



# Organizing, documenting and distributing code

ASPP 2022, Bilbao

***= How to make your  
code (more) usable***

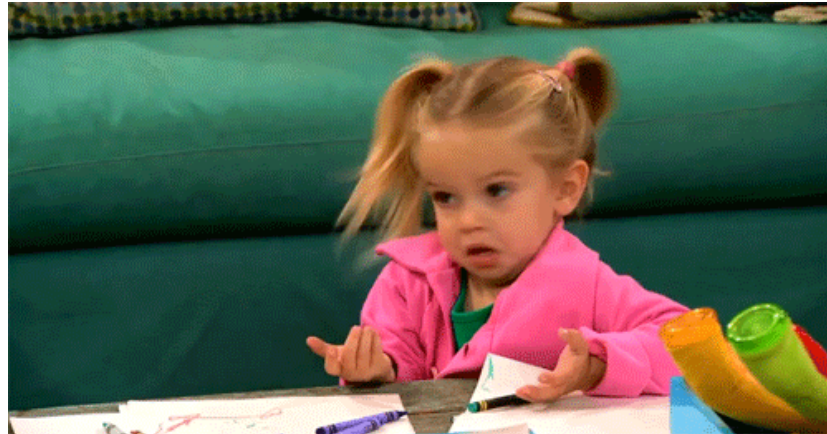


# Why bother?





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# Contents

usability features:

1) folder and file structure

2) error-free importing and installation

3) isolated, protected code

4) readability



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1) folder and file structure

2) error-free importing and installation

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4) readability





?

Folder structure

code

algorithm.py

calculations.py

data.npy

figure (1).png

figure (2).png

figure (3).png

figure.png

params.npy

processing.py

result.h5

run.ipynb

run.py

tests.py

tools.py

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  - algorithm.py
  - calculations.py
  - processing.py
  - tools.py
  - > data
  - > figures
  - LICENSE
  - pyproject.toml
  - README.md
  - > results
  - > scripts/notebooks
  - setup.cfg
  - > tests



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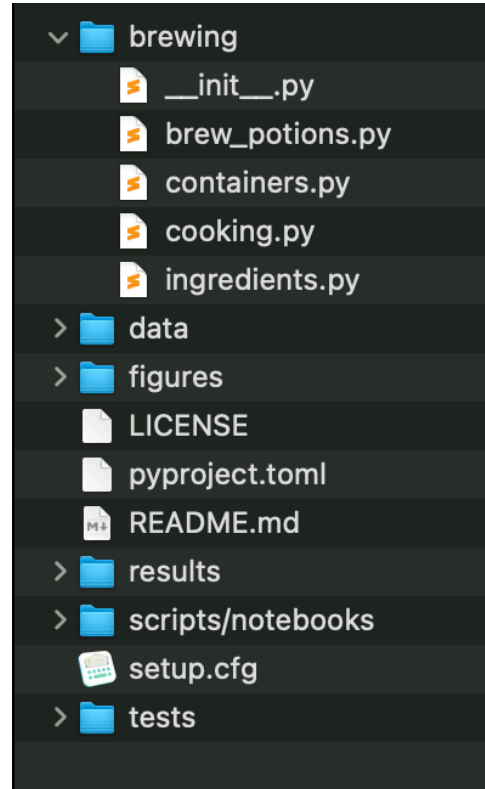
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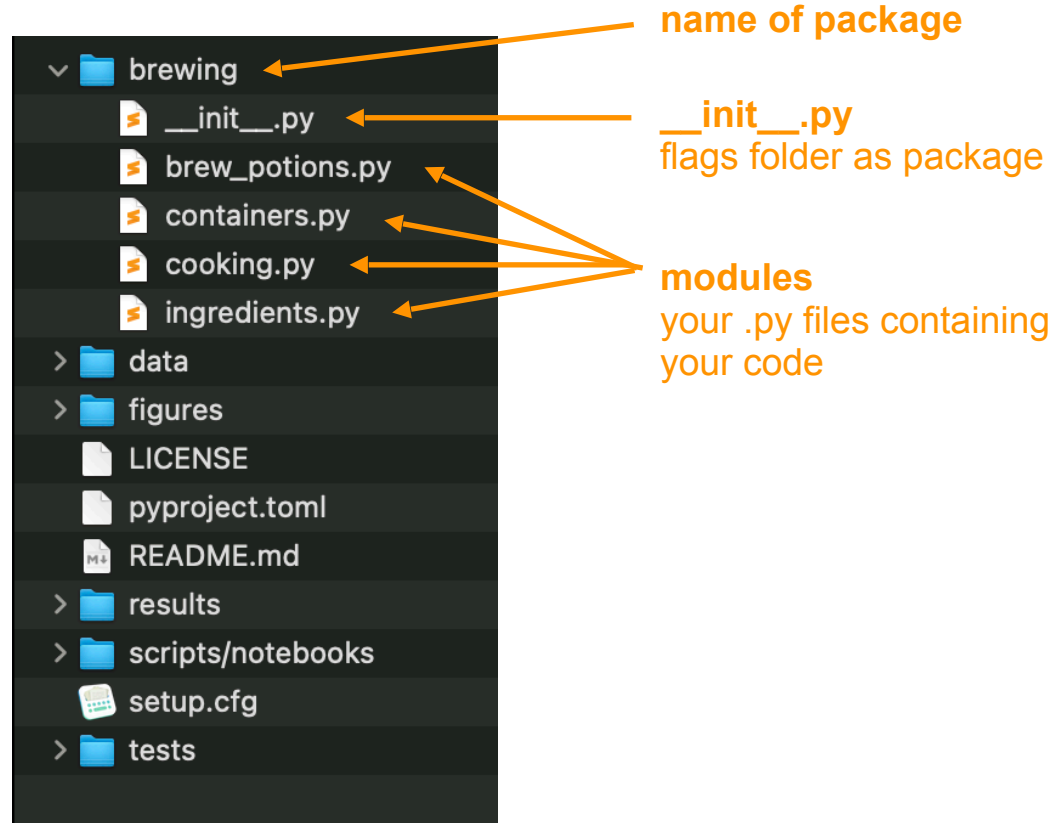
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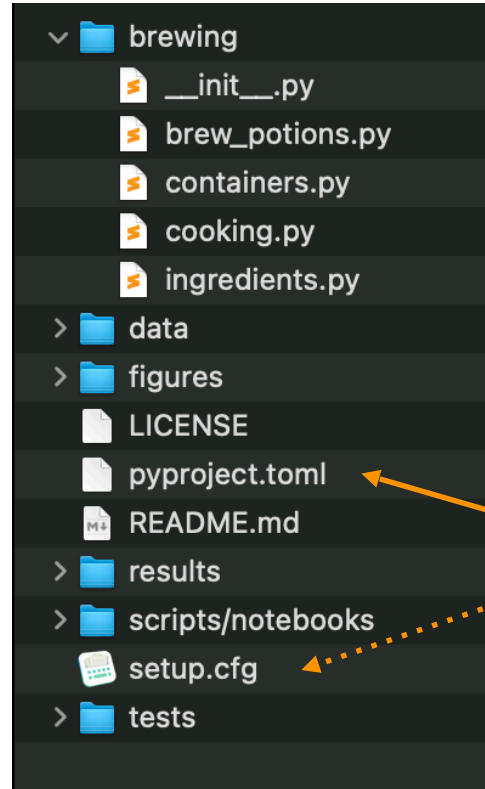
# Python package structure



