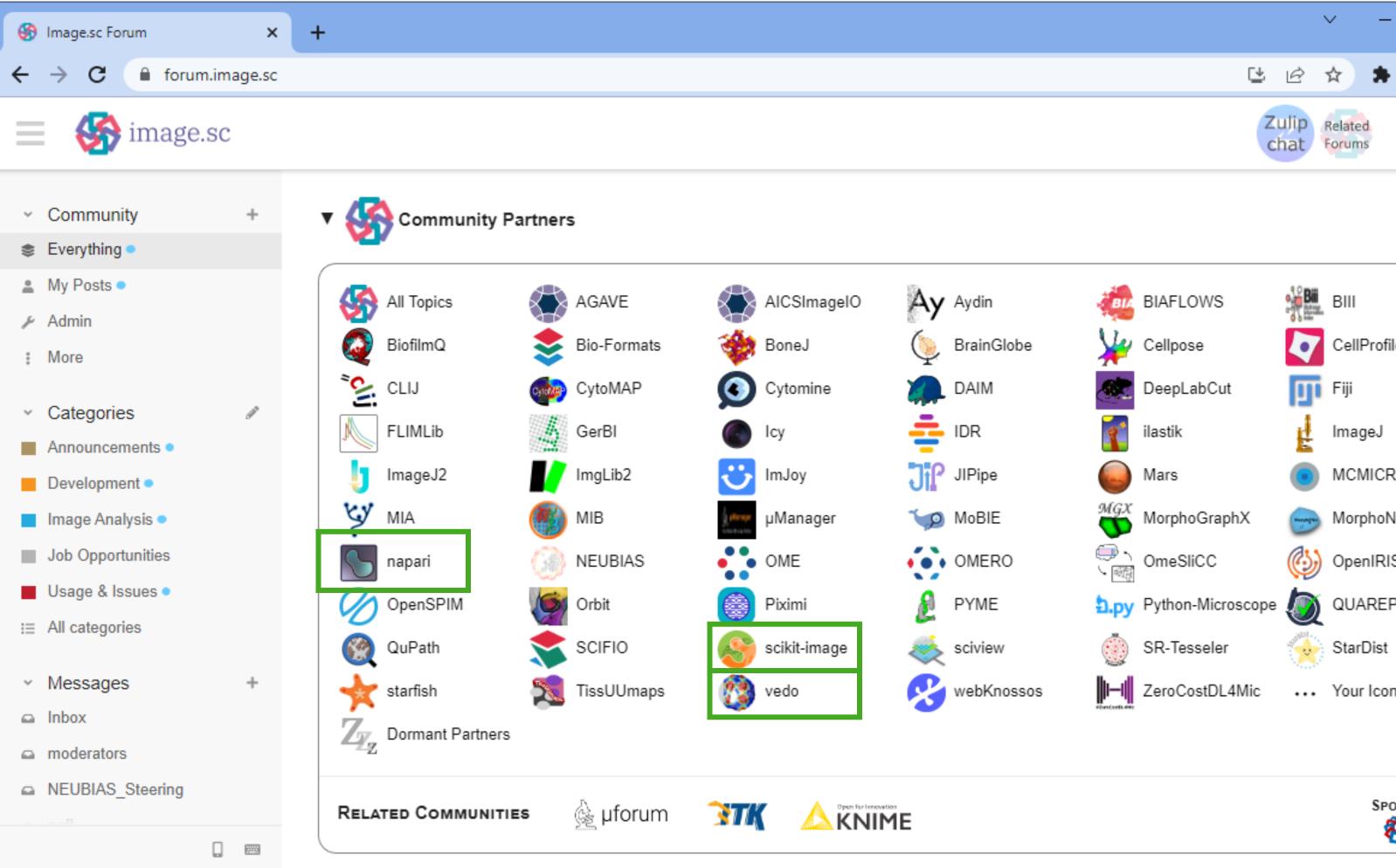


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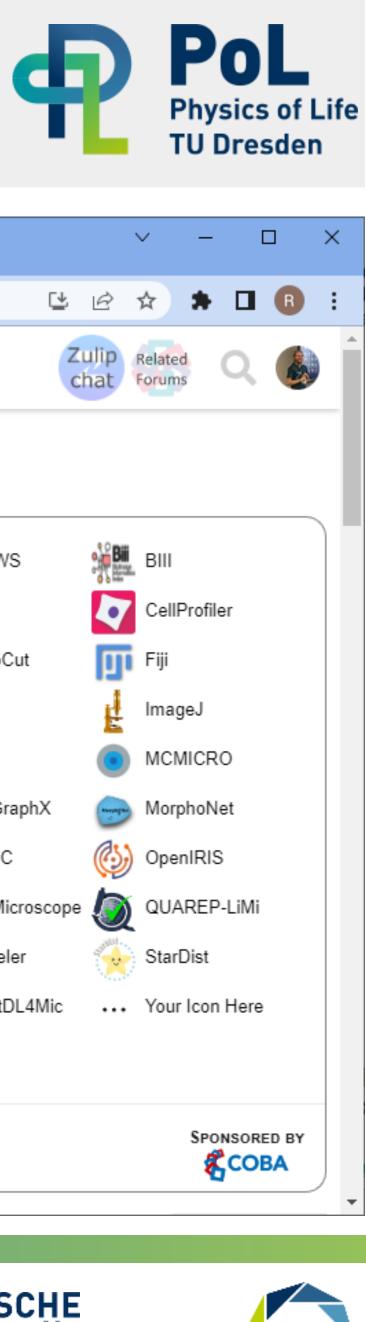


• Community actively involved









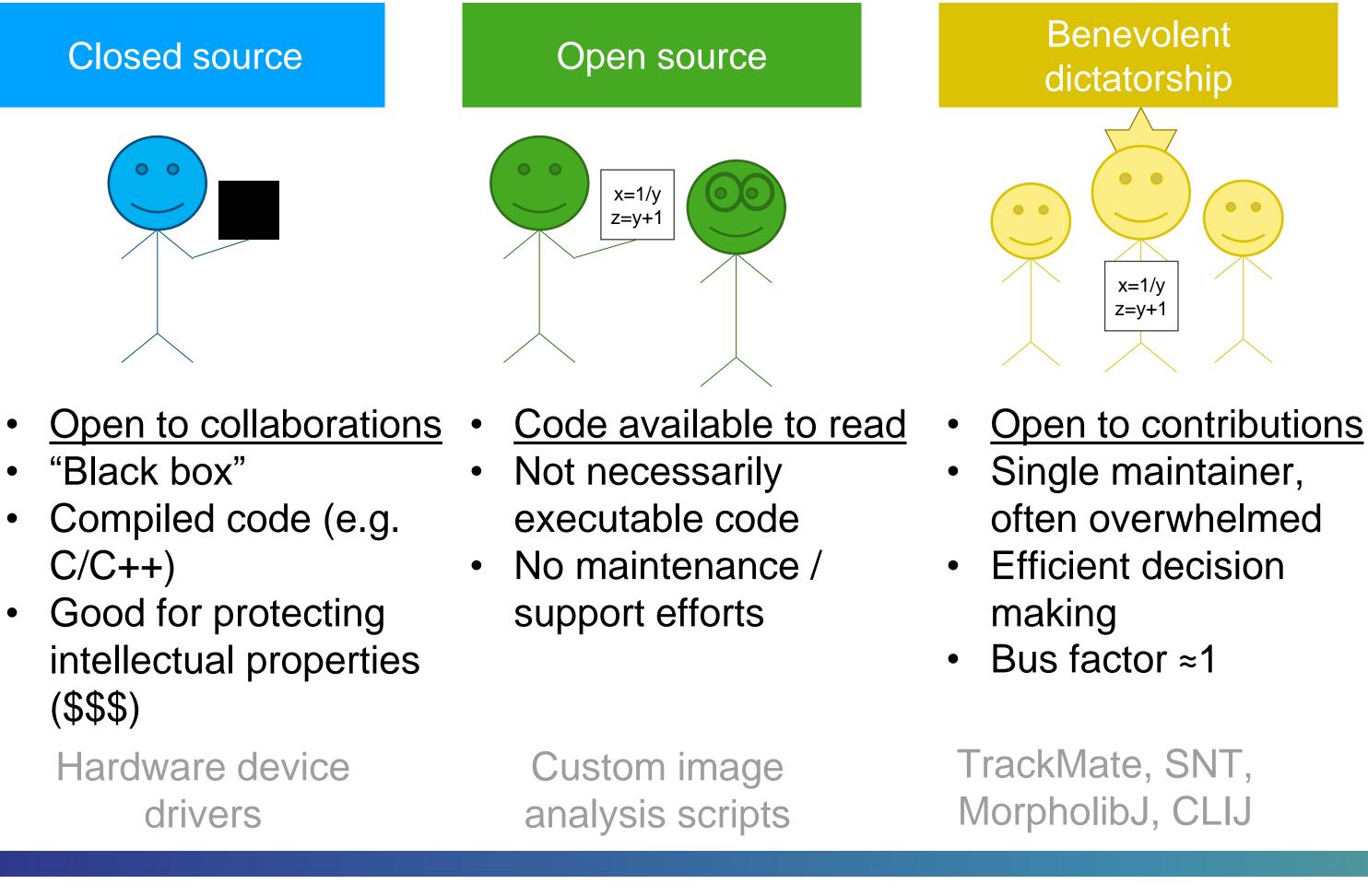
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https://image.sc/



Openness of software / projects

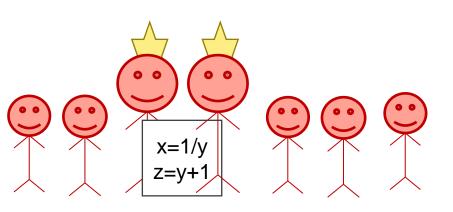
Choose your project's level wisely, and communicate it clearly





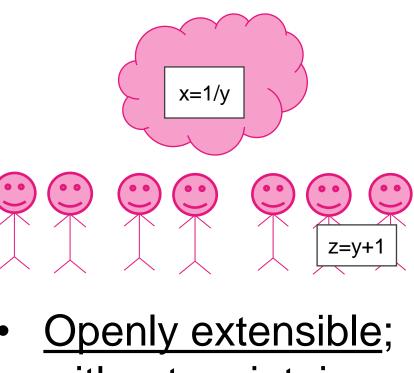


Community driven



- Open to contributions
- Partially democratic
- Board of maintainers (core developers)
- Long-winded decision making

Openly extensible



- without maintainers involved
- Partially community driven

scikit-image, scipy, **OpenCL**

ImageJ, Python, numpy











Take home message

When using [open-source] software, make sure

- it's maintained
- used by others
- supported by an active community
- well-documented



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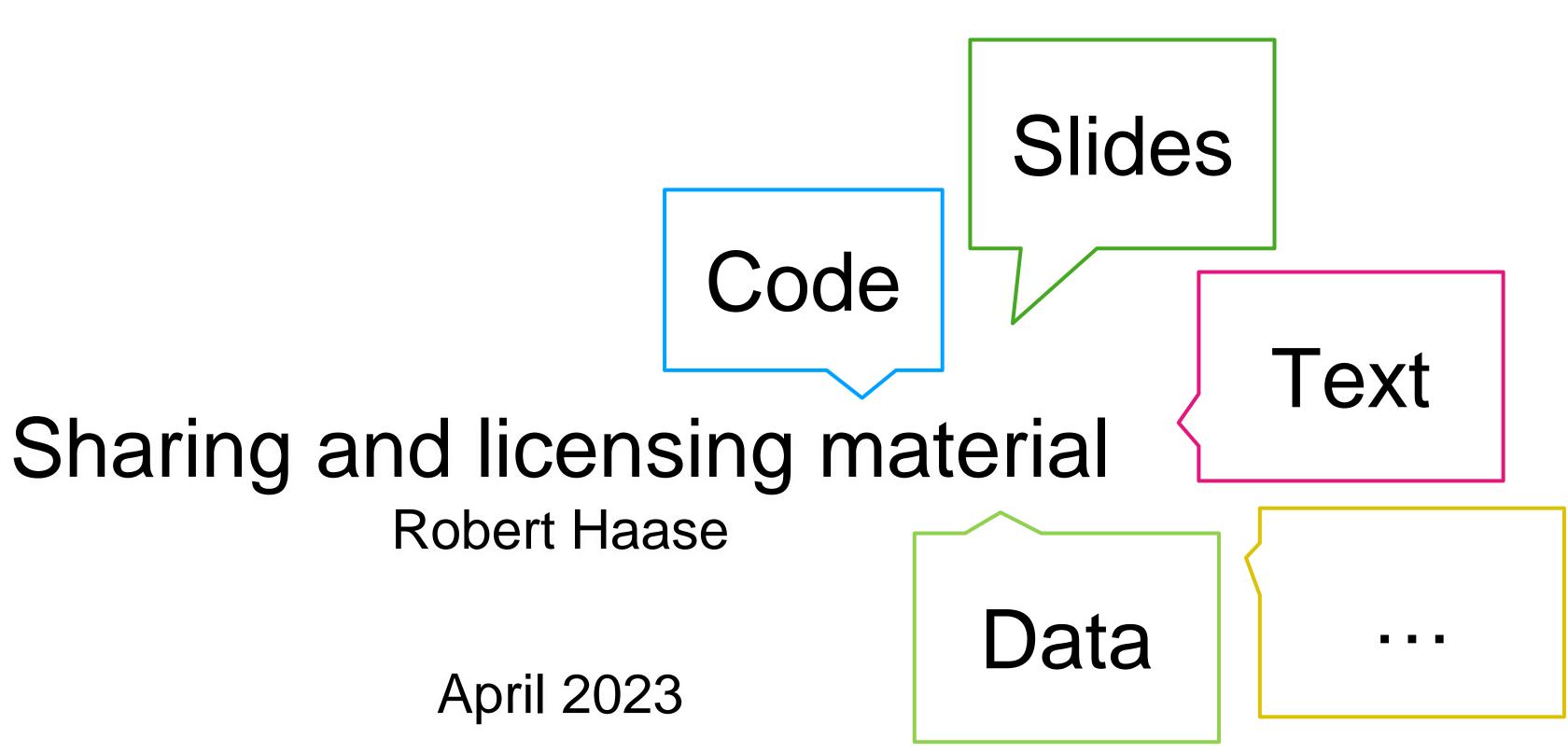






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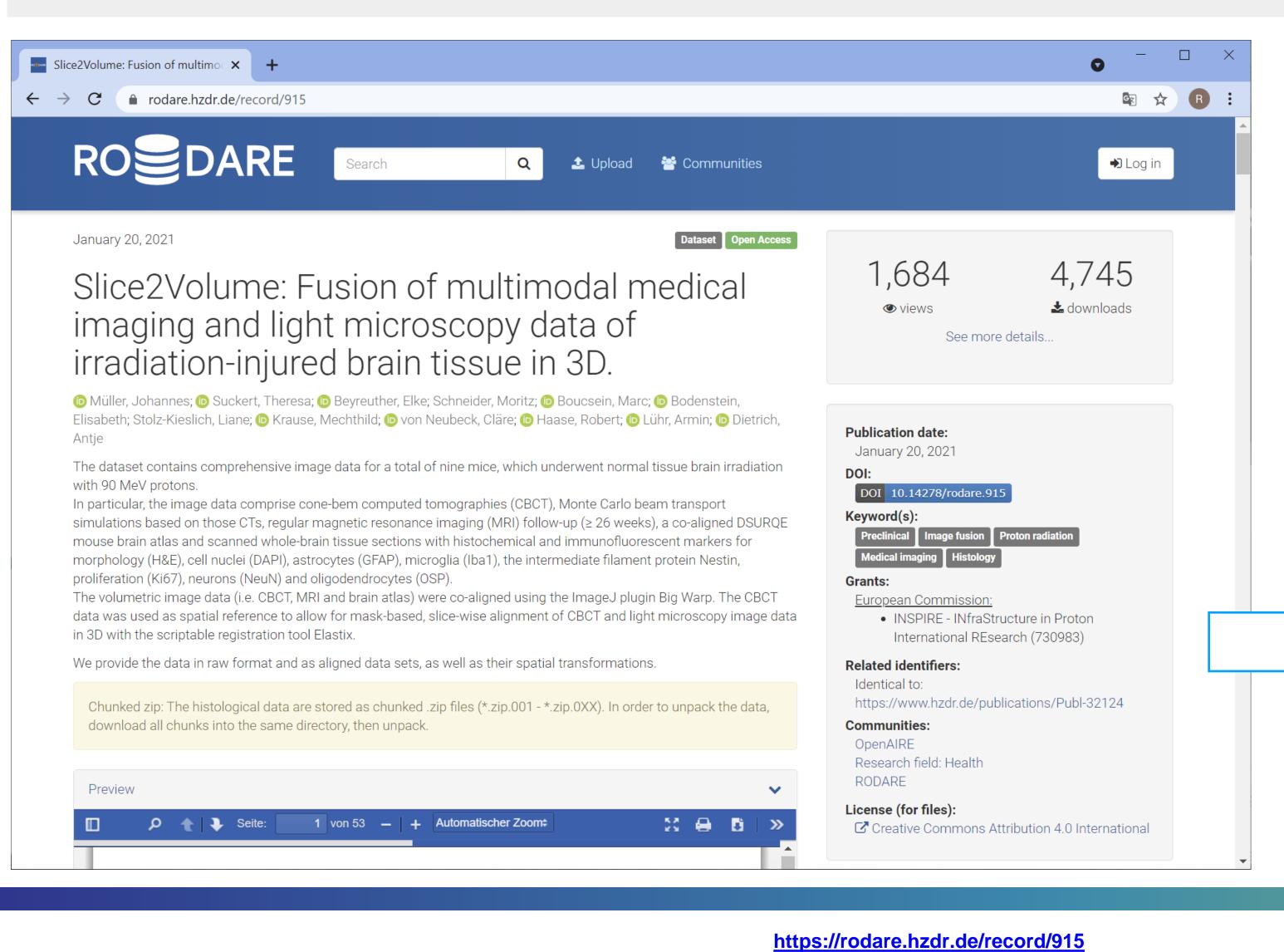








Use cases: Data





https://twitter.com/nKiaru/status/1409194004219142148?s=20



Unique datasets Valuable for biologists Valuable for software developers Institutional servers / services <u>https://idr.openmicroscopy.org/</u> https://zenodo.org



Nicolas Chiaruttini @nKiaru · Jun 27 awesome open access dataset is from @SuckertTheresa and @jm_mightypirate (rodare.hzdr.de/record/915)



TECHNISCHE

UNIVERSITÄT

DRESDEN



Use cases: Manuscripts

Preprints —Accessible / reusable <u>https://arxiv.org/</u> <u>https://biorxiv.org/</u> <u>https://medrxiv.org/</u> Journals

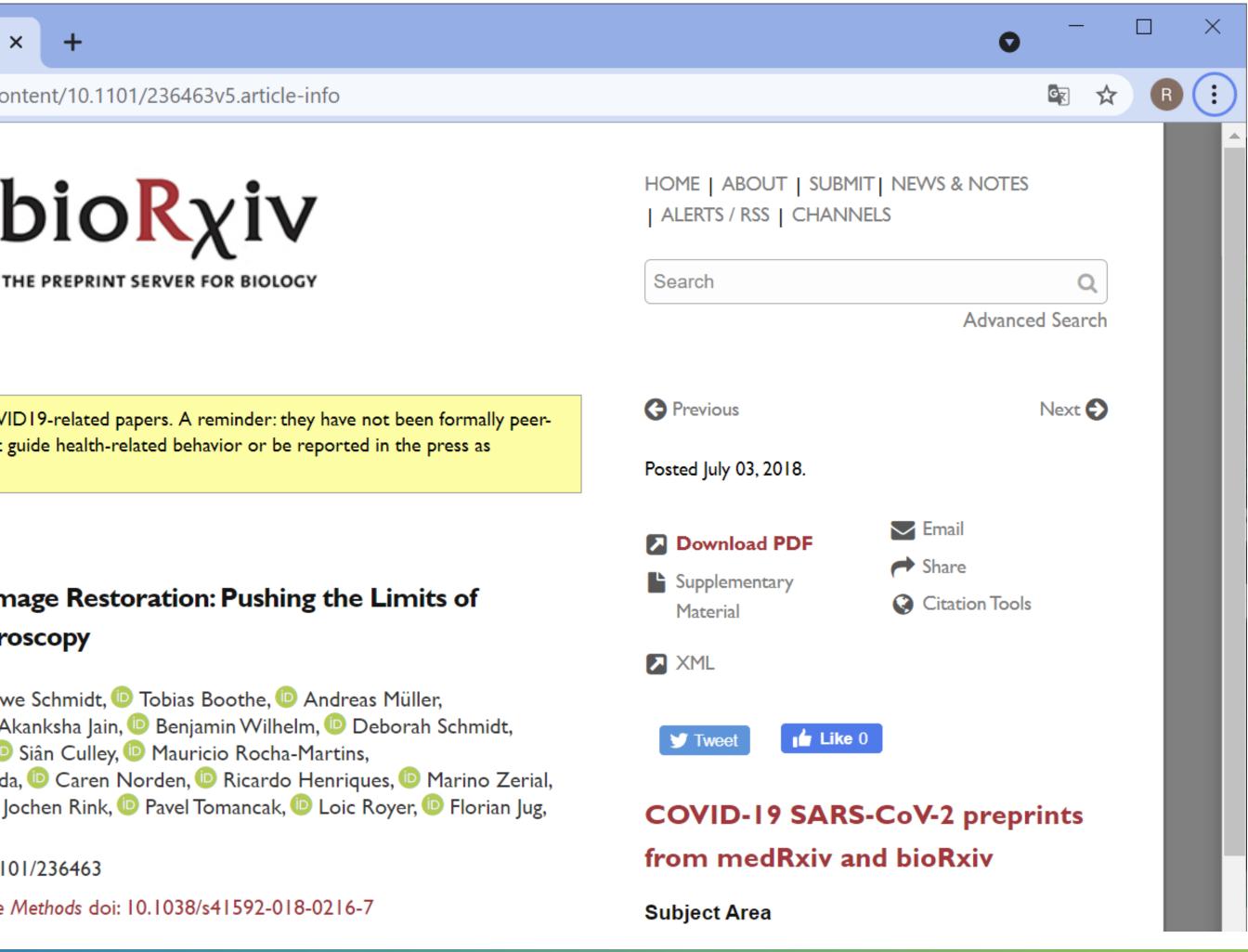
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https://www.biorxiv.org/content/10.1101/236463v5.article-info





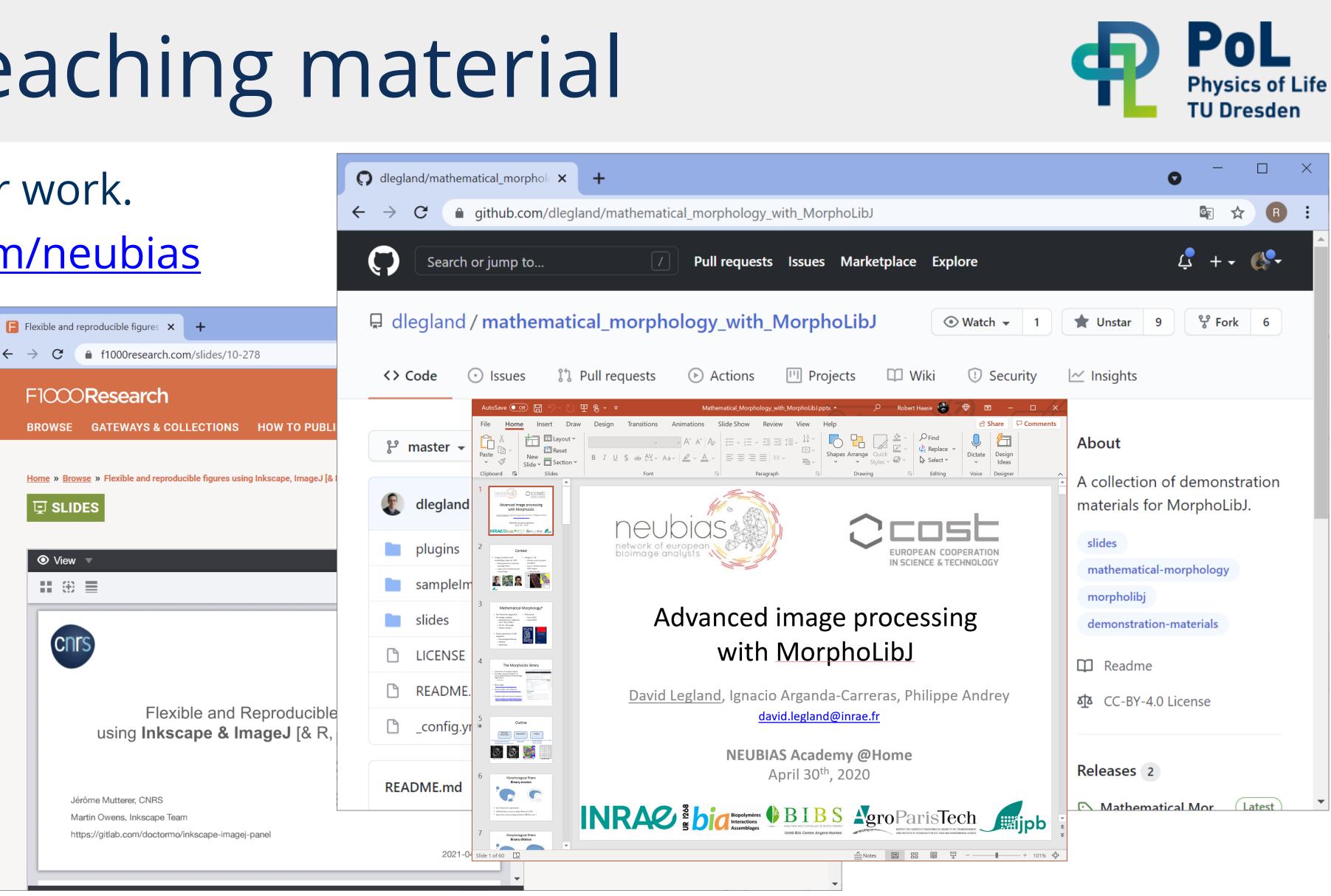






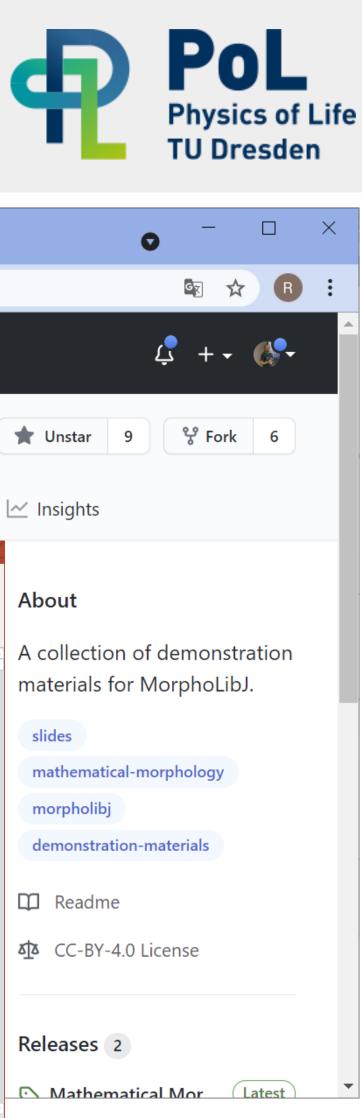
Use cases: Teaching material

Re-using, advertising your work. https://f1000research.com/neubias https://figshare.com https://github.com F1000Research



https://f1000research.com/slides/10-278 https://github.com/dlegland/mathematical_morphology_with_MorphoLibJ









Use cases: Figures

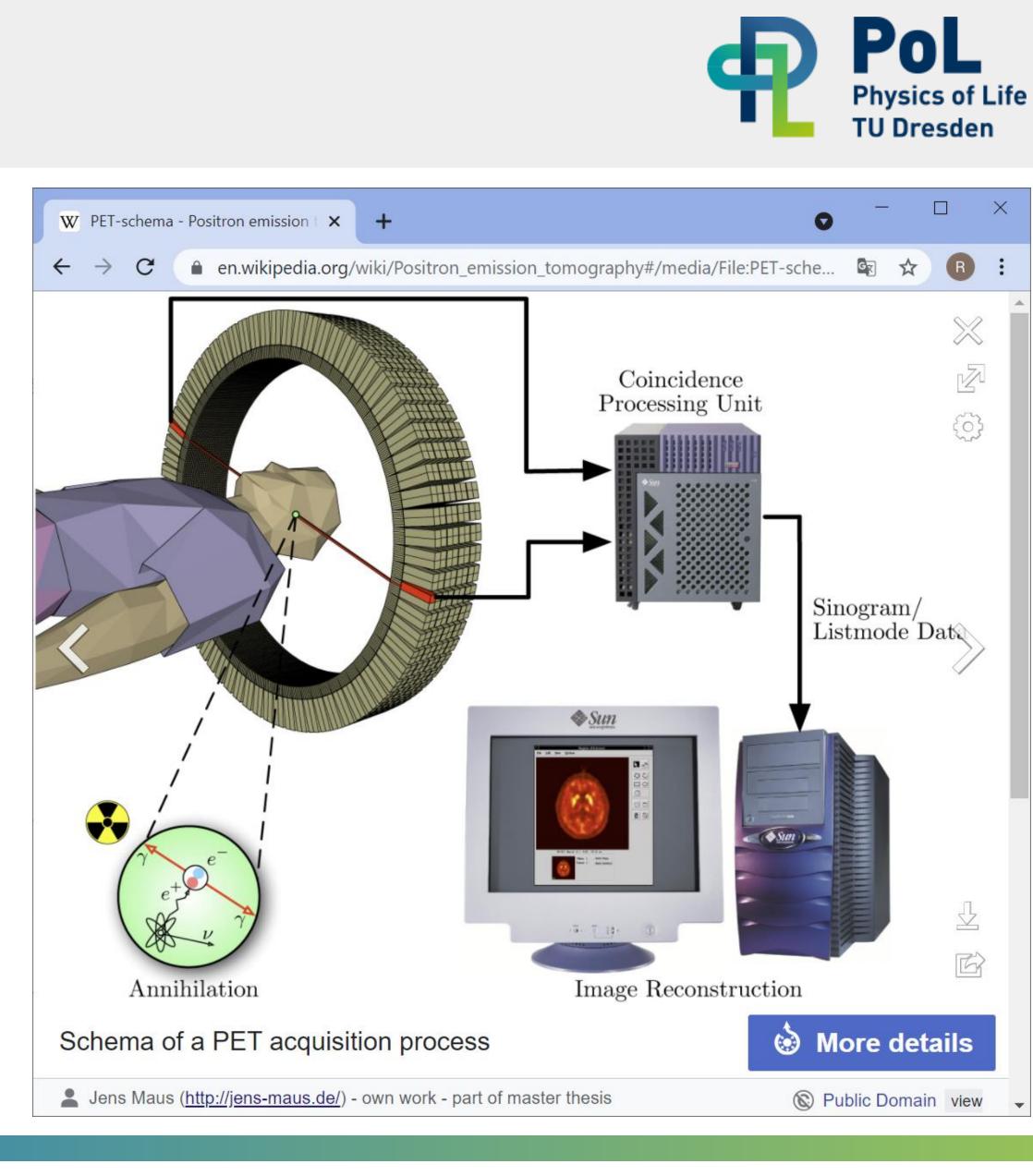
Share efforts

- —Talk about each others' work
- Advertise your work
- ... because our work is often publicly funded