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**name of package**

**`__init__.py`**  
flags folder as package

**modules**  
your .py files containing  
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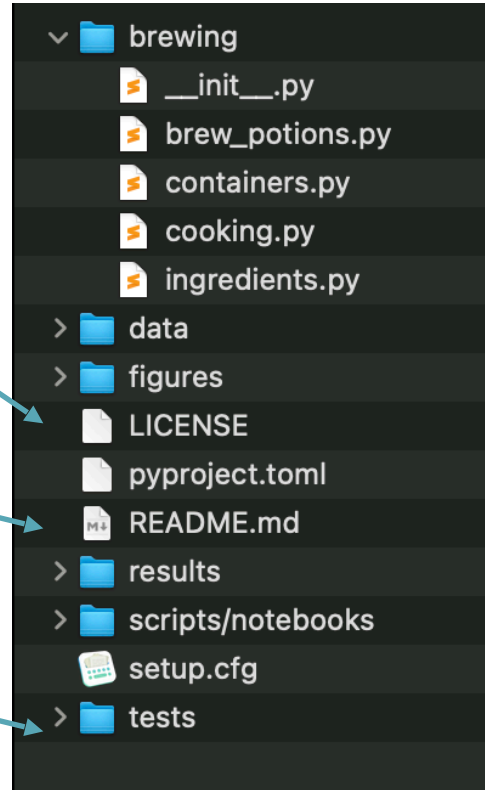
**build instructions &  
package metadata**  
will explain more later :)

# Python package structure

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**README**  
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# Advantage 1

—> know where to find items

e.g. wardrobe

- suit, shirts
- towels
- socks

same concept applies to code

—> use meaningful  
file names



# Advantage 2

- it makes all of your code **installable\***
- which makes all of your code **importable**

```
Terminal
> pip install brewing
>
> python
>>> import brewing
>>> brewing.brew_a_potion()
```

\* (need a few other changes we will go over)

# Advantage 2

- it makes all of your code **installable\***
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Importing

# Brewing package

- content of brewing package
  - walk through code
  - run `brew_potions.py`
  - point out files for exercise

**brewing  
package**

# Importing



- Follow the instructions in  
**Exercise 1 Importing.md**

(There is no need to submit a pull request for this exercise)

# names & mains

any code running under `if __name__ == "__main__":`

- will be ignored when importing
- will be executed when the module is run as a script

```
if name == "__main__":  
    i_will_not_be_imported = True  
    print("Not printing when importing")  
    print("But printing when run as script")
```

# Importing code

- you can always import code from your **current directory**
  - by calling `import brew_potions`, Python will look for
    - a module called `brew_potions.py` inside the **current directory**
    - a package called `brew_potions` inside in the **current directory** (= folder called `brewing` with an `__init__.py` file)
- Importing a module will execute all the code in the module (including imports, print statements)



# Importing modules

- you can always import code from other modules (.py files) in your ***current directory***
- Options for e.g. importing *eternal\_flame*

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1. `import cooking`

2. `import cooking as cook`

3. `from cooking import eternal_flame`

4. `from cooking import *`

# Importing modules

- you can always import code from other modules (.py files) in your **current directory**
- Options for e.g. importing *eternal\_flame*

1. `import cooking` + `cooking.eternal_flame`

2. `import cooking as cook` + `cook.eternal_flame`

3. `from cooking import eternal_flame` + `eternal_flame`

4. `from cooking import *` + `eternal_flame`

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2. <code>import cooking as cook</code>	+ <code>cook.eternal_flame</code> + <code>cook.fire</code>
3. <code>from cooking import eternal_flame</code>	+ <code>eternal_flame</code> X <code>fire</code>
4. <code>from cooking import *</code>	+ <code>eternal_flame</code> + <code>fire</code>

# Importing a package

- you can always import a package located in your current directory
- Modules in the package are bound to the package name

1. `import package`

2. `import package.module`

3. `from package.module import  
object`

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1. `import package`

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2. `import package.module`

+ `package.module.object`

3. `from package.module import  
object`

+ `object`

# Importing



- Thought(?) exercise:  
**Exercise 1 Importing.md**

Is there a way to get

*a) any 2*

*b) all 3*

exercises to work simultaneously?



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editable installation

# Knowledge needed

- **what packages are available?**
- what does an editable pip installation do?
- what are the requirements for this?

# Available packages

- **core packages** e.g. time, math, os, ...  
(come with Python, no installation needed)
  - **installed packages** e.g. numpy, scipy, ...  
(packages are downloaded to a system location  
e.g. /Library/Frameworks/Python.framework/Versions/3.9/lib/python3.9/site-packages  
which is on the Pythonpath => Python can find it)
  - **current directory**
- All packages which fall under these categories can be imported

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# Installing other packages

- Options to install a package using **pip**

**Option 1:** if package is included in PyPI

```
pip install numpy
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**Option 2:** install from a VCS like git

```
pip install git+https://github.com/<user>/<package-name>.git
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# Installing other packages

- You can install Python packages in your terminal using a package manager

## **pip**

standard package manager for  
Python

can install packages from PyPI  
(Python Package Index) or from VCS  
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open source package manager/  
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# Pip editable install

You can import the package you are currently working on as if it were a package you downloaded.