https://commons.wikimedia.org/wiki/Main_Page https://figshare.com





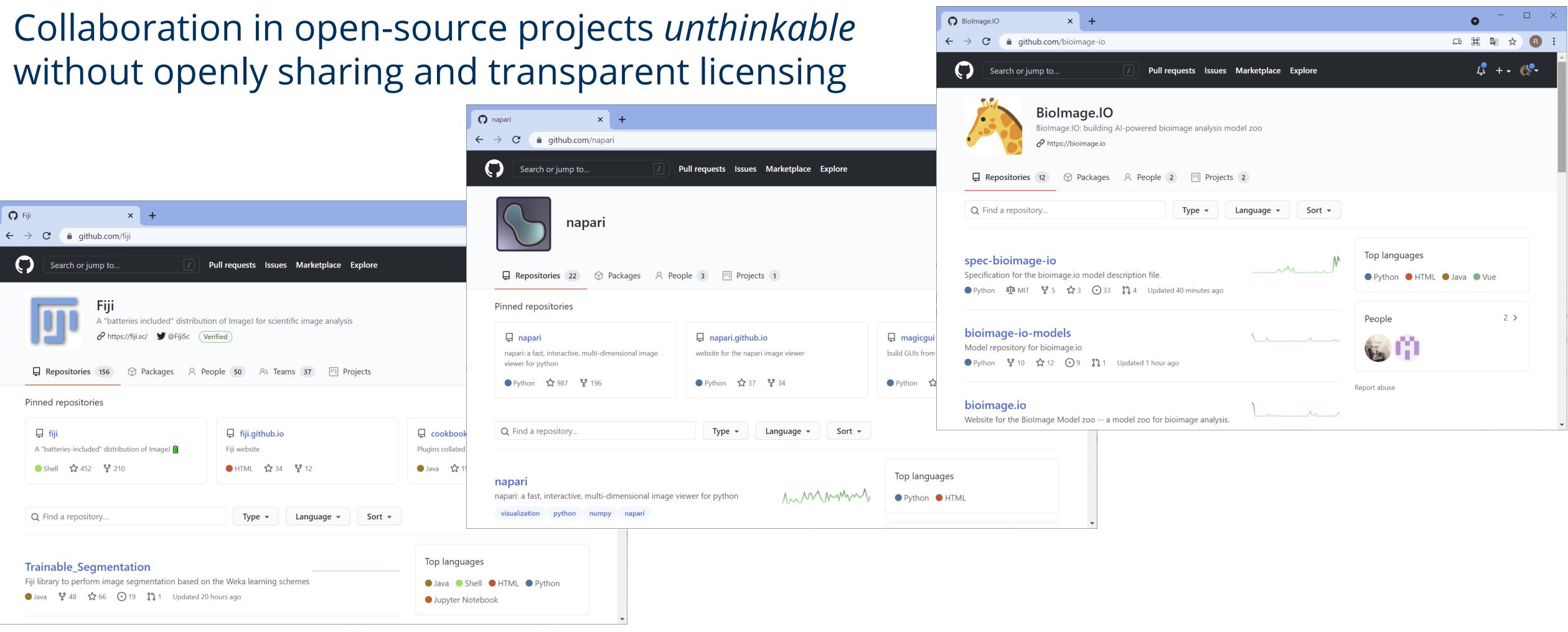




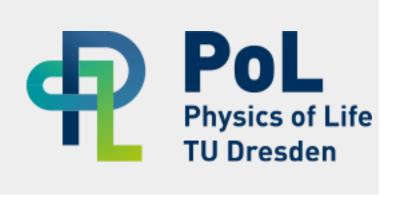




Use cases: Code



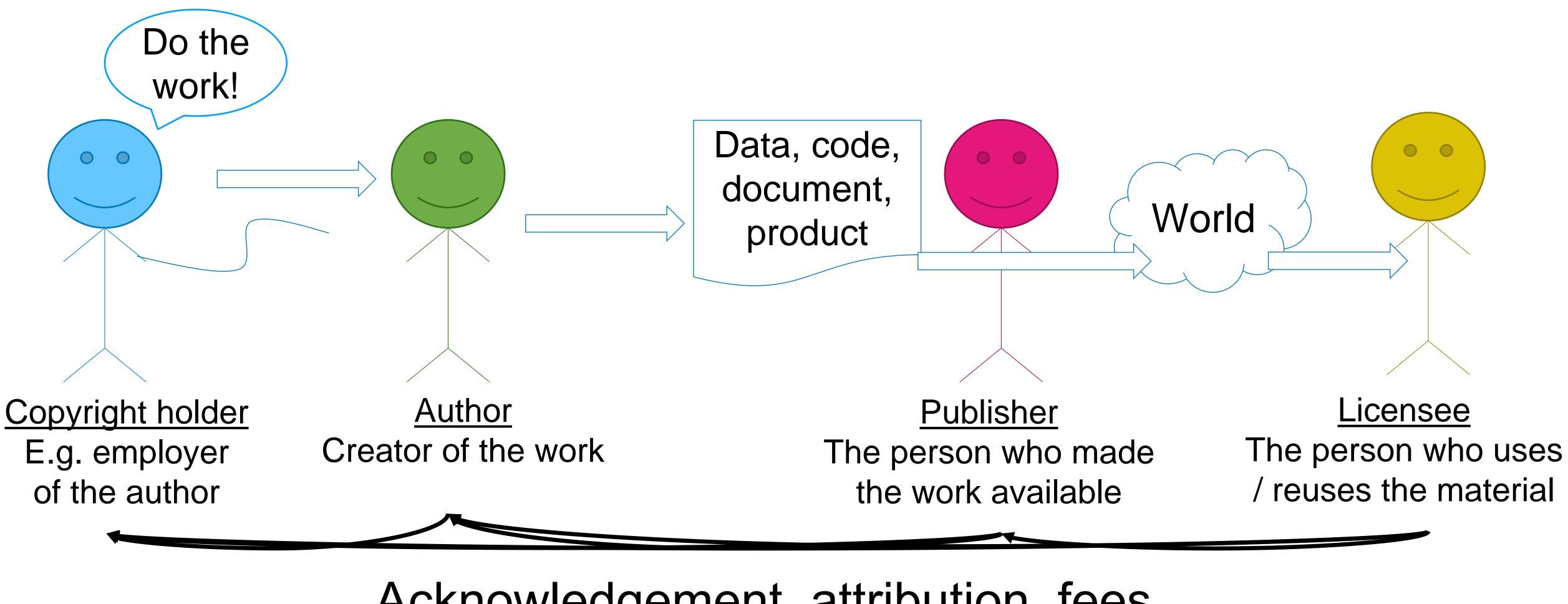








Terminology







Acknowledgement, attribution, fees, ...





FAIR principles

- <u>Findable</u>
- Accessible
- Interoperable
- Reusable





=> State-of-the-art Research Data Management (RDM)

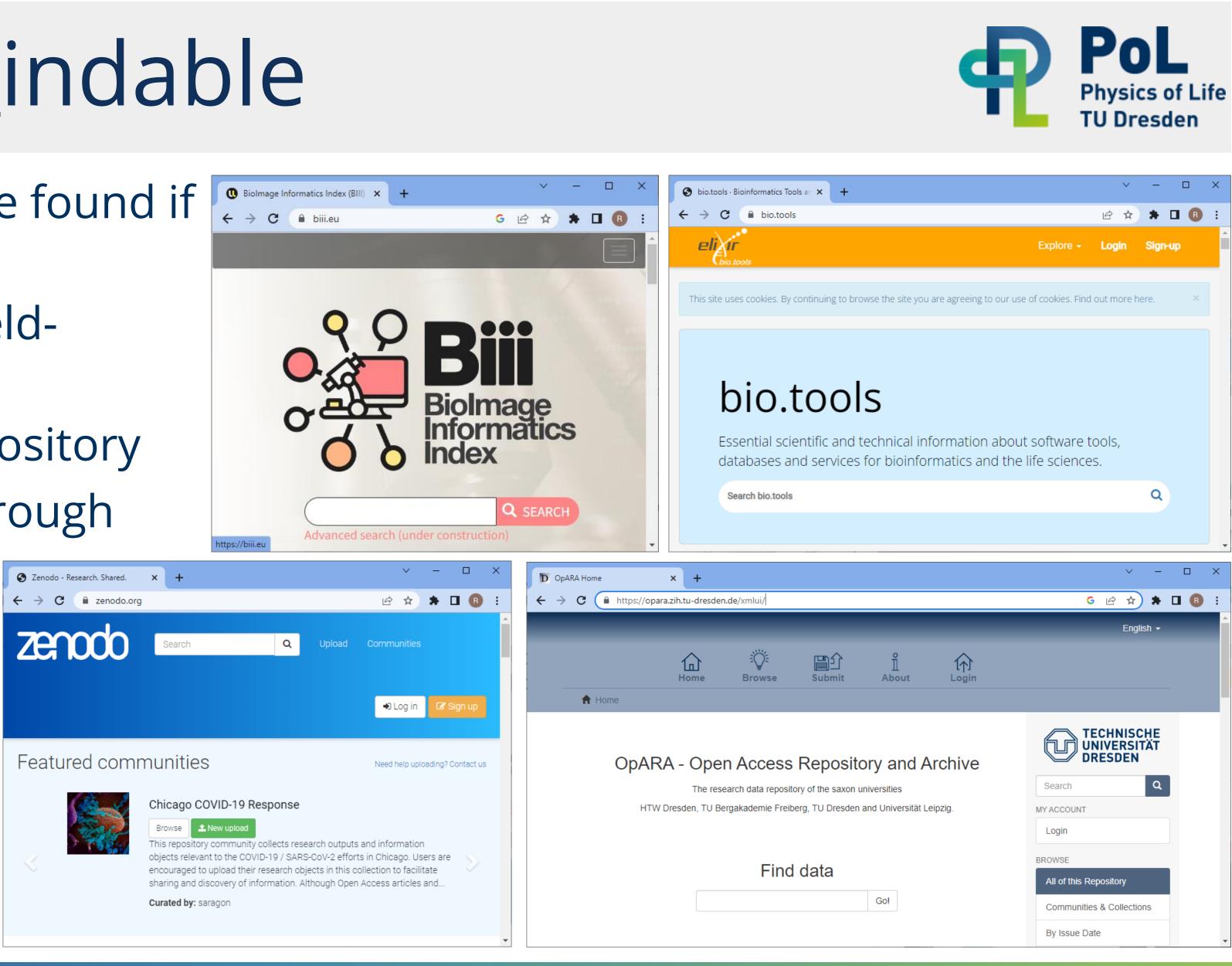


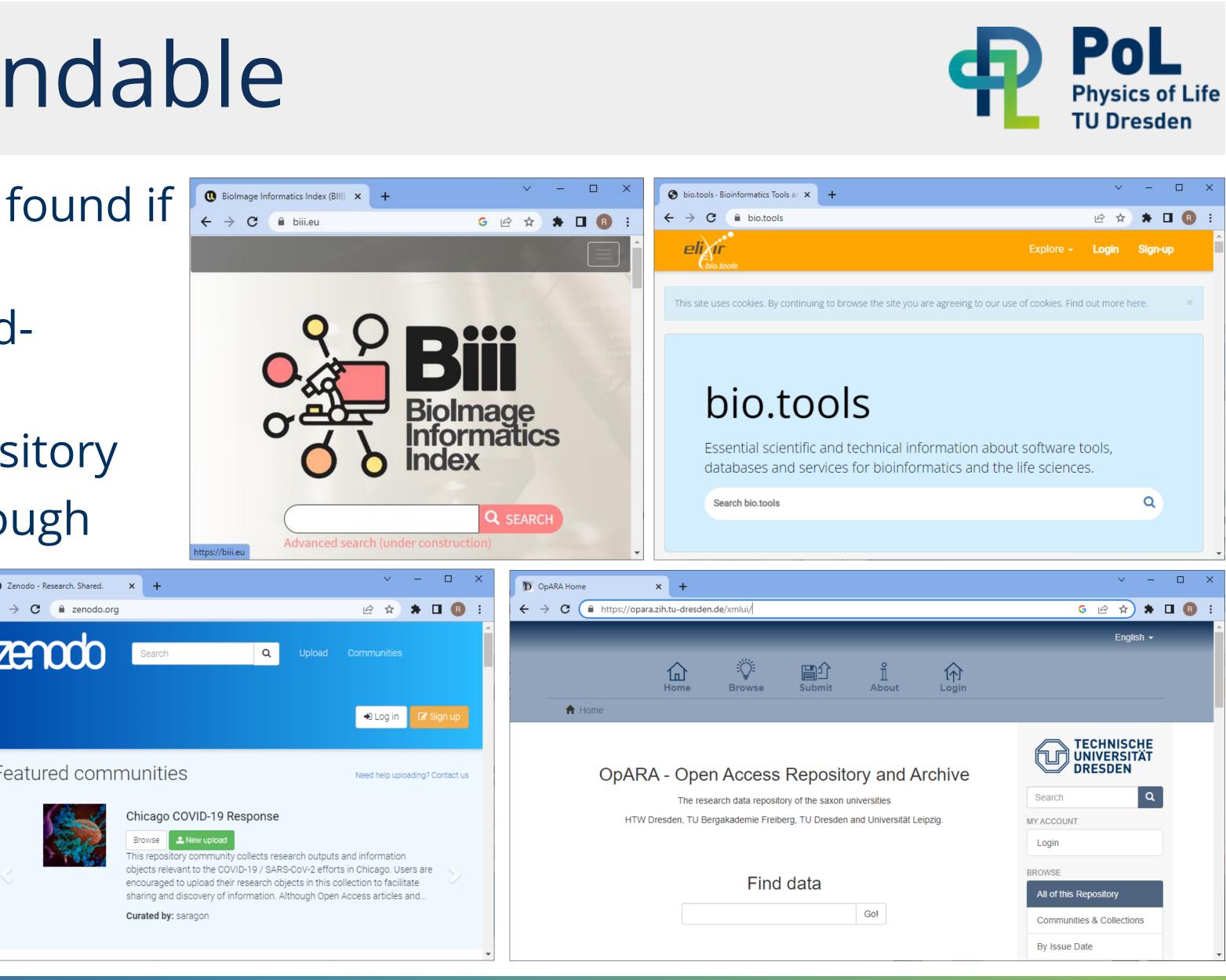




FAIR principles: <u>Findable</u>

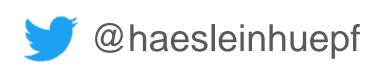
- Research data / code / ... can be found if it's listed in *repositories*
 - Preferably: global, public, fieldspecific repository
 - Alternative: institutional repository
- Findability can be improved through attaching
 - meta data
 - unique digital object *identifiers* (DOI)

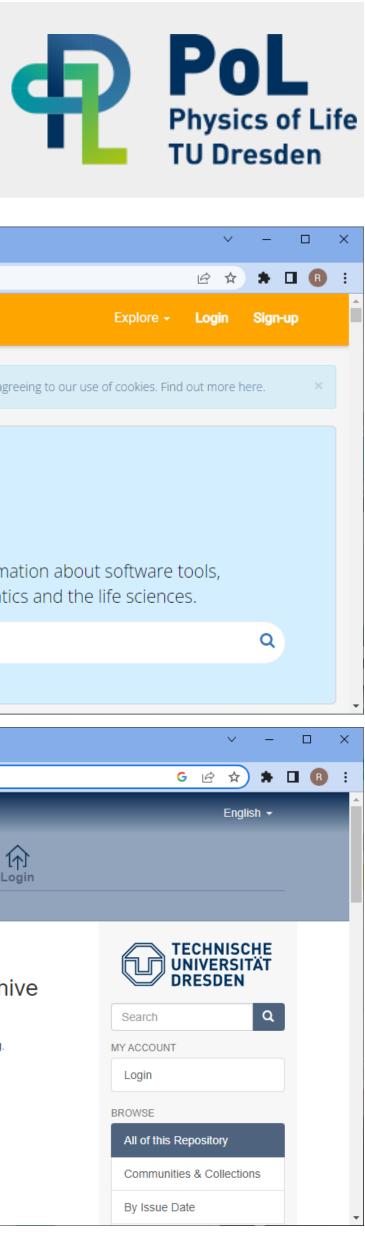
















Quiz: Digital object identifiers

Which of these is a *unique* digital object identifier?

https://twitter.com/haesleinhuepf/status/891596662782779392

https://doi.org/10.5281/zenodo.28325

https://github.com/haesleinhuepf/devbio-napari

https://napari.org/







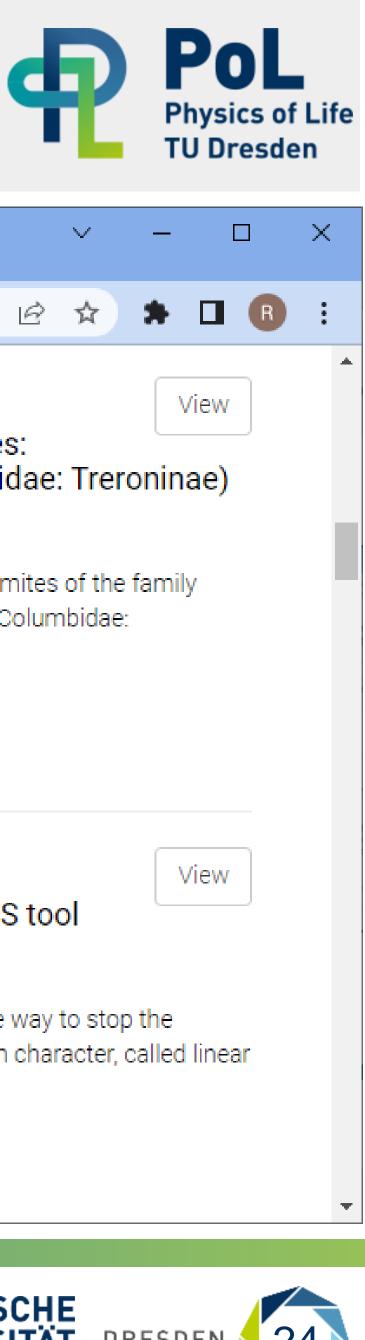


FAIR principles: <u>Accessible</u>

- Research data can be made accessible (after it was found by potential users)
 - Open Access is just one form of accessibility
 - Authentication enables other forms









December 31, 2014 (v1) Journal article Closed Access

Two new species of quill mites of the family Syringophilidae (Acariformes: Cheyletoidea) associated with treronine doves (Columbiformes: Columbidae: Treroninae)

Kaszewska, Katarzyna; Kavetska, Katarzyna; Skoracki, Maciej;

Kaszewska, Katarzyna, Kavetska, Katarzyna, Skoracki, Maciej (2014): Two new species of quill mites of the family Syringophilidae (Acariformes: Cheyletoidea) associated with treronine doves (Columbiformes: Columbidae: Treroninae). Zootaxa 3846 (2): 293-300, DOI: http://dx.doi.org/10.11646/zootaxa.384

Uploaded on January 5, 2017

Published in Zootaxa, vol. 3846, issue 2, pp. 293-300.

April 5, 2018 (v1) Journal article Open Access

Modeling potential tree belt functions in rural landscapes using a new GIS tool

Nowak, Maciej Marcin; Pędziwiatr, Katarzyna;

The increasing human pressure on the environment requires effective protection activities. One way to stop the degradation of natural resources is the presence of woody vegetation networks, mainly linear in character, called linear woody features, greenways or tree belts. These objects, thanks to th

Uploaded on April 16, 2018

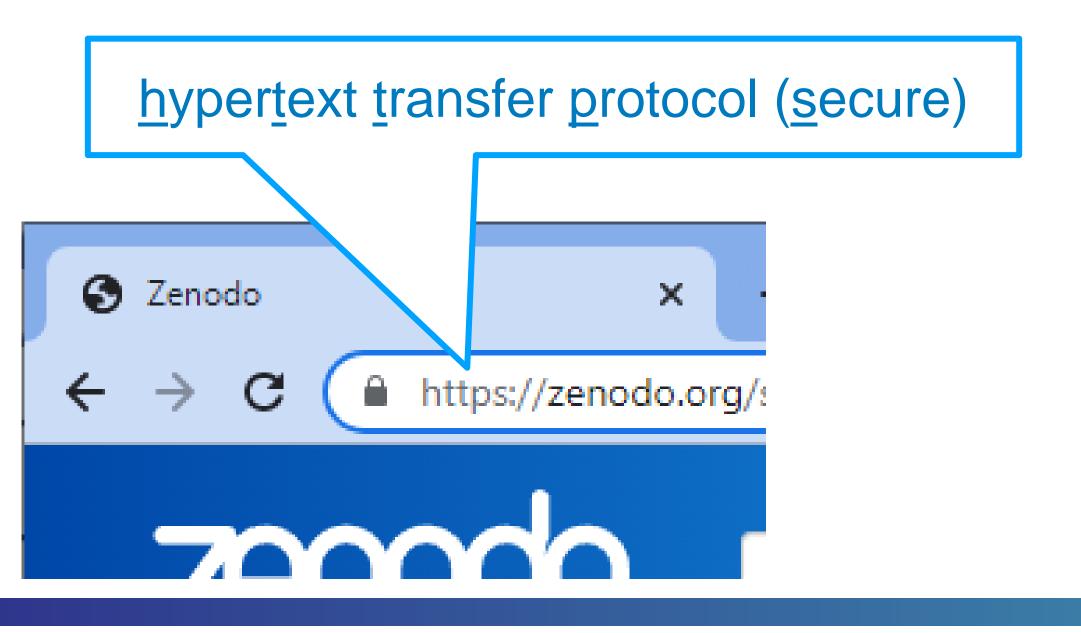
Published in Journal of Environmental Management, vol. 217, pp. 315-326.



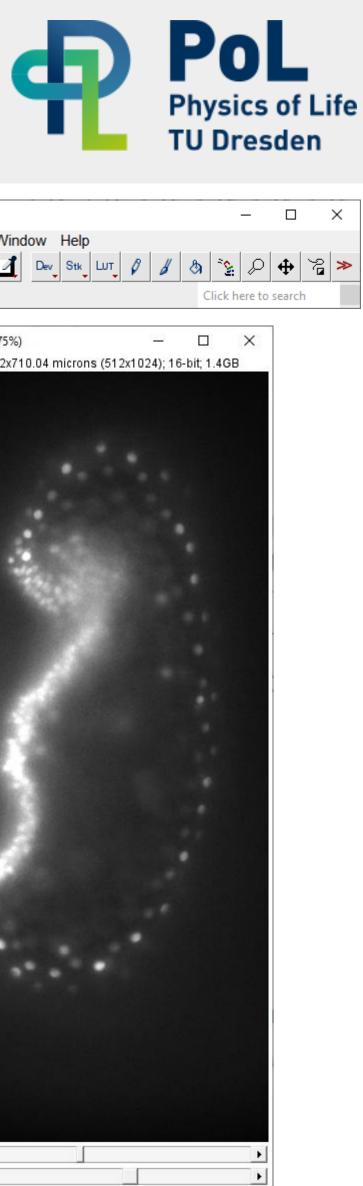
FAIR principles: Interoperable

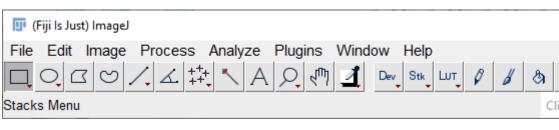
Data can be opened in multiple software through open and documented...

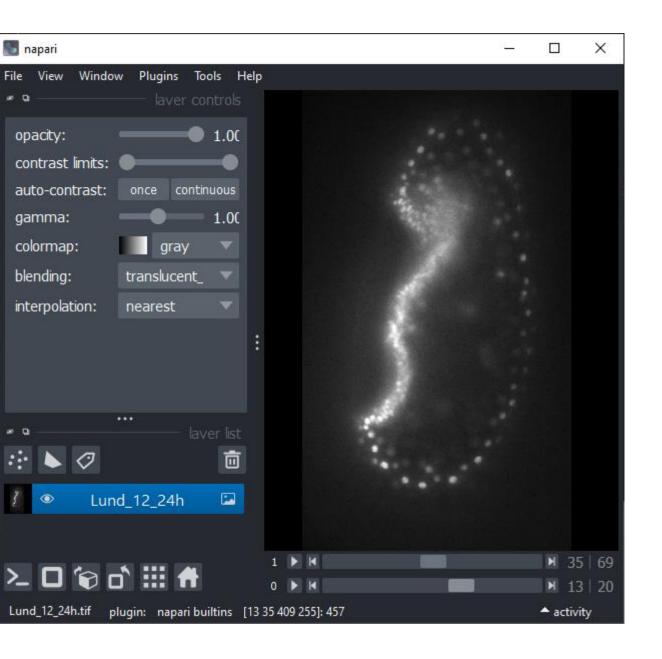
- file-formats
- protocols

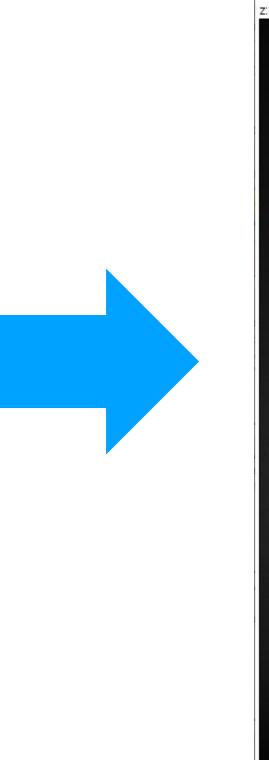


@haesleinhuepf















FAIR principles: <u>Reusable</u>

Data can be reused if

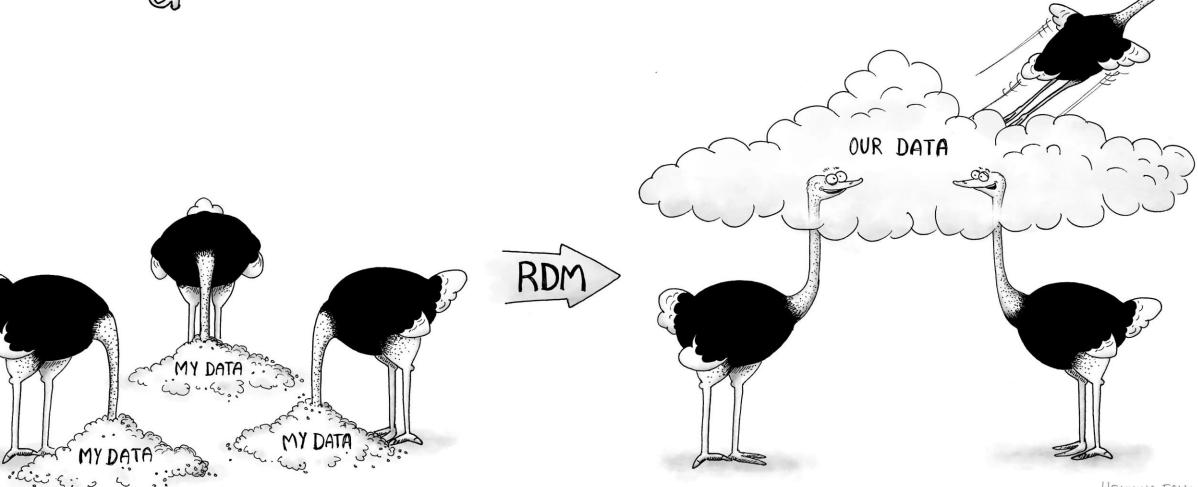
- Other FAIR principles are fulfilled
- Data is properly licensed
 - copyright statement is given
 - No copyright statement means: You do not have the right to copy







IMAGINE THE FUTURE.



HENNING FALK

Image source: \bigcirc @DrHenningFalk, licensed CC-BY 4.0

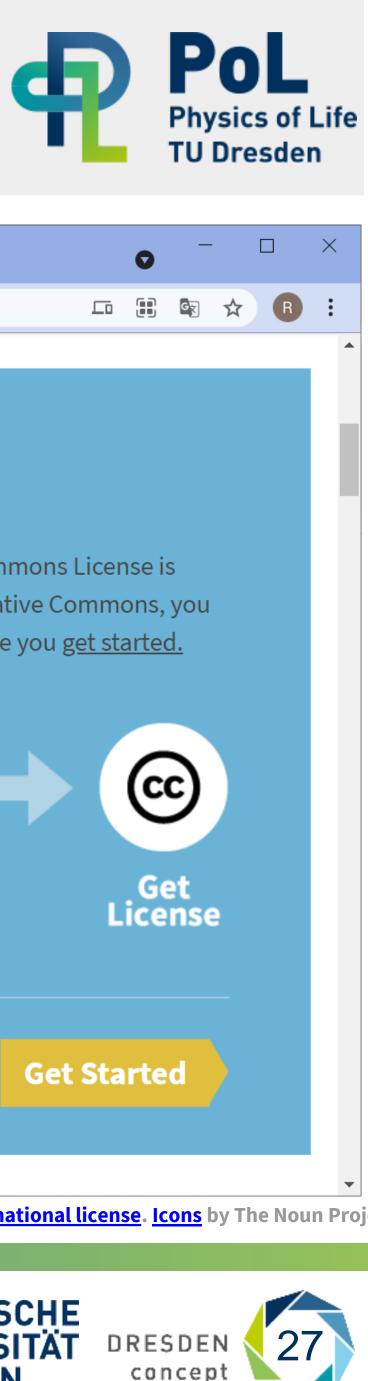


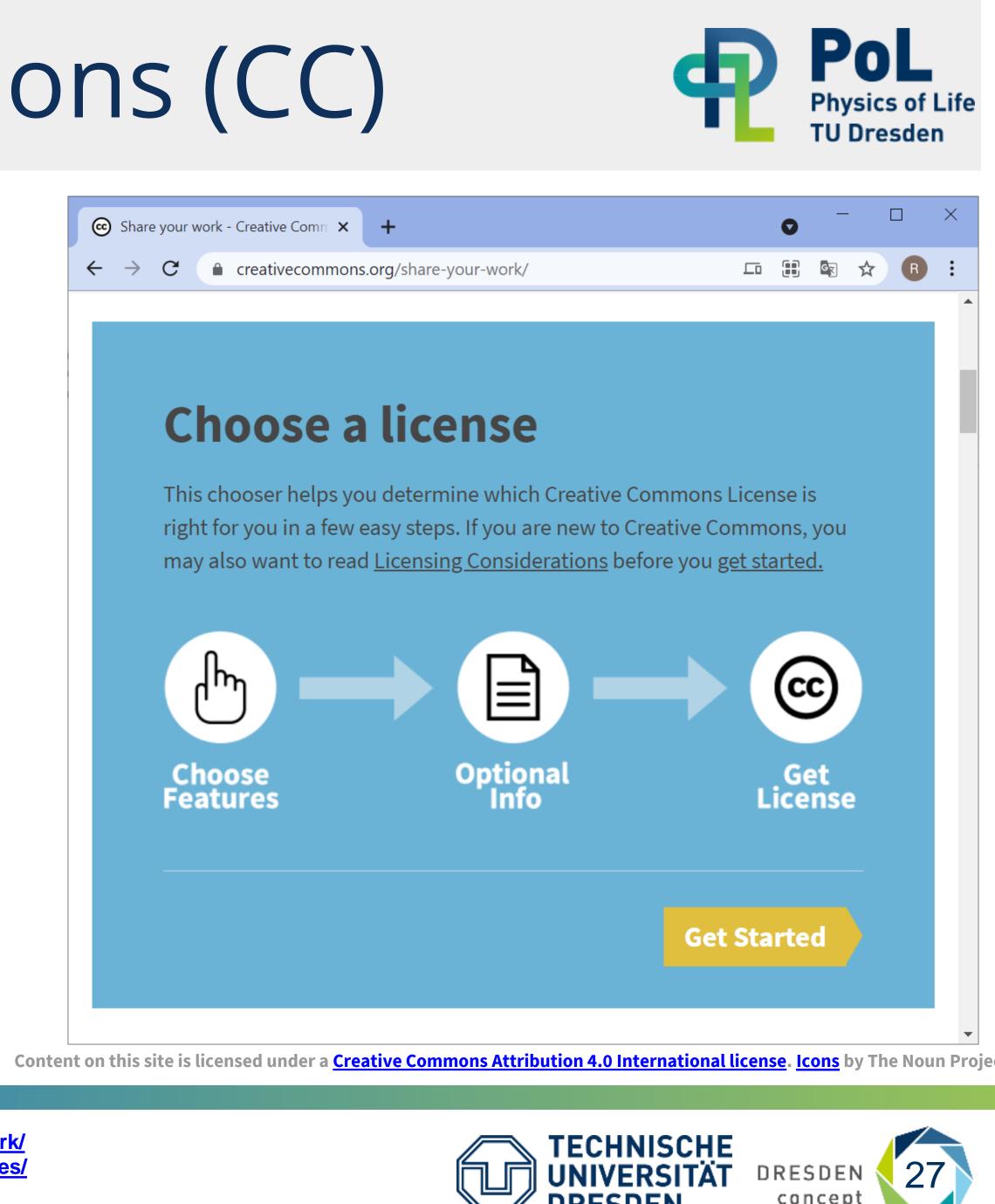


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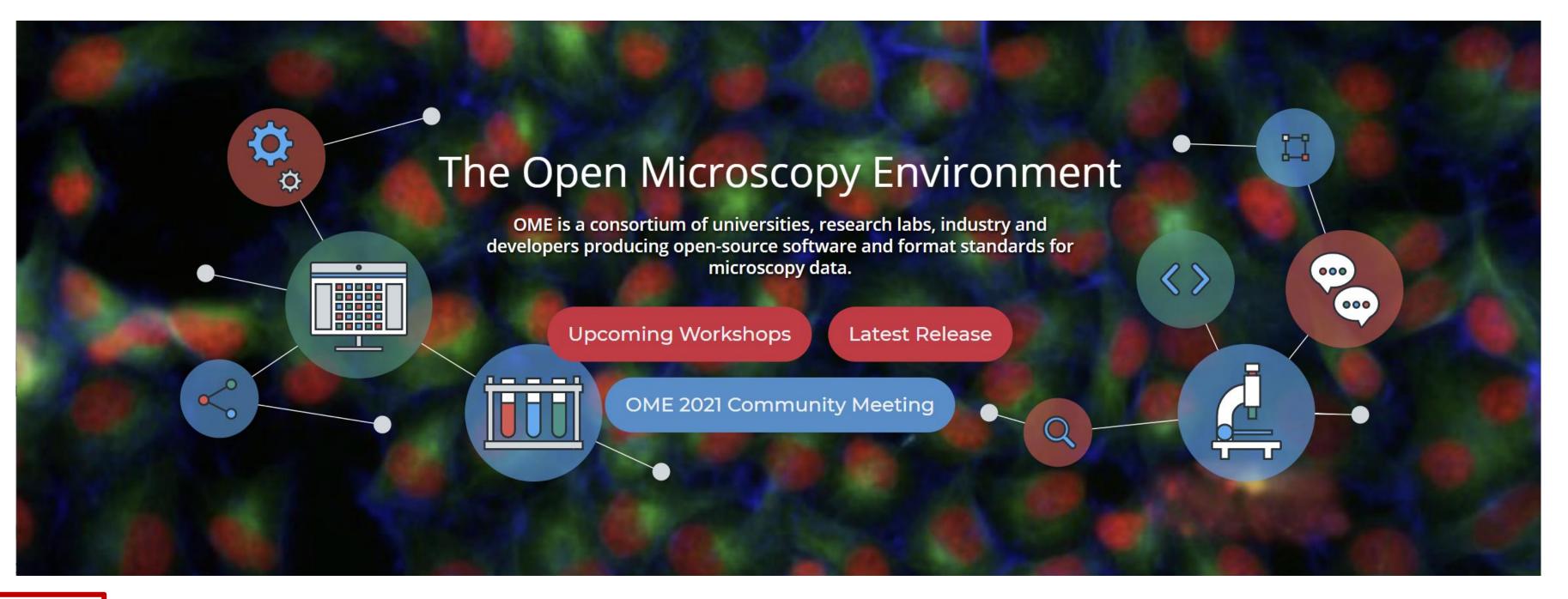








Example



You must put such a sentence and keep the link to CC-BY

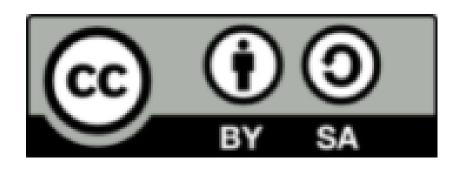
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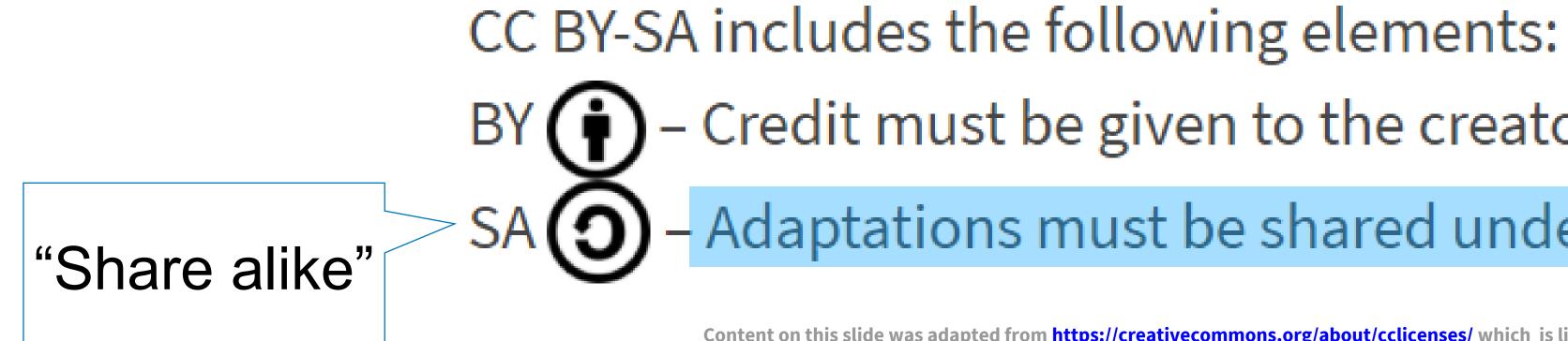