—> This lets you use your own code as any other package you installed

Advantages:

1. you can **import** the objects in the package **from any directory**  
(no longer bound to the directory which contains the package)
2. at the same time you can keep your project in your current directory
3. you use your code as someone else would use it, which forces you to write it in a more usable way

# Importing own project

- Options to install a package using **pip**

**Option 1:** if package is included in PyPI

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pip install numpy
```

**Option 2:** install from a VCS like git

```
pip install git+https://github.com/<user>/<package-name>.git
```

**Option 3:** install your package with -e (--editable) option

```
pip install -e <path-to-package>
```

# Knowledge needed

- what packages are available?
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# Knowledge needed

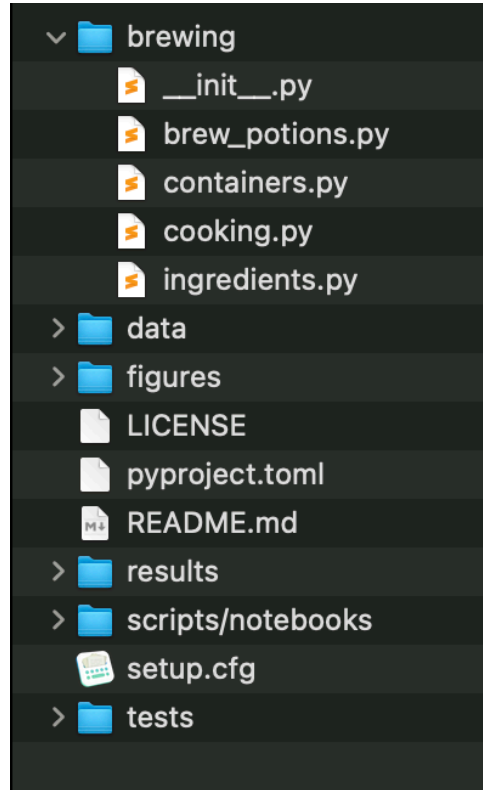
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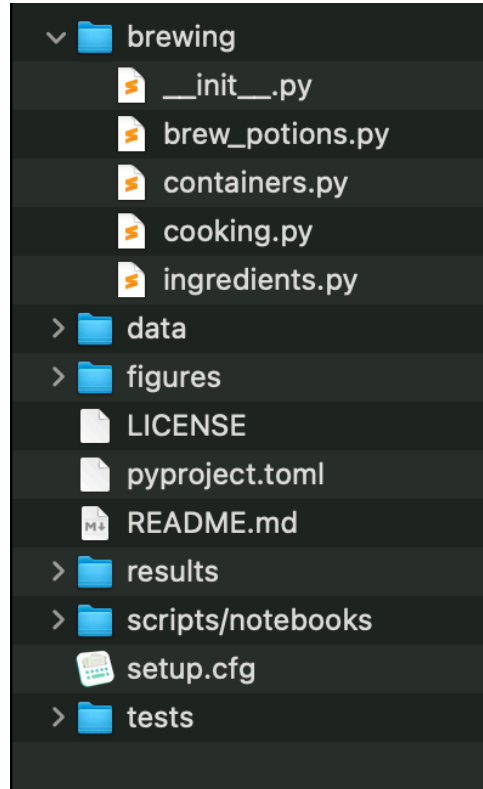
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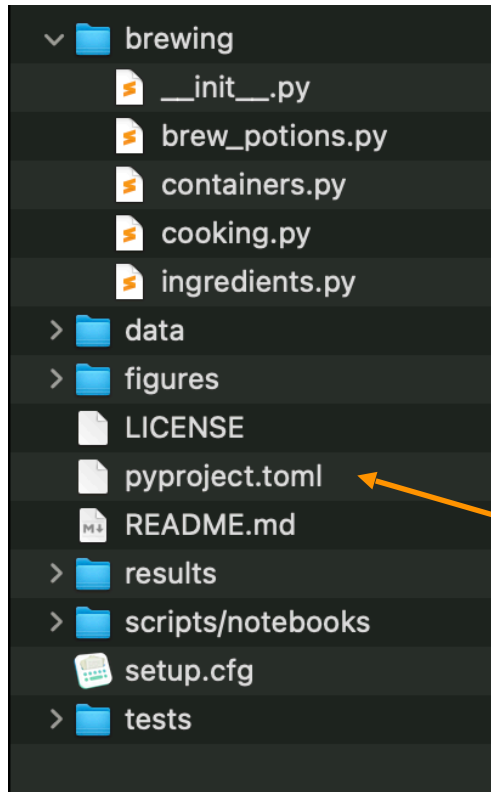
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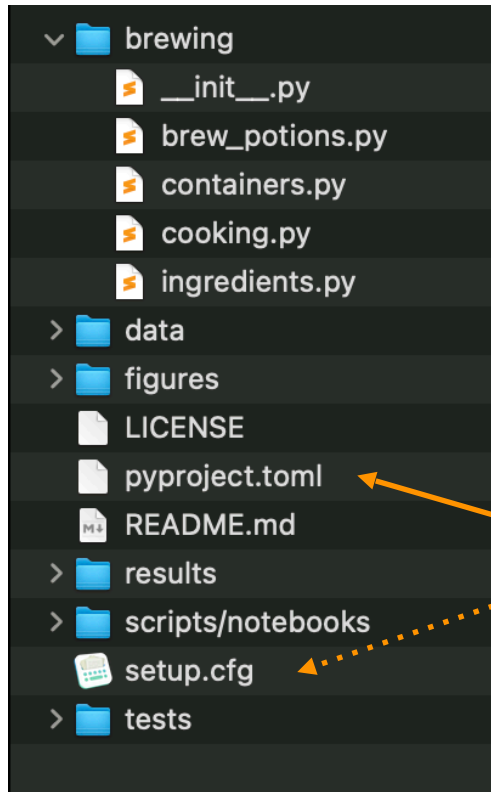
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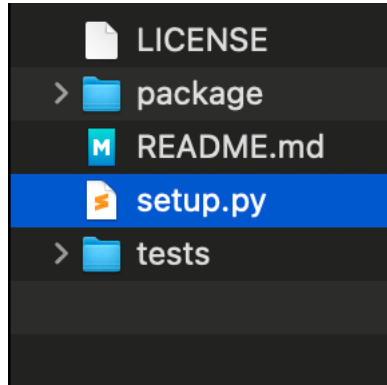
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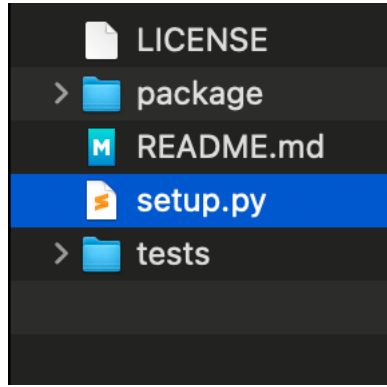
how it started



still the case for a lot of  
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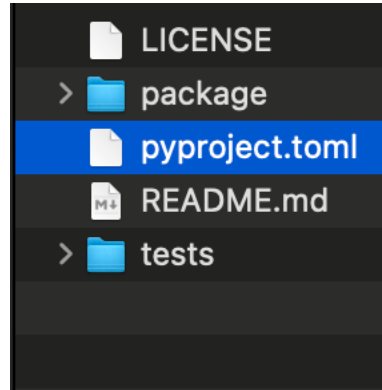
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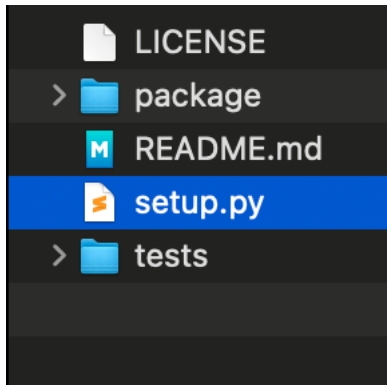
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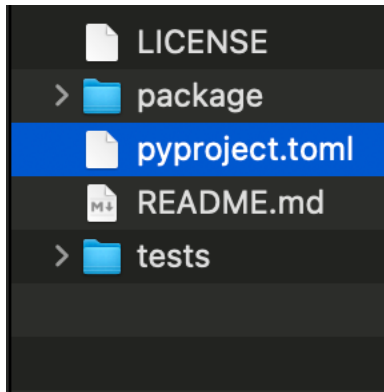
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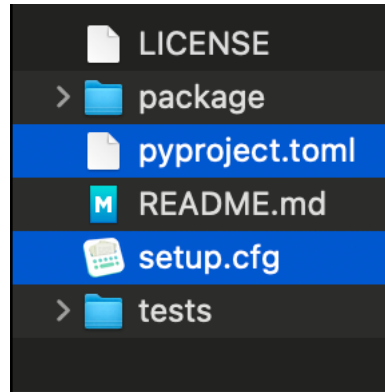
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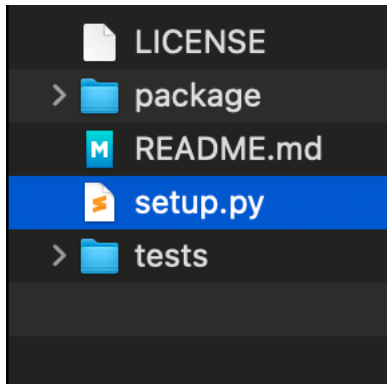
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pyproject.toml currently  
not supported across all  
systems for editable  
install, fix by adding an  
**empty** setup.cfg file

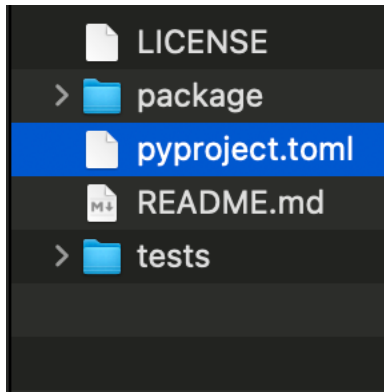
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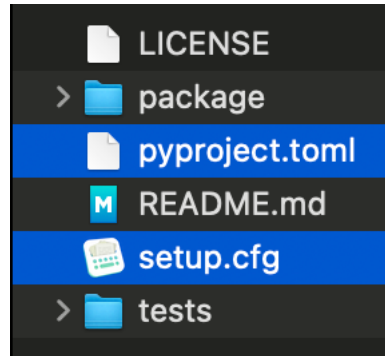
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-> can also go into separate requirements.txt file

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name = "brewing"
version = "0.1.0"
description = "a python package for brewing potions"
authors = [{ name = "H. Granger", email = "h.granger@hogwarts.ac.uk" }]
license = { file = "LICENSE" }
readme = "README.md"
requires-python = ">=3.7"
dependencies = ["numpy", "matplotlib >= 3.0.0", "pytest"]
classifiers = [
    "Programming Language :: Python :: 3",
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[tool.setuptools]
packages = ["brewing"]

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build-backend = "setuptools.build_meta"
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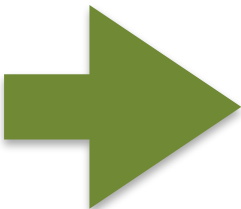
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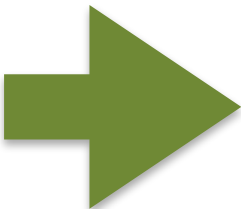
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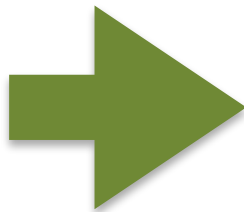
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- “build-system” defines which system is used to install the package
- “setuptools” is the default, but there are others, e.g. poetry
- No need to worry about the build system if there are no special requirements- BUT if you do change it, the necessary other keys may change (e.g. tools.setuptools key)



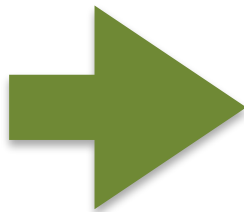
```
[project]
name = "brewing"
version = "0.1.0"
description = "a python package for brewing potions"
authors = [{ name = "H. Granger", email = "h.granger@hogwarts.ac.uk" }]
license = { file = "LICENSE" }
readme = "README.md"
requires-python = ">=3.7"
dependencies = ["numpy", "matplotlib >= 3.0.0", "pytest"]
classifiers = [
    "Programming Language :: Python :: 3",
    "License :: OSI Approved :: BSD License",
    "Operating System :: OS Independent"
]