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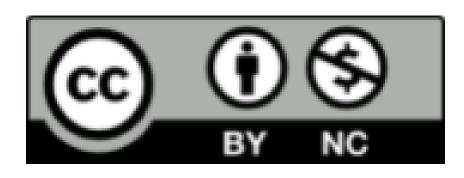
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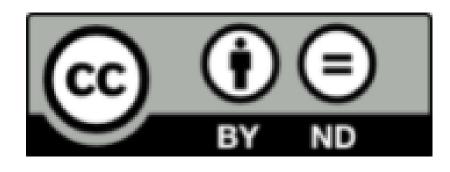
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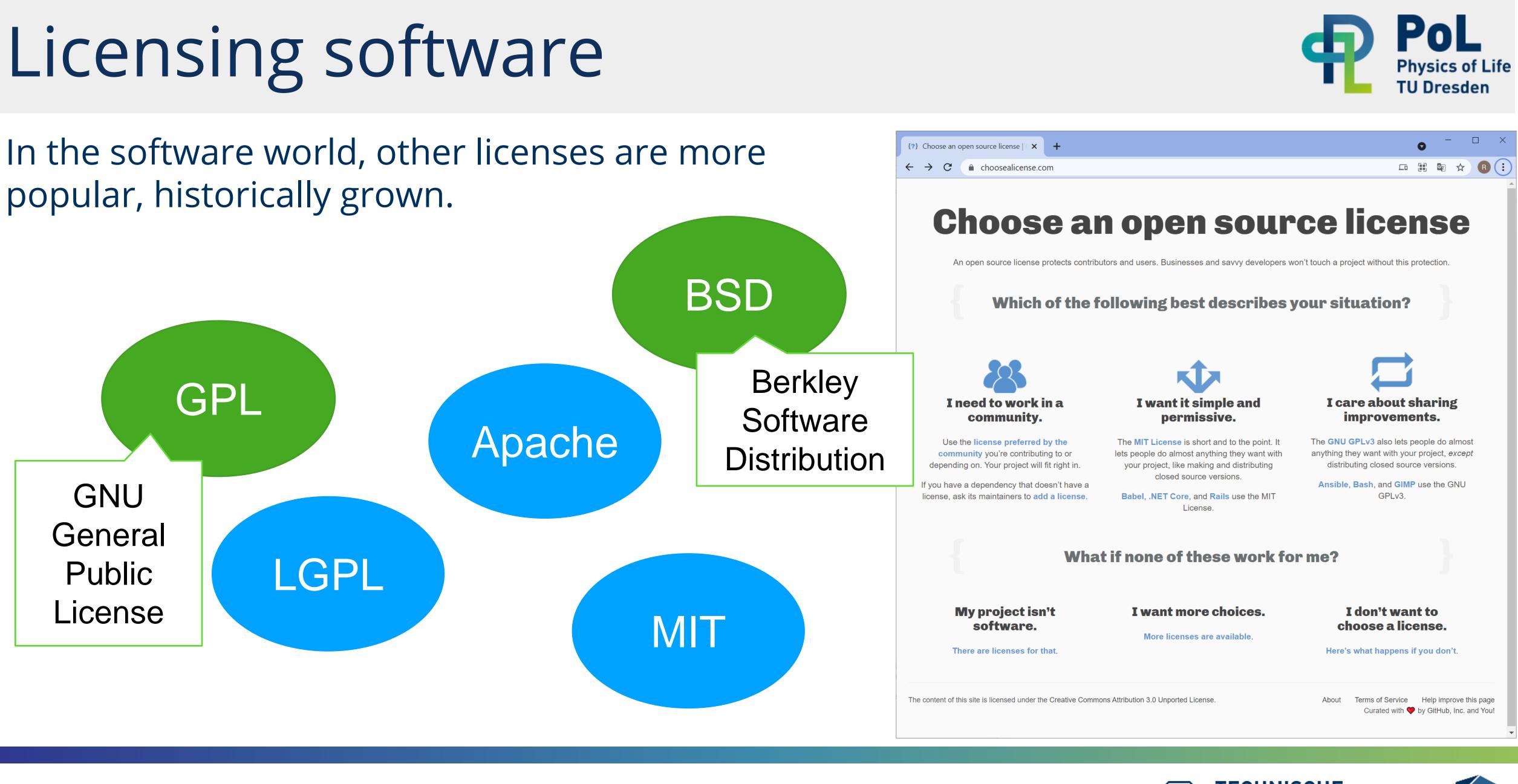
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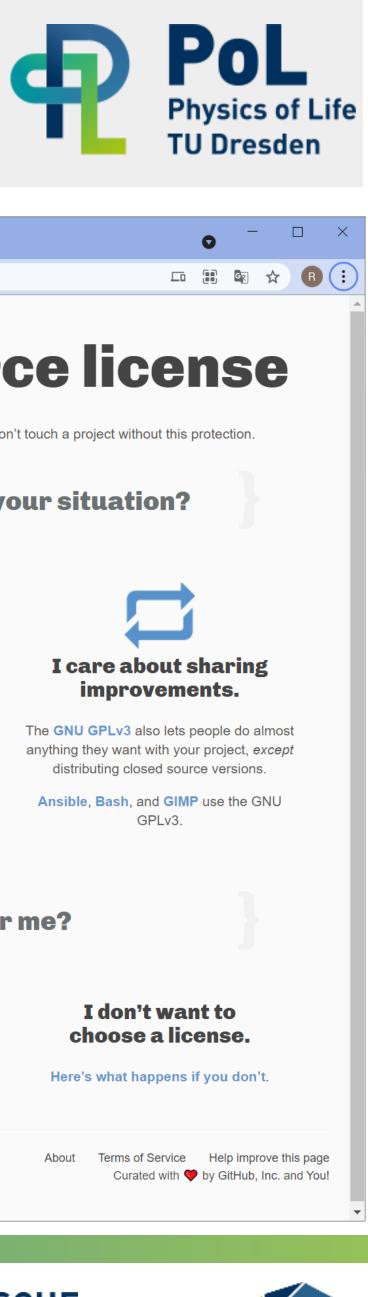








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Preamble

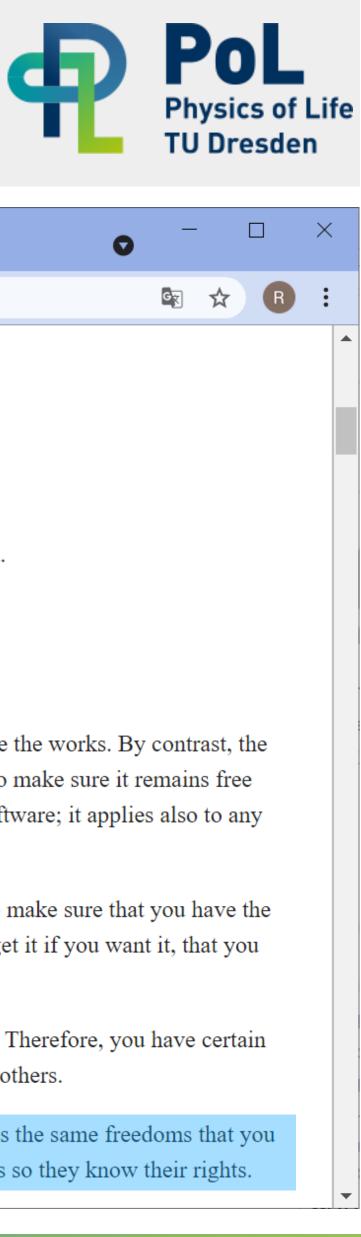
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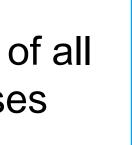














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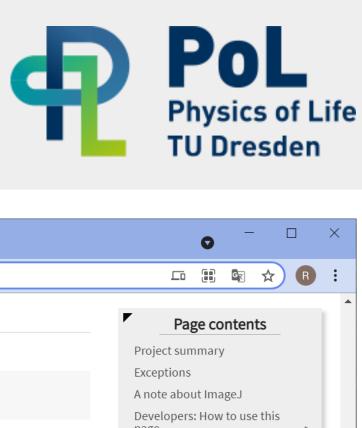
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• Choose a license compatible with your ecosystem

When?

- When the project starts
- As early as possible
- Changing the license later may be hard.
- Beware: Your employer might be the copyright holder. They have the final word on how to license, publish and make accessible your work!

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Quiz



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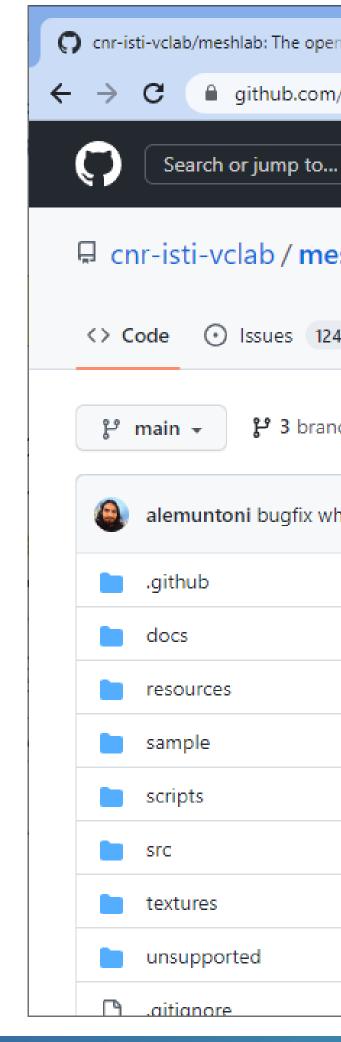




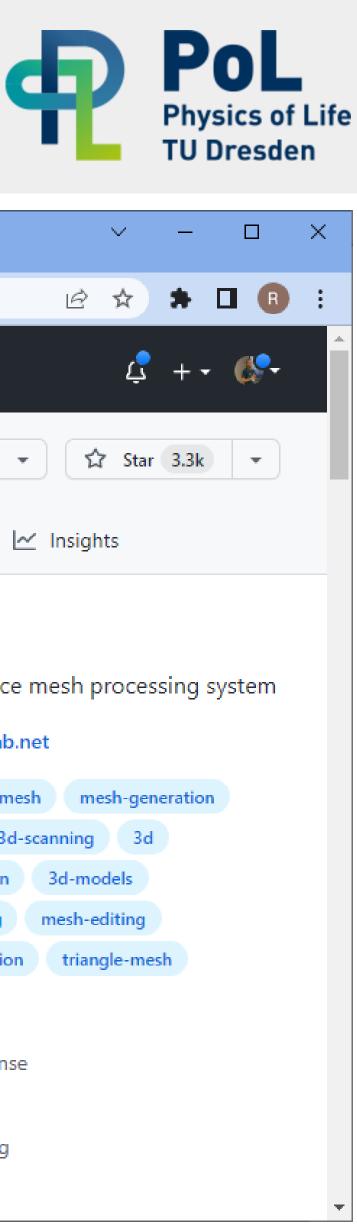
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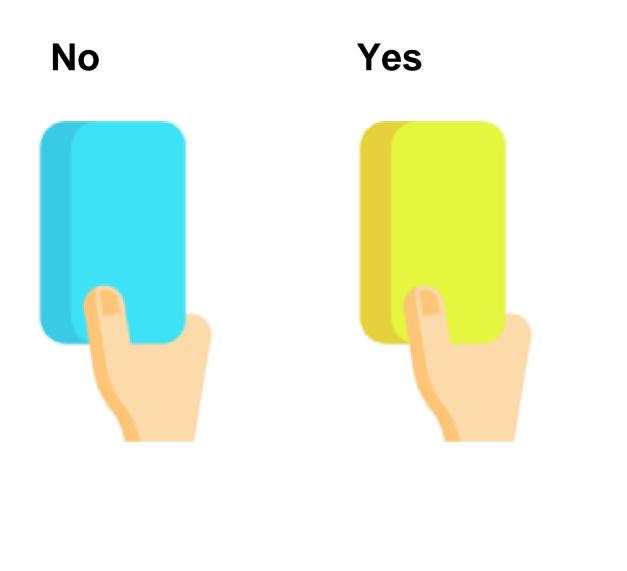
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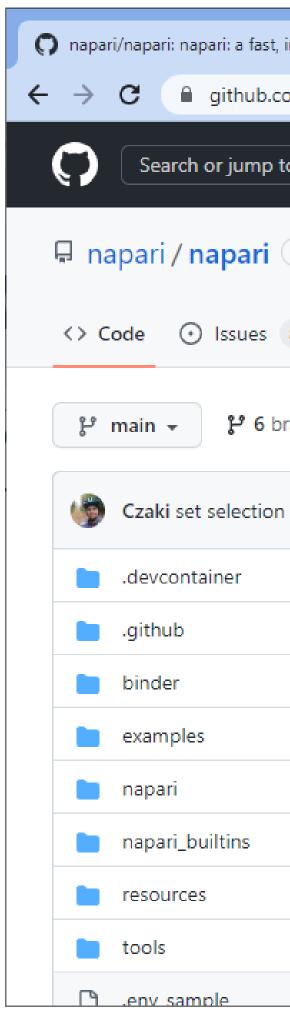




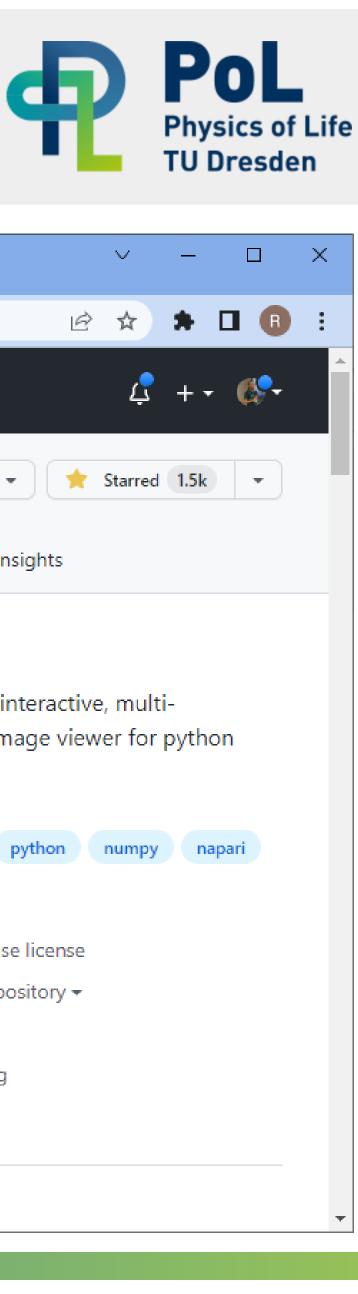


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Split out builtins into another top-level module (#4706) 3 months ago 3 to 45 watching		
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Python Algorithms: Conditions, loops, functions and custom libraries **Robert Haase**

April 2023

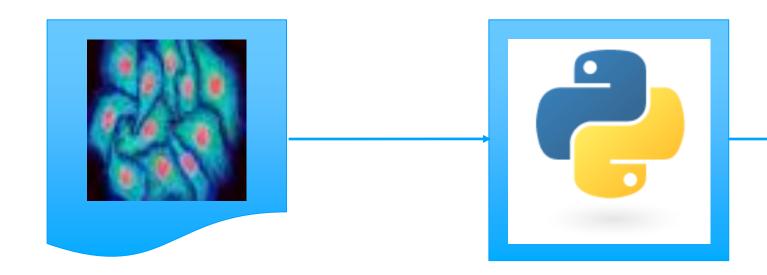






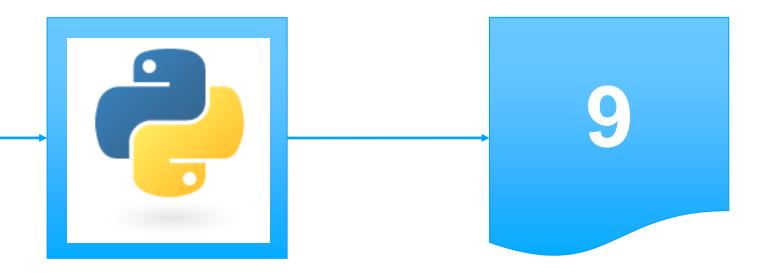
Conditions

Data science workflows *rarely* look like this









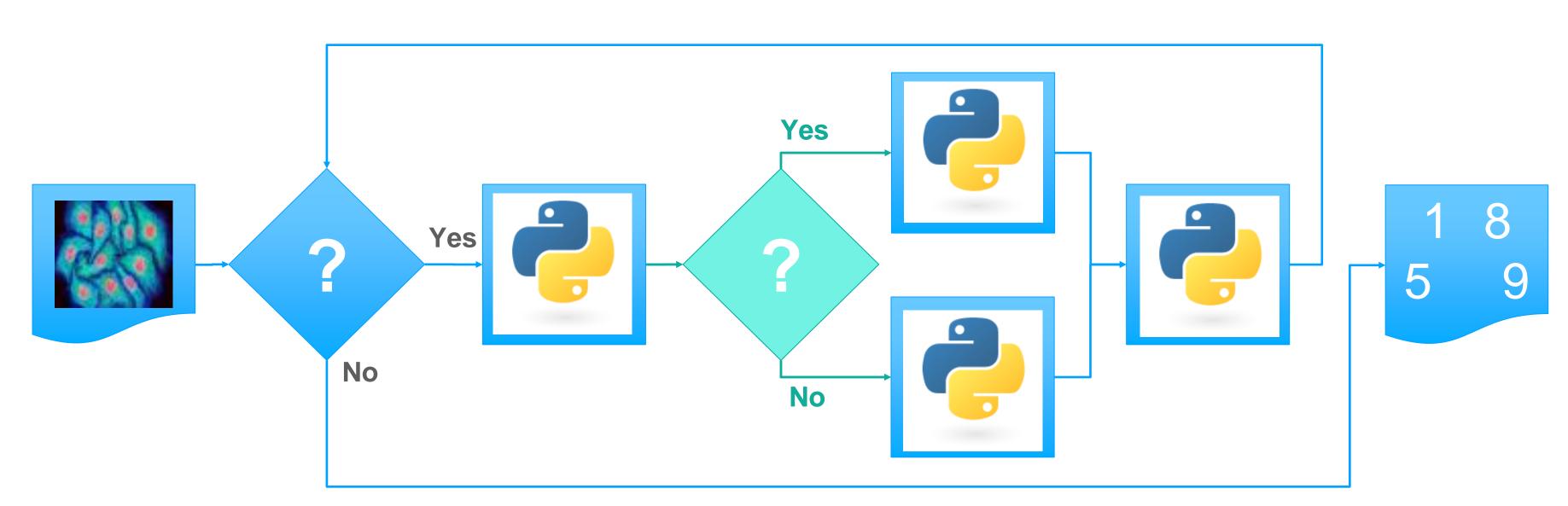




Conditions

Data science workflows *rather* look like this

Conditional statement











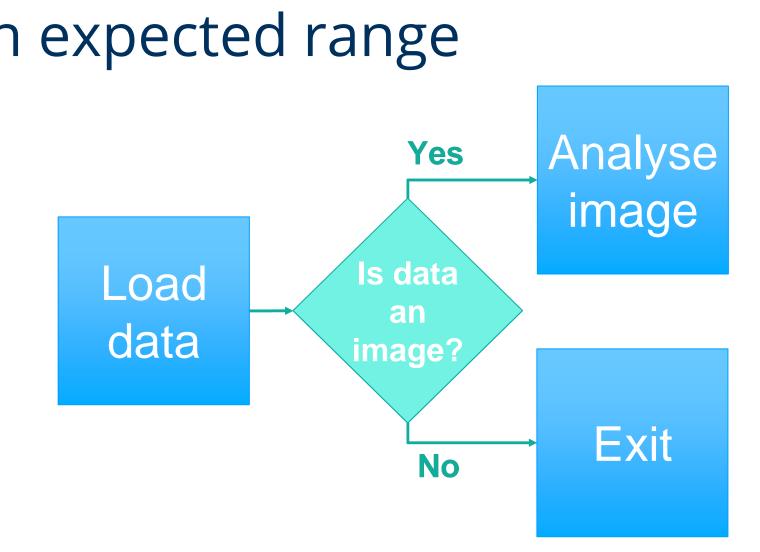
Conditions

Conditional statements can be used to

- Check if pre-requisites are met
- Check if data has the right format
- Check if processing results are within an expected range
- Check for errors