[tool.setuptools]
packages = ["brewing"]

[build-system]
requires = ["setuptools>=42"]
build-backend = "setuptools.build_meta"
```

# pyproject.toml

- “build-system” defines which system is used to install the package
- “setuptools” is the default, but there are others, e.g. poetry
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    "Programming Language :: Python :: 3",
    "License :: OSI Approved :: BSD License",
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]

[tool.setuptools]
packages = ["brewing"]

[build-system]
requires = ["setuptools>=42"]
build-backend = "setuptools.build_meta"
```

# Pip editable installation



- `pip install -e <path-to-folder-above-brewing>`

or in the directory above brewing

```
pip install -e .
```

- Follow the instructions in  
**Exercise: Editable installation**

(There is no need to submit a pull request for this exercise)



?

how to develop code if it's in a package

# Using the editable installation

- You set your imports once and then never worry about them again
- You have not lost any capability, you only gained usability
- If you absolutely must use notebooks, then you can import your code from your modules into your notebook much easier

# Workflow (realistic?)

## ① Create

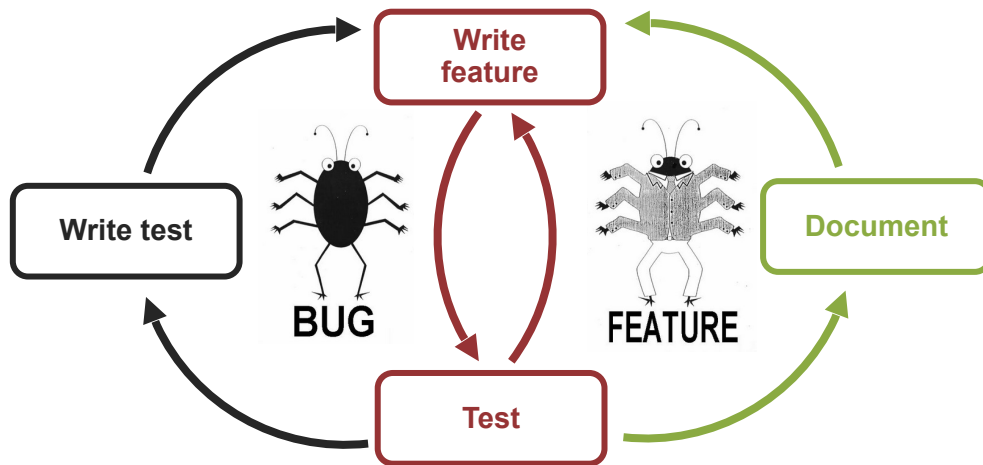
Set up structure

Create files:

```
__init__.py  
pyproject.toml  
setup.cfg  
README  
LICENSE
```

Make installable  
at this point

## ② Build & Test



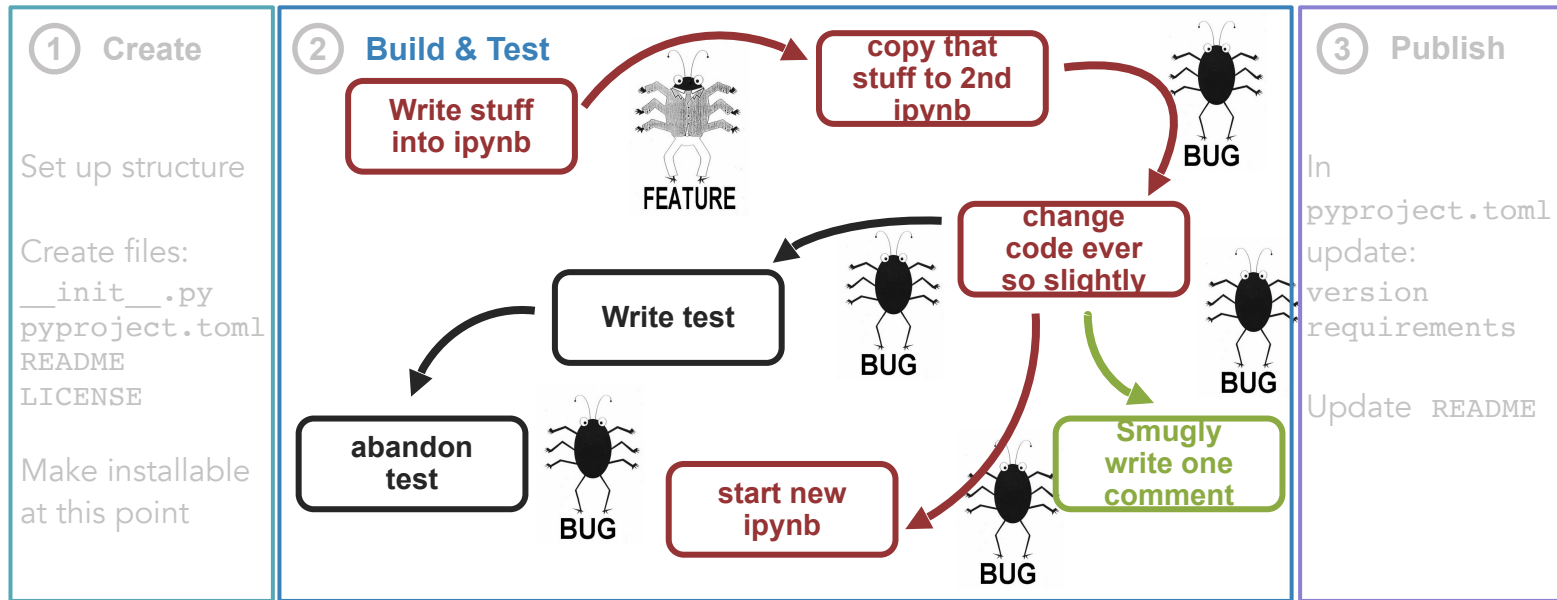
## ③ Publish

In  
`pyproject.toml`  
update:  
version  
requirements

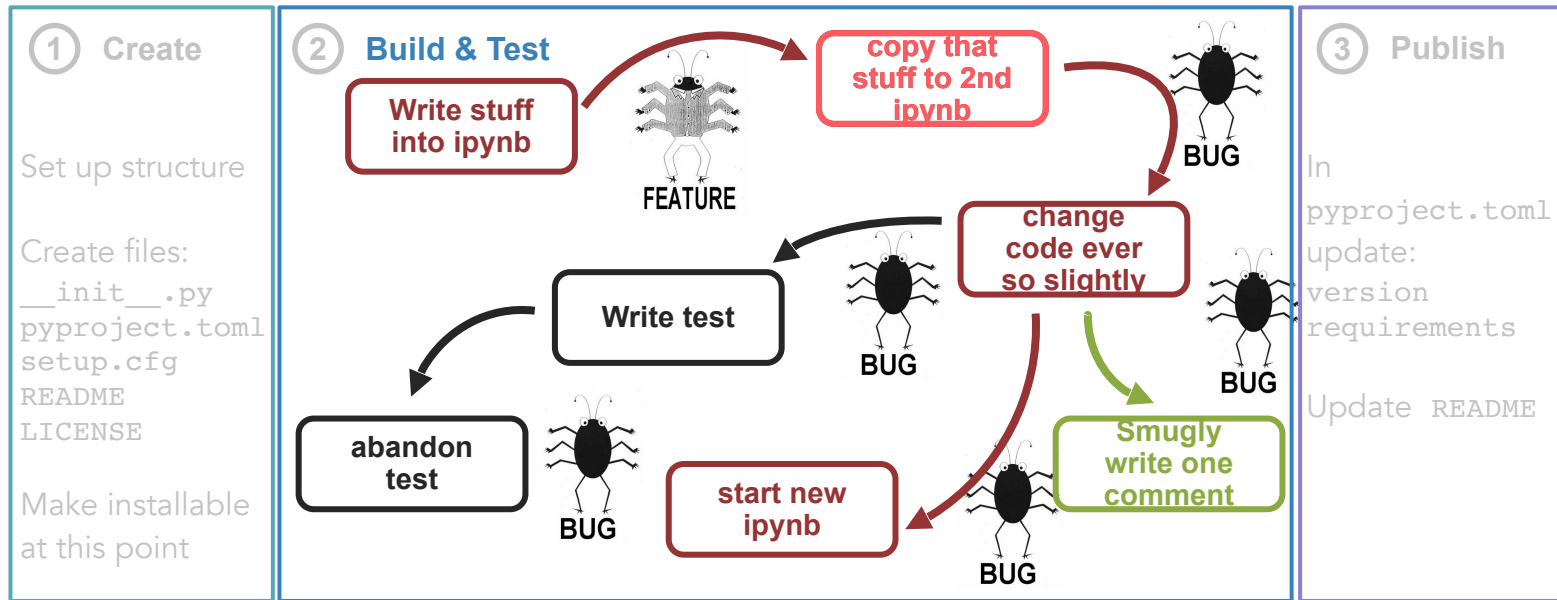
Update README



# Workflow (realistic?)



# Workflow (realistic?)



# Workflow (realistic?)

## ① Create

Set up structure

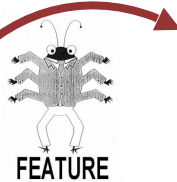
Create files:

```
__init__.py  
pyproject.toml  
setup.cfg  
README  
LICENSE
```

Make installable  
at this point

## ② Build & Test

Write stuff  