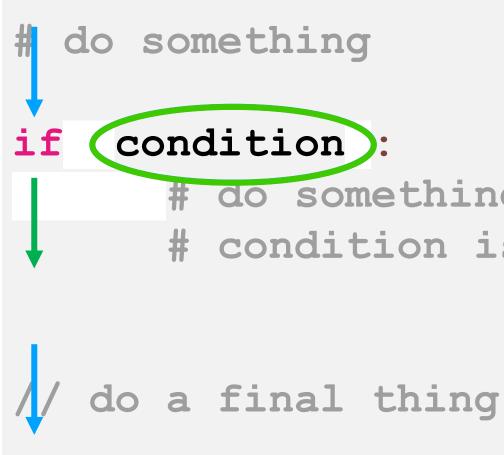






lf-statement

Depending on a condition, some lines of code are executed or not.







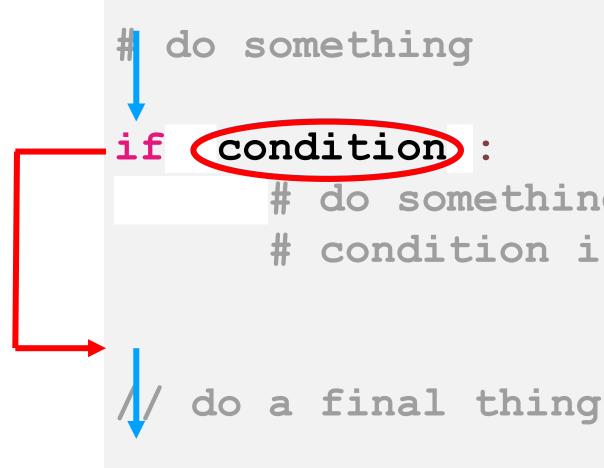
do something if # condition is true





lf-statement

Depending on a condition, some lines of code are executed or not.







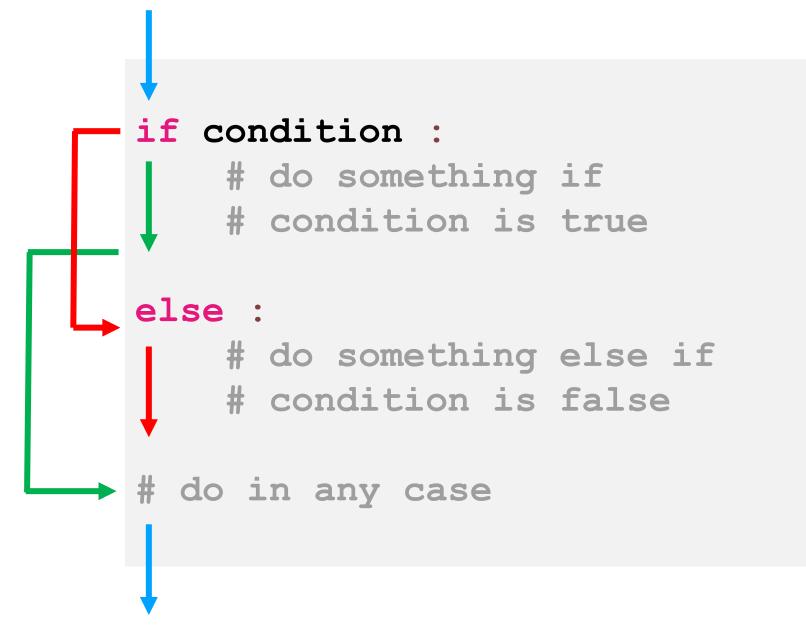
do something if # condition is true





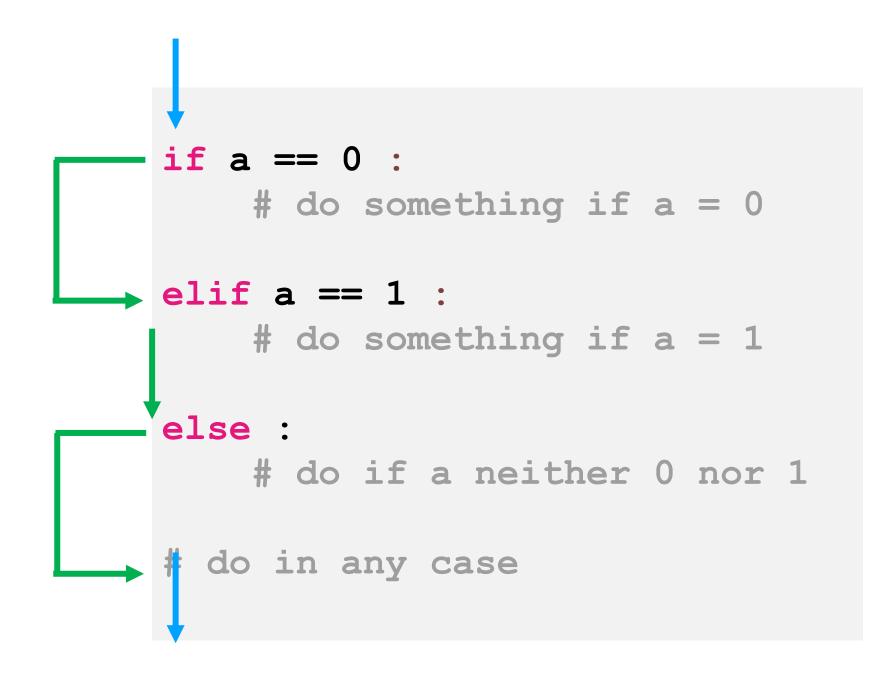
If-statement

The **if / elif / else** statement allows to program alternatives. Depending on conditions, only one block is computed Indentation is used to mark where a block starts and ends. Indentation helps reading blocks,









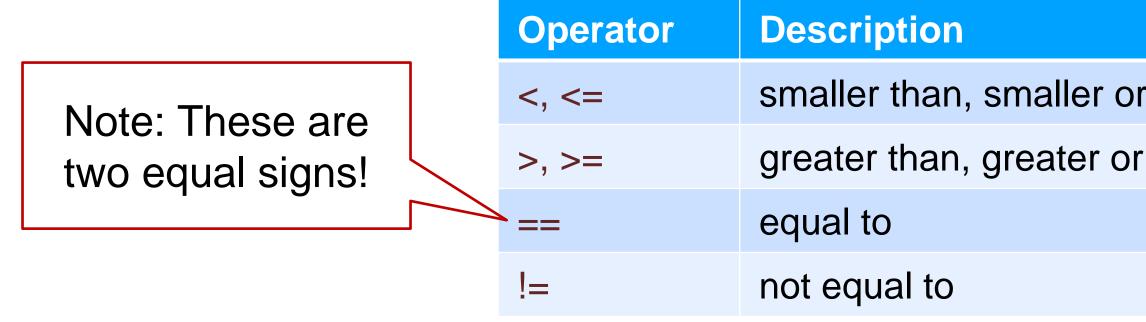




If-statement

Comparison operators always have True (1) or False (0) as results.

```
# initialise program
quality = 99.5
 evaluate result
#
if quality > 99.9:
    print("Everything is fine.")
else :
    print("We need to improve!")
```









	Example
r equal to	a < b
r equal to	a > b
	a == b
	a != 1





Combined conditions

Logic operators always take conditions as operands and result in a condition.

- and
- or
- not

Also combined conditions can be either True (1) or False (0).

```
# initialise program
quality = 99.9
age = 3
if quality >= 99.9 and age > 5:
   print("The item is ok.")
```

@haesleinhuepf



```
# initialise program
quality = 99.9
```

```
if not quality < 99.9 :
   print("The item is ok.")
```





Conditions with arrays

Checking contents of lists can be done intuitively using the in statement

```
# initialise program
my_{list} = [1, 5, 7, 8]
item = 3
if item in my_list :
    print("The item is in the list.")
else :
    print("There is no", item, "in", my_list )
```

item = 3







```
# initialise program
my_{list} = [1, 5, 7, 8]
if item not in my_list :
    print("There is no", item, "in", my_list )
else :
    print("The item is in the list.")
```





Readable code

- <u>Every command belongs on its own line</u>
- Insert <u>empty lines to separate</u> important processing steps
- Put <u>spaces</u> between operators and operands, because:

This is easier to read thanthat, or isnt'it?

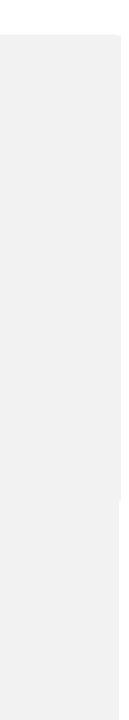
<u>Indent</u> every conditional block (if/else) using the TAB • key





```
# initialise program
a = 5
b = 3
c = 8
# execute algorithm
d = (a + b) / c
# evaluate result
if a == 5 :
   print("Yin")
else :
    print("Yang")
```

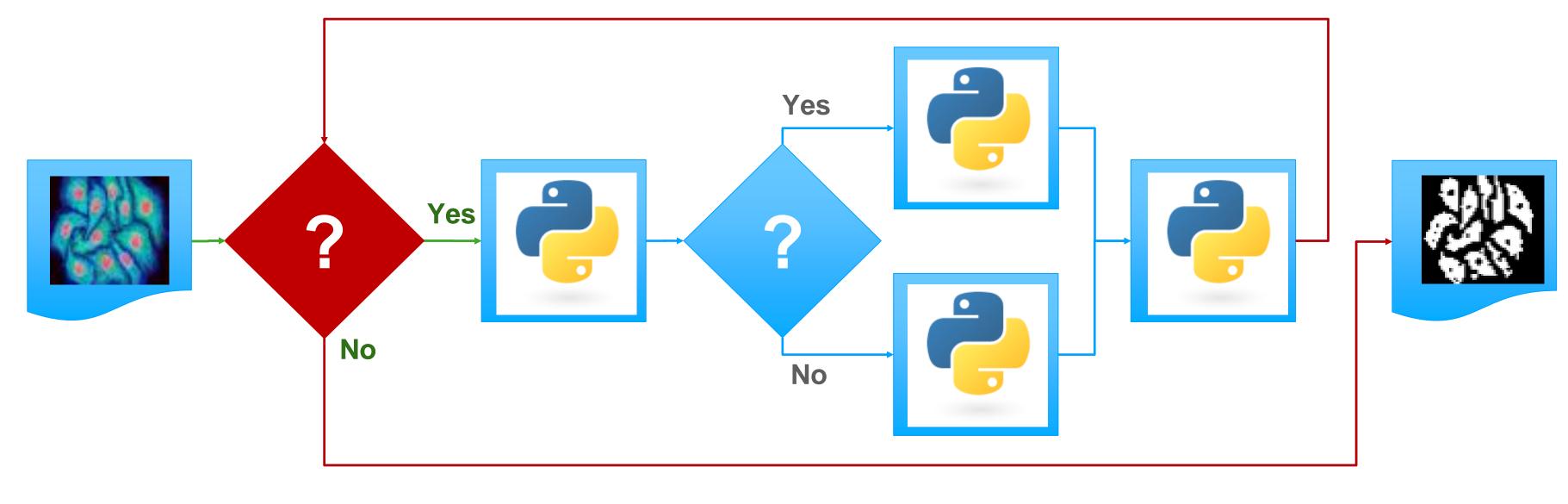








To repeat actions, you run code in loops



Loop statement









Loops

The for statement allows us to execute some lines of code for several times, typically for all items in an array-like thing (lists, tuples, images)





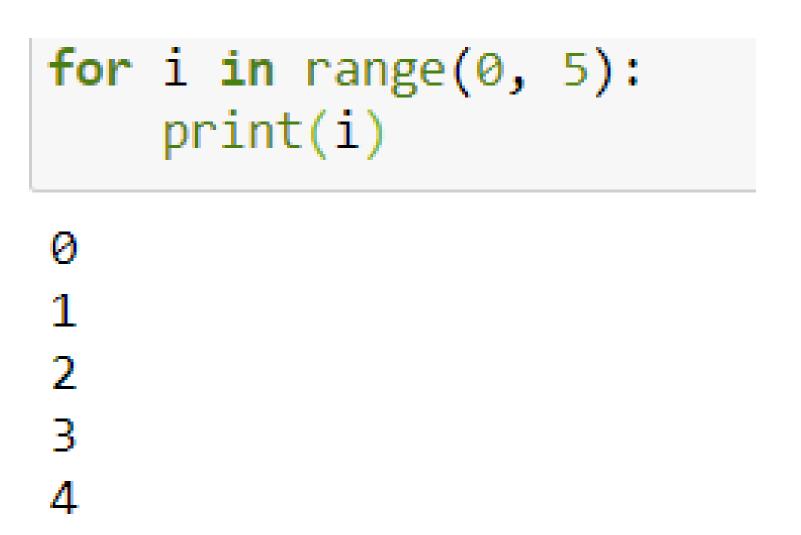






For-loops

Example list:range(start, stop, step)







animal_set = ["Cat", "Dog", "Mouse"] Н

for animal in animal_set: print(animal)

Cat Dog Mouse





For-loops

Indentation means combining operations to a block

```
for i in range(0, 5):
print(i)
```

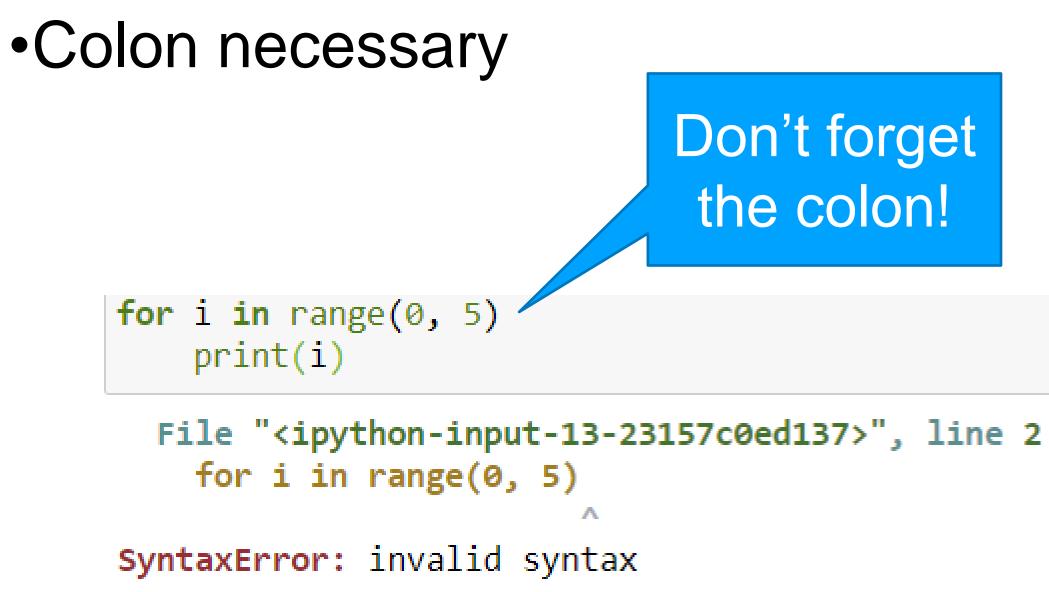
File "<ipython-input-15-59c457ae0ac9>", line 3 print(i)

IndentationError: expected an indented block

Don't forget to indent!