into ipynb



## ③ Publish

```
In  
pyproject.toml  
update:  
version  
requirements
```

Update README

# Workflow (realistic?)

## ① Create

Set up structure

Create files:

```
__init__.py  
pyproject.toml  
setup.cfg  
README  
LICENSE
```

Make installable  
at this point

## ② Build & Test

Write stuff  
into ipynb



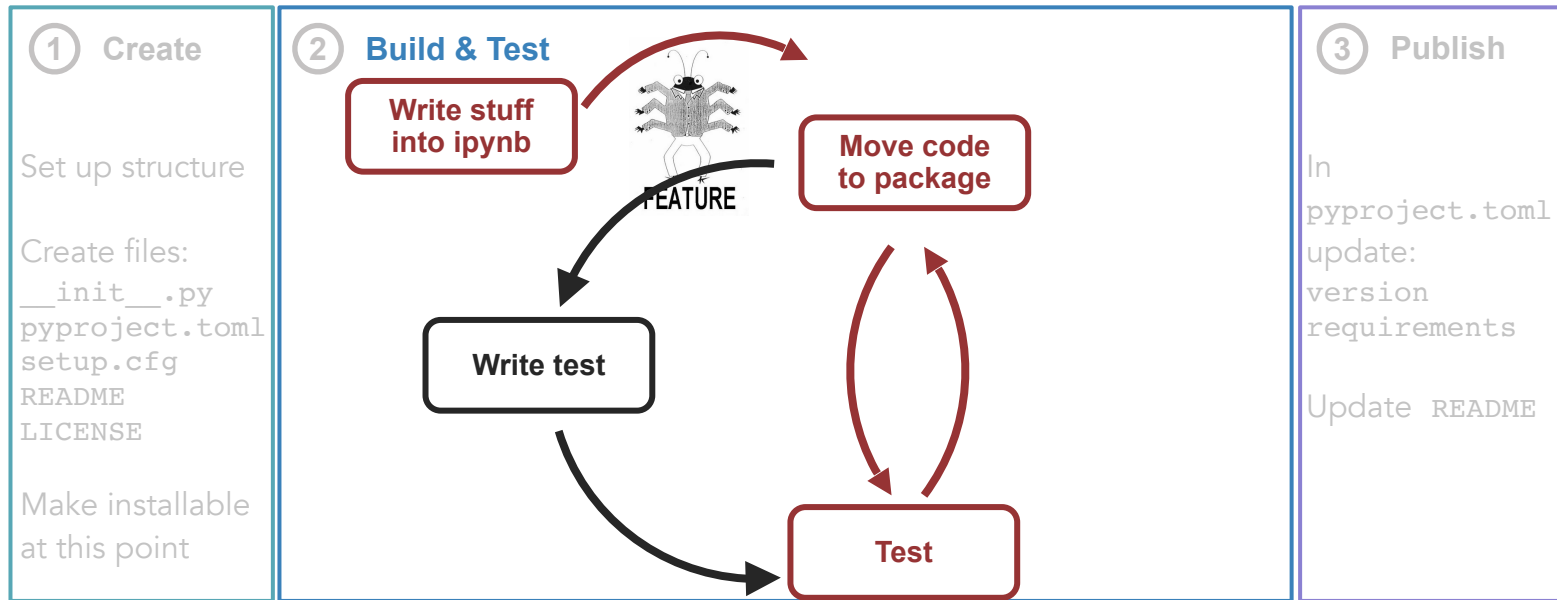
Move code  
to package

## ③ Publish

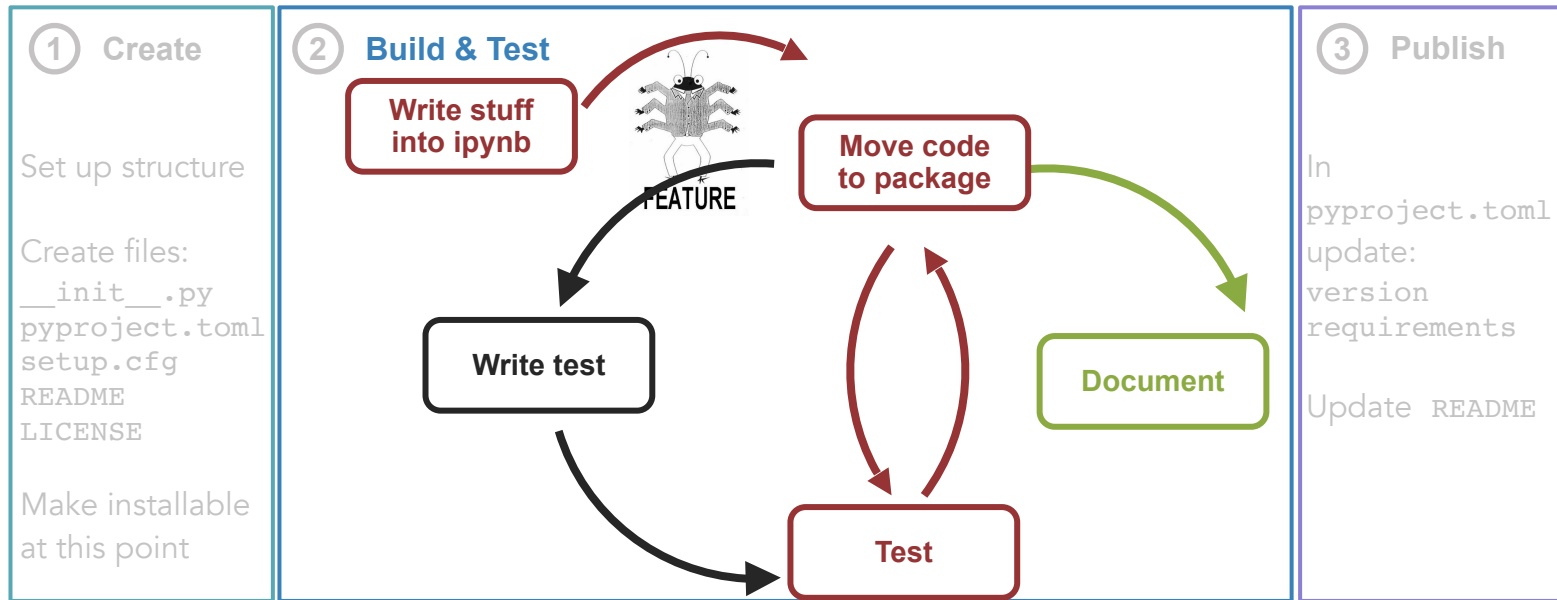
```
In  
pyproject.toml  
update:  
version  
requirements
```