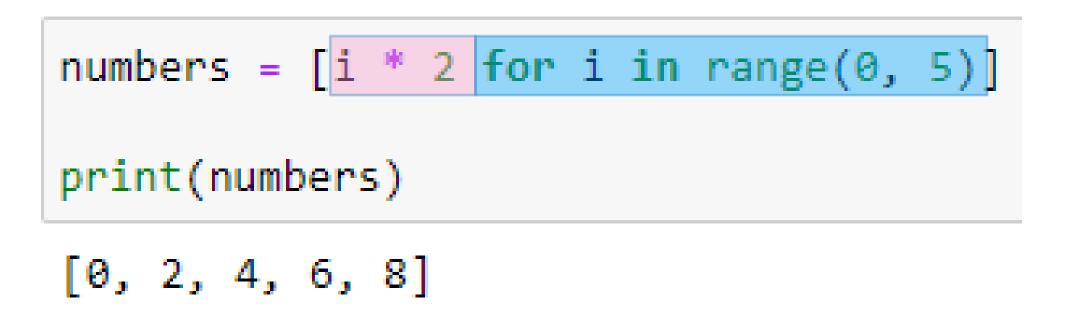
Generating arrays within for-loops

There is a long and a short way for creating arrays with numbers.

```
# we start with an empty list
numbers = []
# and add elements
for i in range(0, 5):
   numbers.append(i * 2)
print(numbers)
```





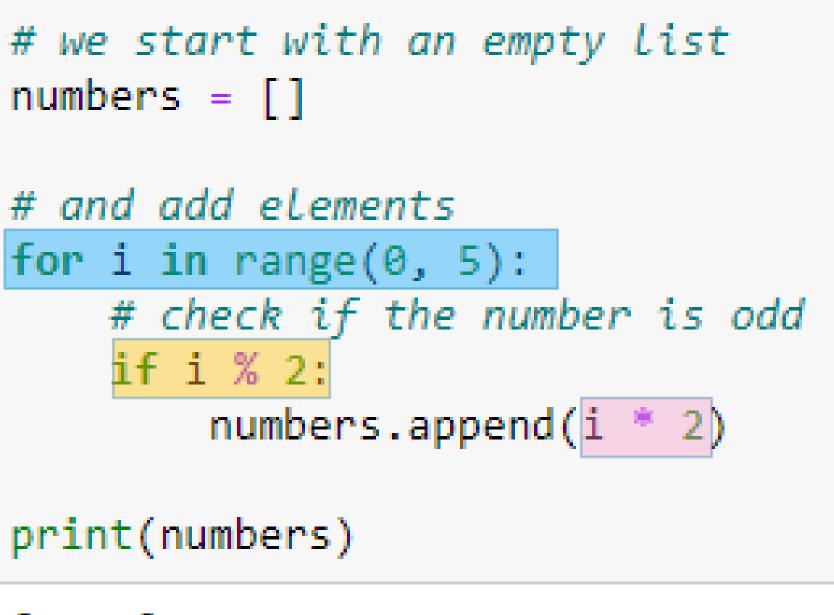






Generating arrays within for-loops

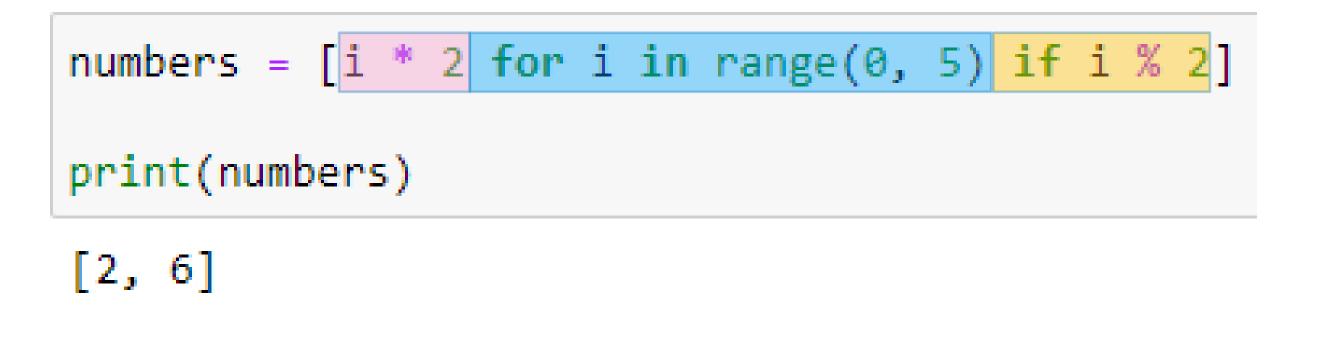
Also a combination with the if-statement is possible



[2, 6]











Listing files in a folder

Common use-case: do something with all *image* files in a folder

for file in file_list: if file.endswith(".tif"): print(file)

- banana0002.tif
- banana0003.tif
- banana0004.tif
- banana0005.tif
- banana0006.tif

image_file_list

image_file_list

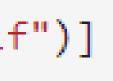
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- 'banana0003.ti
- 'banana0004.ti
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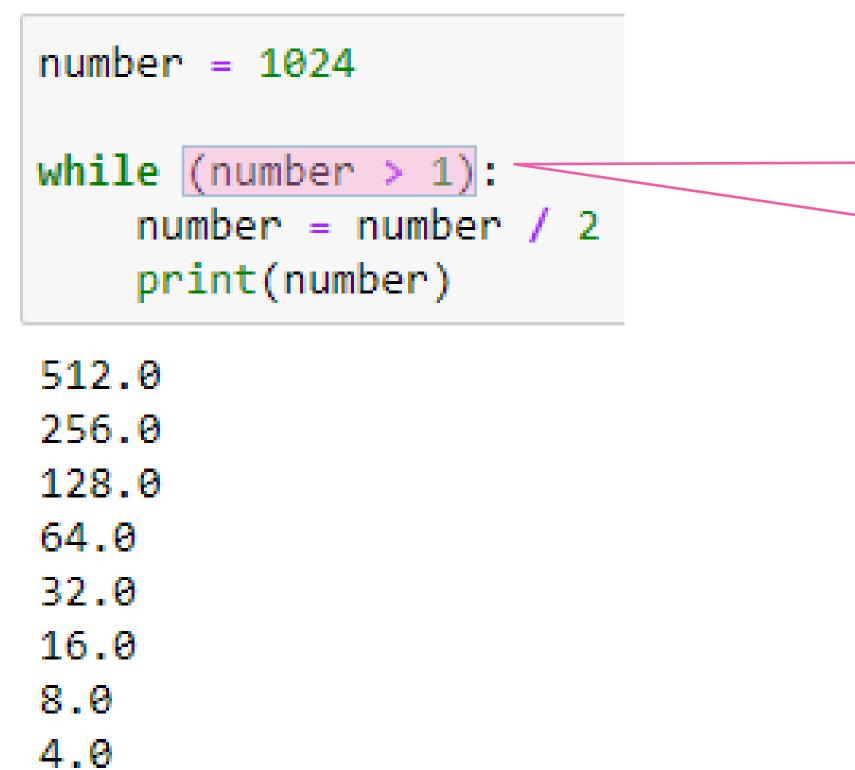






While-loops

While loops keep executing indented code as long as a condition is met:



- 2.0
- 1.0





Works the same as with the if statement





Executing loops

Using the **break** statement, you can leave a loop

```
number = 1024
while (True):
    number = number / 2
    print(number)
    if number < 1:
        break
512.0
256.0
128.0
64.0
32.0
16.0
8.0
4.0
2.0
1.0
0.5
```



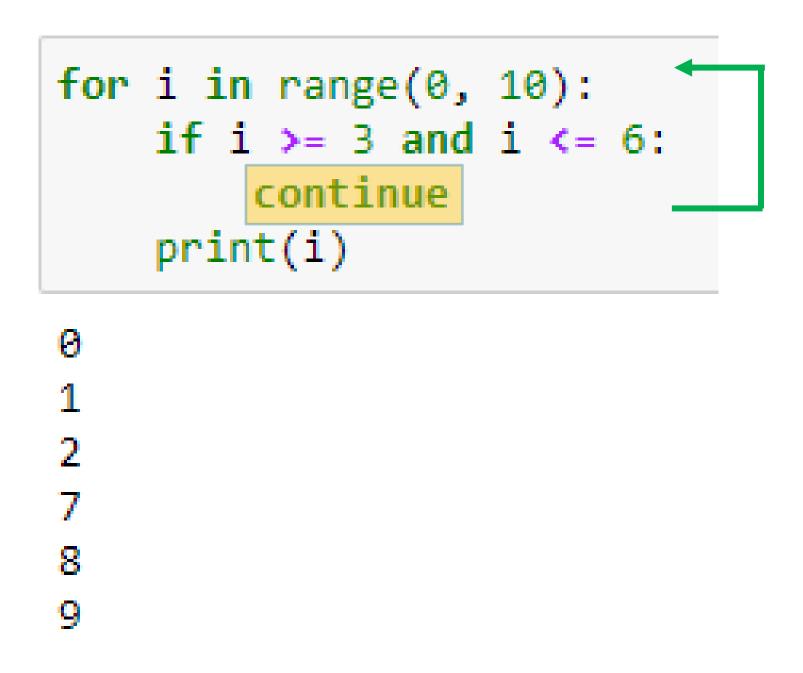






Skipping iterations

The continue statement allows to skip iterations











Functions

- g0.
- Functions allow to re-use code in different contexts.
- Indentation is crucial.
- Functions must be defined before called Definition:

name (parameters) body return statement (optional)





• In case repetitive tasks appear that cannot be handled in a loop, custom functions are the way to

```
Call:
c = sum_numbers(4, 5)
print(c)
 9
sum_numbers(5, 6)
11
sum_numbers(3, 4)
```





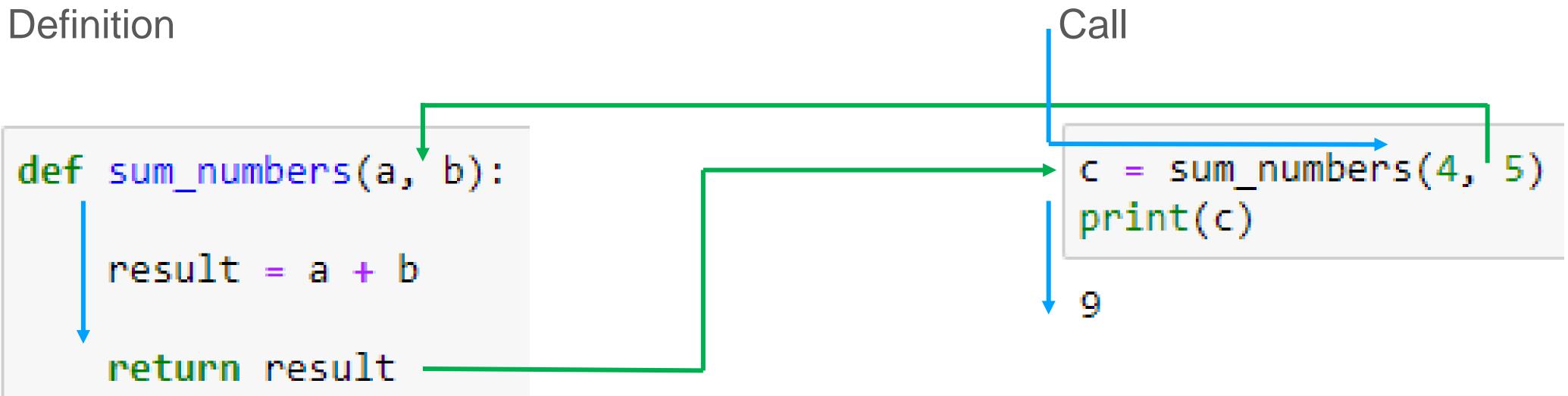


Functions

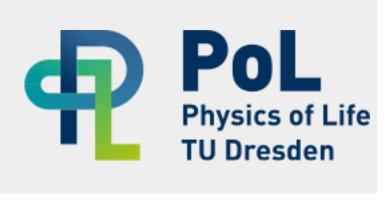
way to go.

Functions allow to re-use code in different contexts. Indentation is crucial.

Functions must be defined before called







- In case repetitive tasks appear that cannot be handled in a loop, custom functions are the







Functions

Document your functions to keep track of what they do. Describe what the functions does and what the parameters are meant to be

```
def square(number):
    Squares a number by multiplying it with itself and returns its result.
    . . .
    return number * number
```

You can then later print the documentation if you can't recall how a function works.

```
square?
Signature: square(number)
Docstring: Squares a number by multiplying it with itself and returns its
result.
```



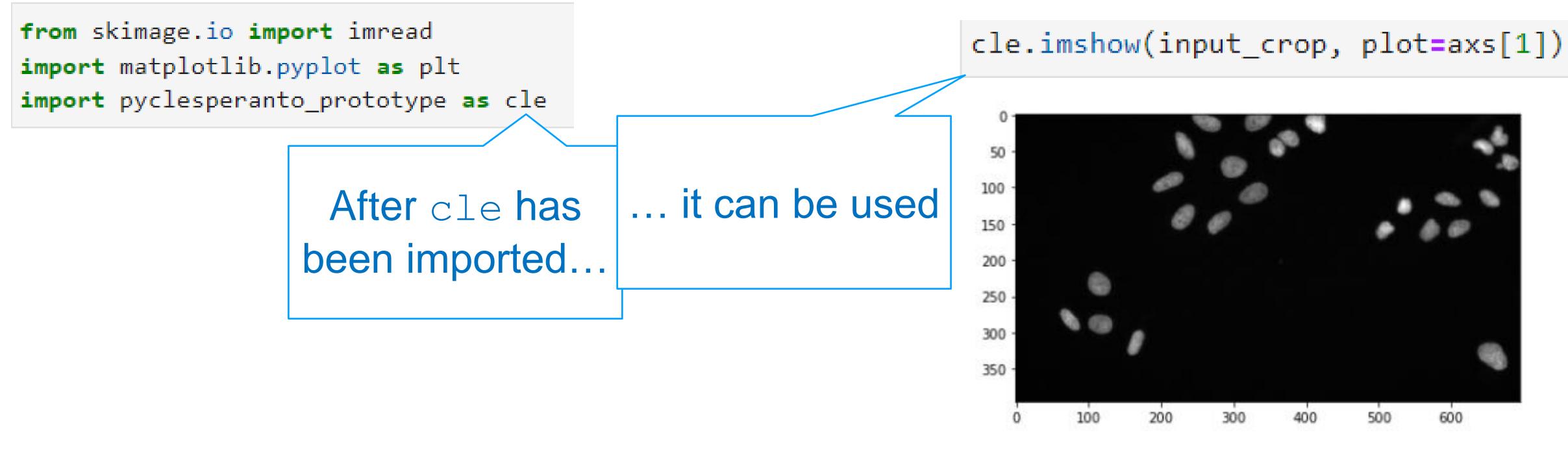






Libraries

- The import statement allows to use functions provided by others.
- Commonly put at the beginning of a notebook or script to make sure everything is installed.







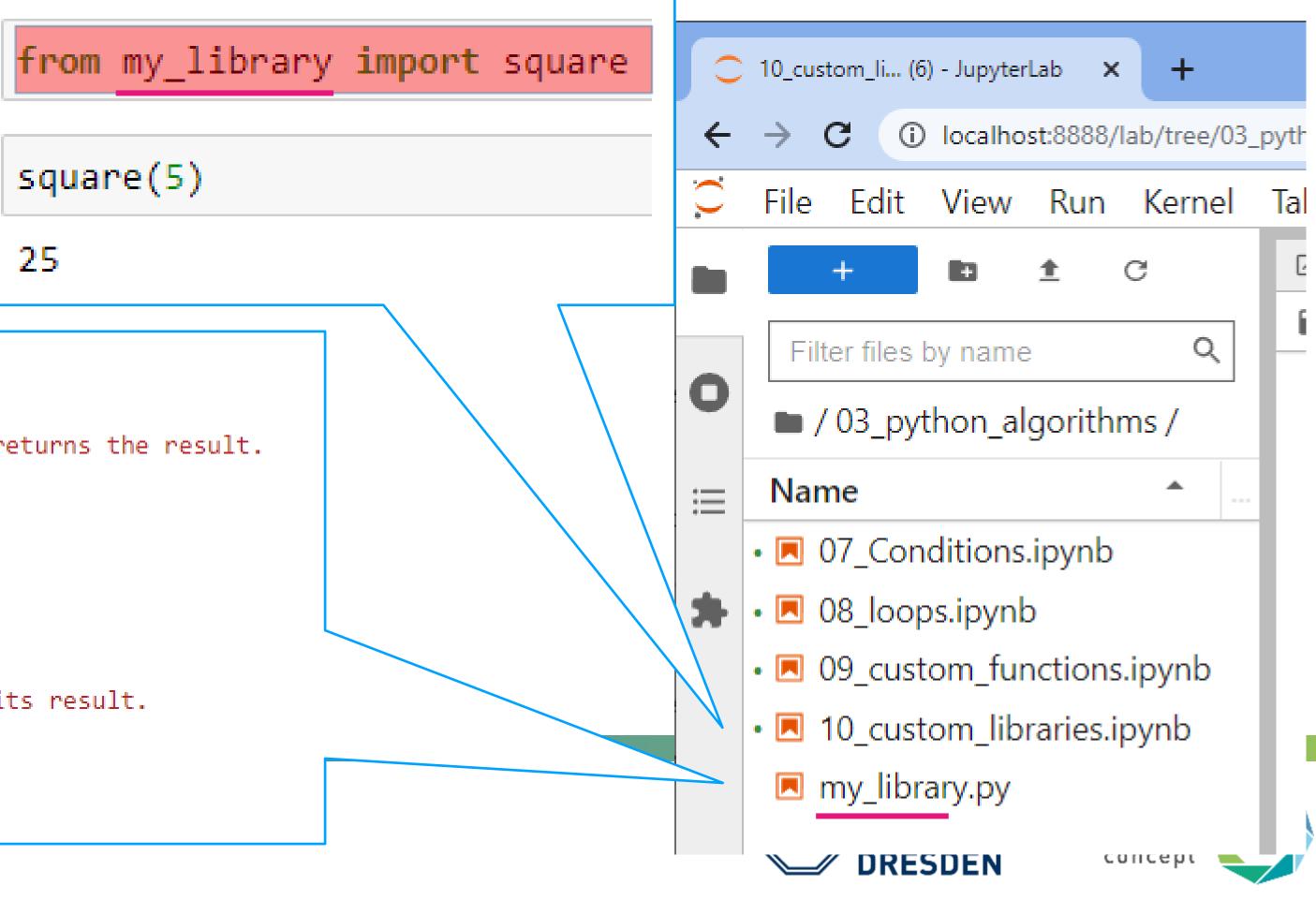






Libraries

For <u>re-using</u> functions between notebooks / projects, use libraries. -> <u>Sustainability</u> Simple python libraries are .py files containing multiple functions. The import statement allows you to import python files from the same folder.



```
def wuzzle(number):
        The wuzzle function manipulates a number in a magic way and returns the result.
        . . .
 4
 5
        import math
 6
        return math.sqrt(number * 1.2)
 8
   def square(number):
10
        Squares a number by multiplying it with itself and returns its result.
11
12
13
        return number * number
14
```

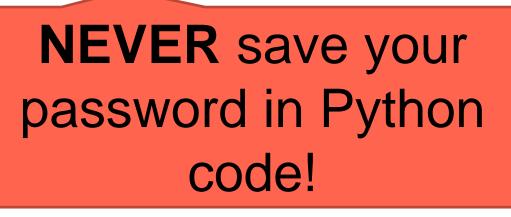


Outlook: The power of Python

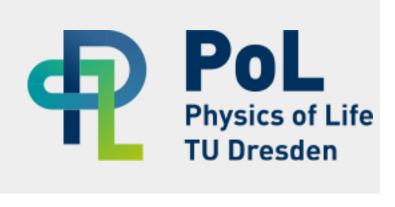
With Python, you can automate many tedious tasks. Example: Downloading files from the owncloud.