Update README

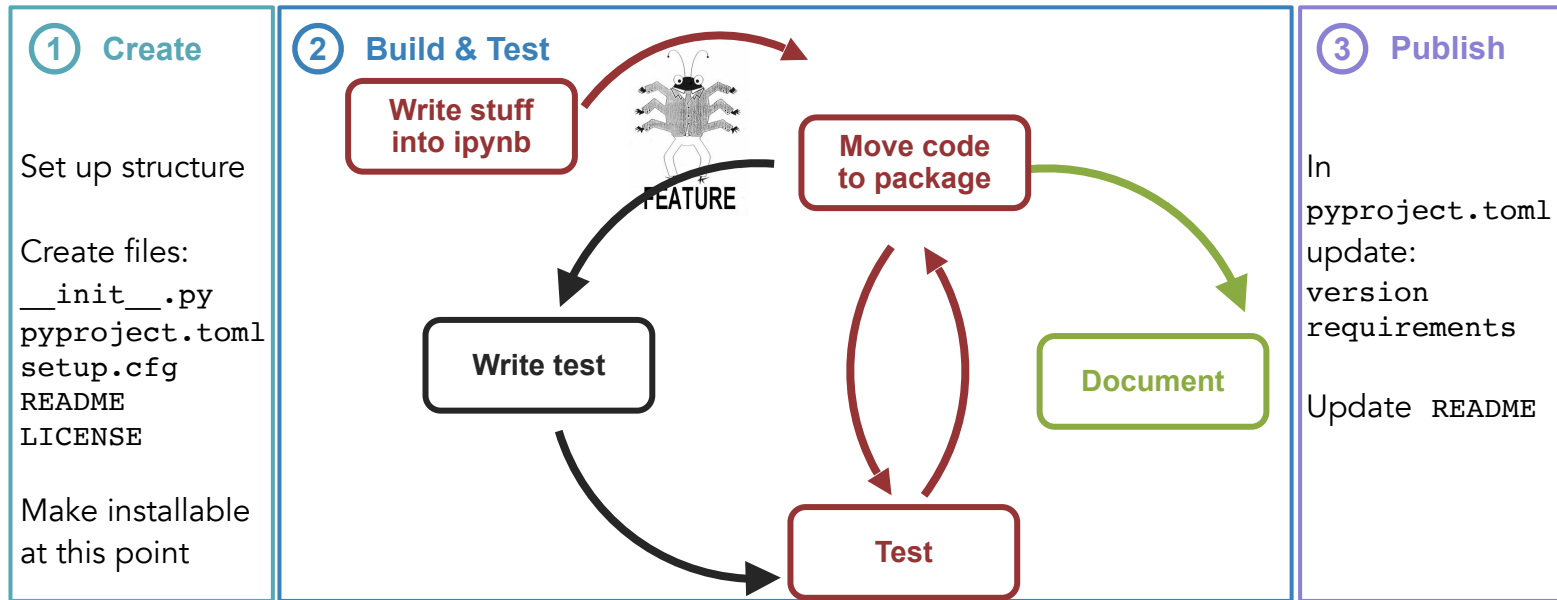
# Workflow (realistic?)



# Workflow (realistic?)



# Workflow (realistic?)



# Write your function

- Write the last remaining **potion making function** we need before sharing the package



Exercise:

- Create a branch with a unique name
- Follow the instructions in **Exercise 3 Workflow** to write and test a function to make a “Python expert” potion
- Create a Pull Request





?

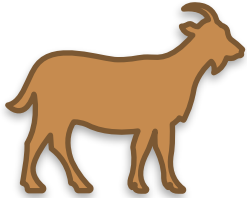
defend your code

# Why environments?

## Project 1

= 1st year

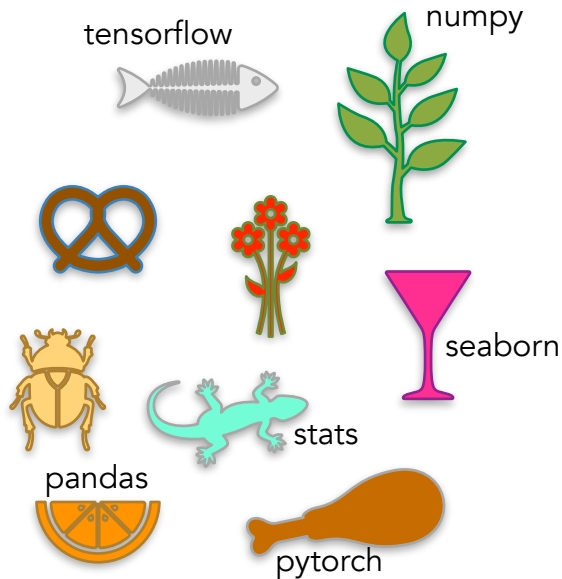
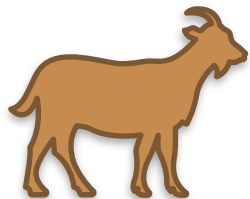
PhD project