Build a login form	List all files
<pre>server_widget = widgets.Text(value='https://cloudstore.zih.tu-dresden. sername_widget = widgets.Text(description='Username:') bassword_widget = widgets.Password(description='Password') vidgets.VBox([server_widget, username_widget, password_widget])</pre>	<pre># enter a folder on to remote_folder = "/" for f in oc.list(remote print (f.path)</pre>
Server https://cloudstore.zih.tu-dresden.d Username: roha044c Password Image: Cloud Store	/BiAPoL/ /Documents/ /Nextcloud Manual.pdf /Nextcloud intro.mp4 /Nextcloud.png
Log in	/Photos/ /Projects/ /Shared/ /Software/

oc = owncloud.Client(server_widget.value) oc.login(username widget.value, password widget.value)







all files in the owncloud

```
lder on the owncloud drive that exists.
r = ''/''
```

```
list(remote_folder):
.path)
```

Download a file

```
# enter the source file here
remote_source_file = '/Nextcloud Manual.pdf'
# enter the destination
local_file = 'Nextcloud Manual.pdf'
```

```
oc.get_file(remote_path=remote_source_file,
            local file=local file)
```

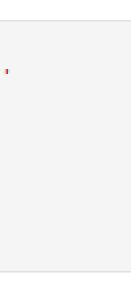
True

The PDF is now located in the same folder as this notebook.

Take care: You can also **DELETE** all files in an owncloud folder using similar code





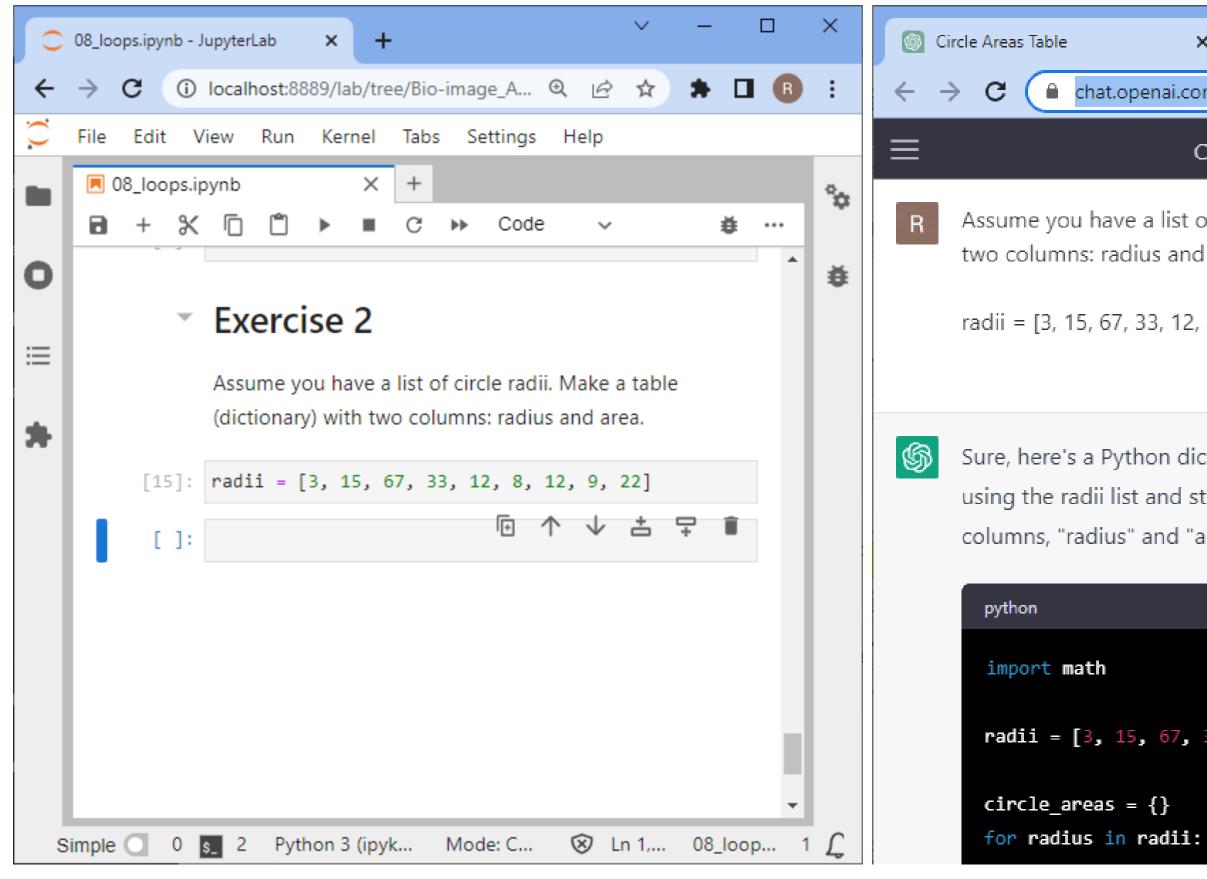






Outlook: The power of Al

Consider: It *lies* from time to time and during the exam it can't help you.





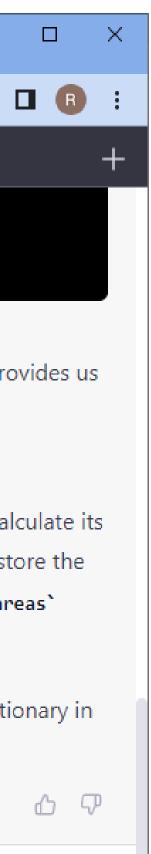
https://chat.openai.com/chat



Feel free to use artificial intelligence during the exercises. Play with it, learn how to exploit it best.

← ~ - □ ×	Sircle Areas Table × +
m/chat 🖻 🖈 🖬 🖪 🔋 :	$\leftarrow \rightarrow \mathbf{C}$ (a chat.openai.com/chat $\textcircled{C} \bigstar$
ircle Areas Table +	E Circle Areas Table
of circle radii. Make a table (dictionary) with area.	8 201.06192982974676 9 254.46900494077323 22 1519.748119012579
8, 12, 9, 22]	In the code above, we first import the math library which pro with the value of pi. We then create an empty dictionary
tionary that calculates the area of each circle cores the values in a dictionary with two rea":	<pre>`circle_areas`. Next, we loop through each radius in the `radii` list and ca area using the formula `math.pi * radius ** 2`. We then si radius as the key and the area as the value in the `circle_area</pre>
Copy code 33, 12, 8, 12, 9, 22]	Finally, we print out the contents of the `circle_areas` dict a formatted table.

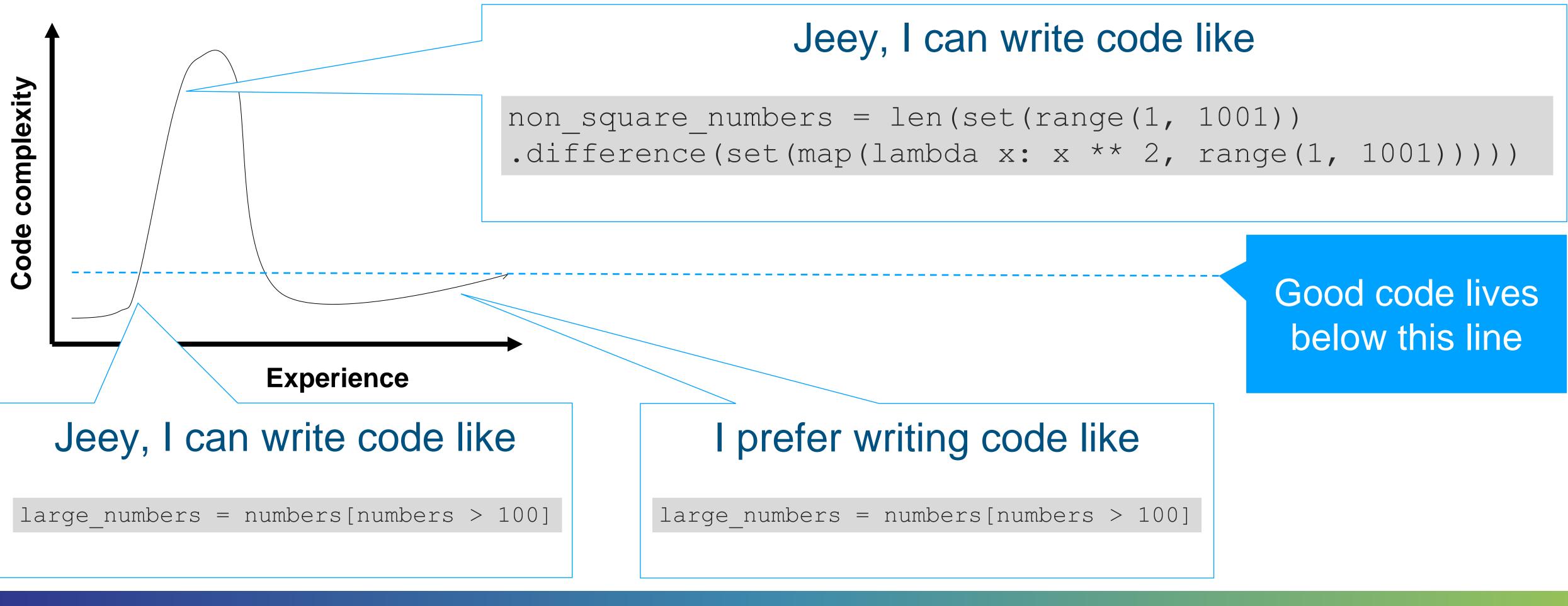






Software quality indicators

Interpretation of "High quality code" changes with experience



https://towardsdatascience.com/how-to-write-high-quality-python-as-a-data-scientistcde99f582675?gi=11843badbb14 https://en.wikipedia.org/wiki/Dunning%E2%80%93Kruger_effect











Summary

Today you learned:

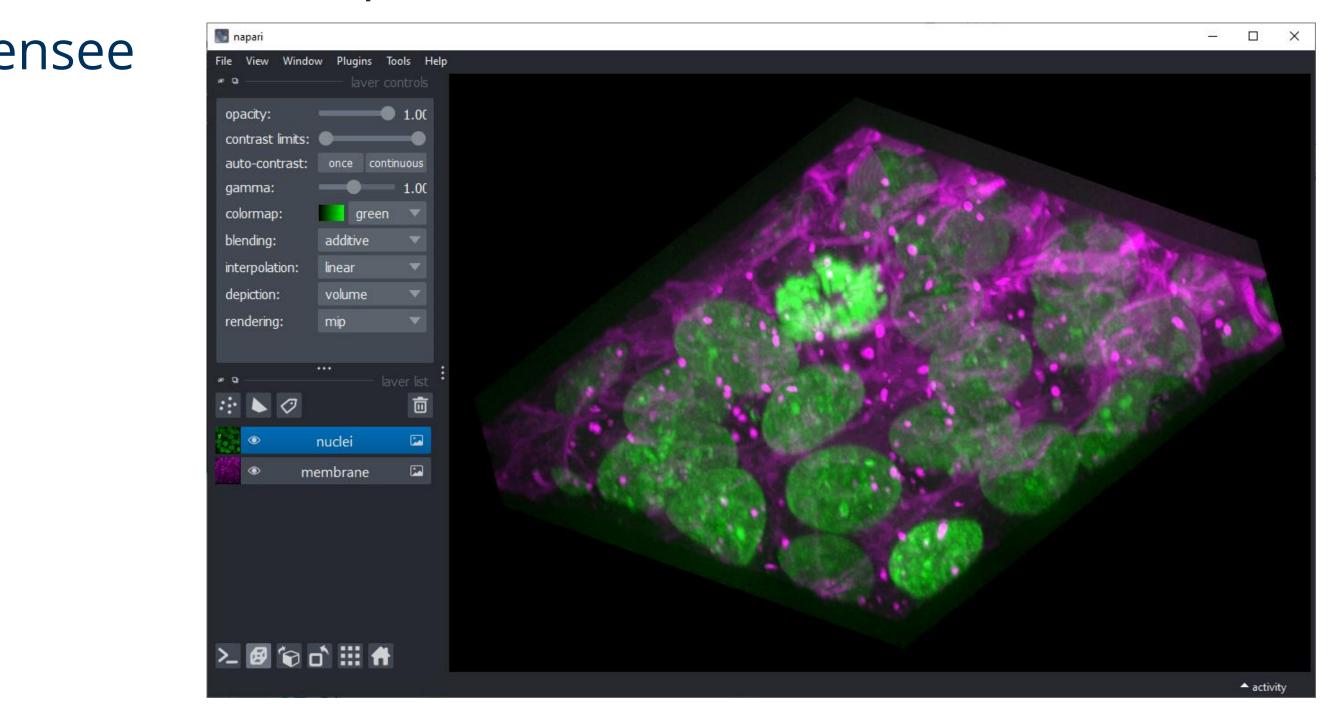
- Document what *dependencies* you use!
- Sharing / licensing terminology
 - Levels of openness
 - Copyright holder / Author / Publisher / Licensee
 - FAIR principles (findable, accessible, interoperable, reusable)
- Python algorithms
 - Loops
 - Conditions
 - Functions
 - Libraries





Coming up next:

- Image processing
- Image filtering
- Napari

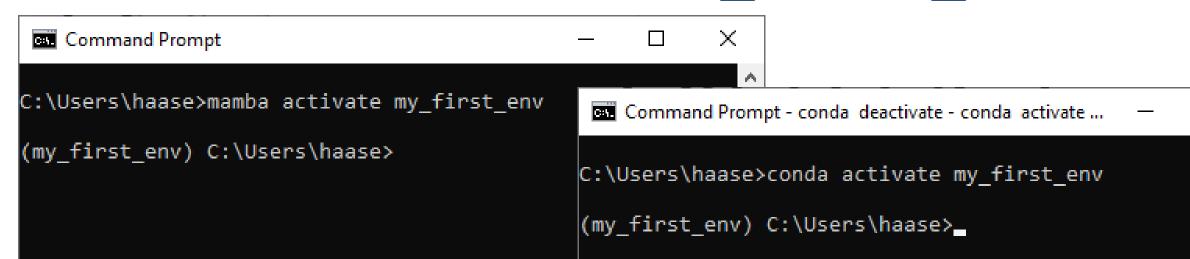




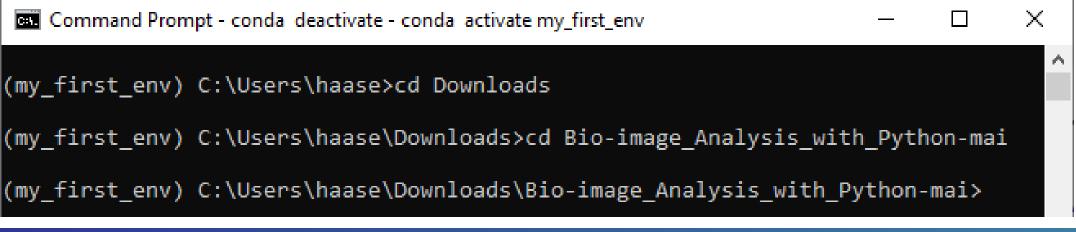


Exercises

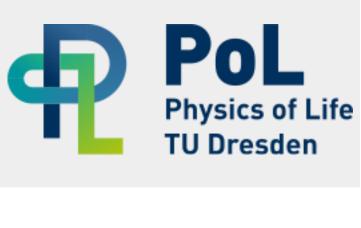
- Check the 02 python algorithms folder online https://github.com/BiAPoL/Bio-image_Analysis_with_Python
- 1. Start up a terminal
- 2. Activate the environment using conda activate my first env



3. Use the cd command to navigate to the exercise folder



@haesleinhuepf



4. Start up jupyter lab

 \times