# Why environments?

## Project 1

= 1st year  
PhD project

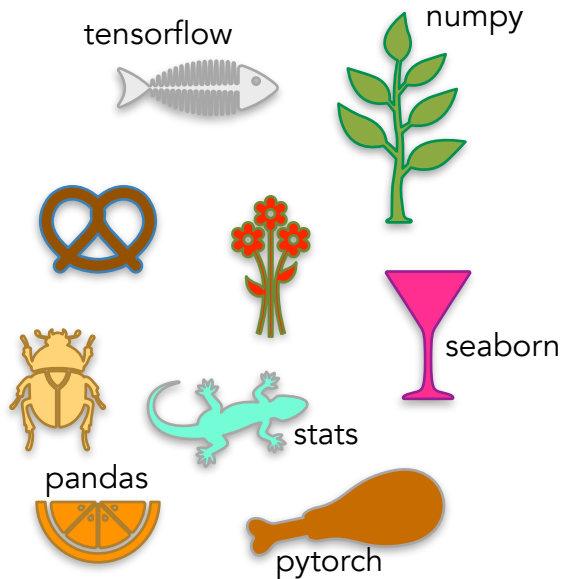
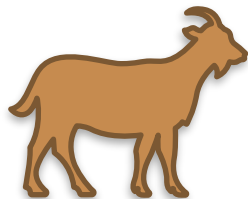


dependencies

# Why environments?

## Project 1

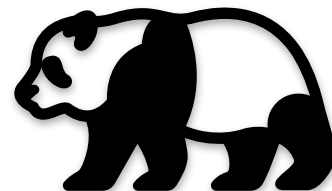
= 1st year  
PhD project



dependencies

## Project 2

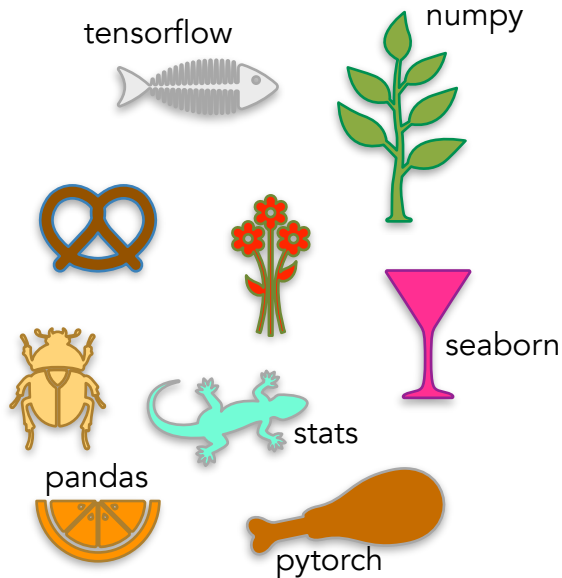
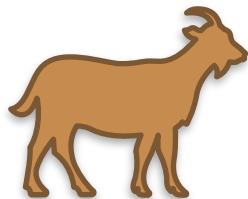
= collaboration  
with another lab



# Why environments?

## Project 1

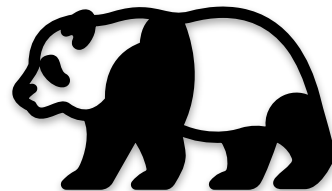
= 1st year  
PhD project



dependencies

## Project 2

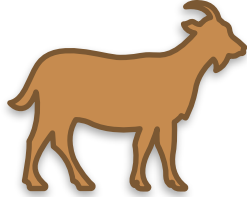
= collaboration  
with another lab



# Why environments?

## Project 1

= 1st year  
PhD project



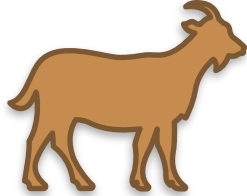
pandas = 1.2.4

dependencies

# Why environments?

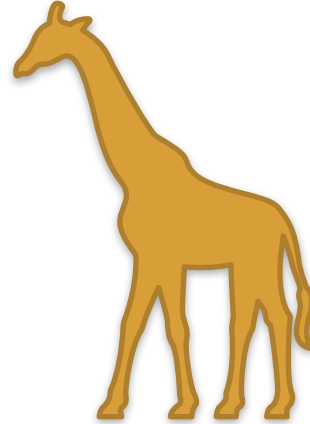
## Project 1

= 1st year  
PhD project



pandas = 1.2.4

dependencies



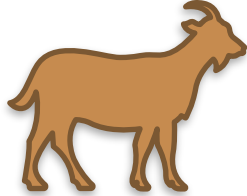
## Project 2

= 2nd year  
PhD project

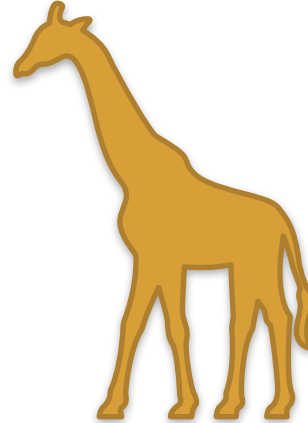
# Why environments?

## Project 1

= 1st year  
PhD project



pandas = 1.3.0



## Project 2

= 2nd year  
PhD project

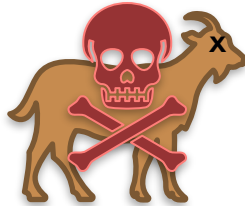
dependencies



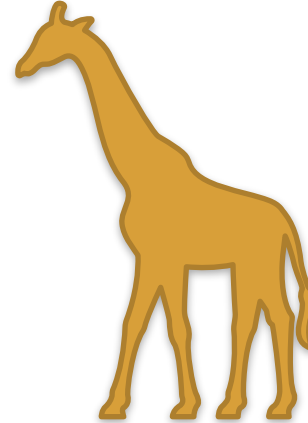
# Why environments?

## Project 1

= 1st year  
PhD project



pandas = 1.3.0



## Project 2

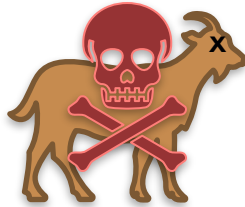
= 2nd year  
PhD project

dependencies

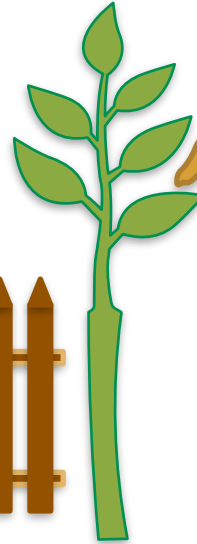
# Why environments?

## Project 1

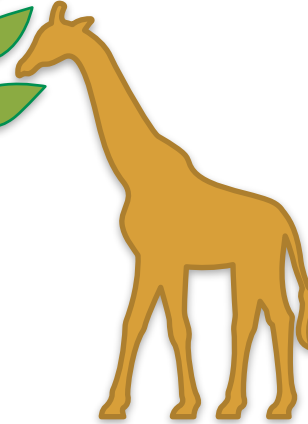
= 1st year  
PhD project



pandas = 1.2.4



pandas = 1.3.0



dependencies

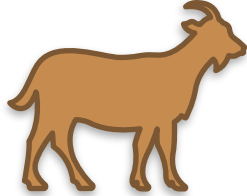
## Project 2

= 2nd year  
PhD project

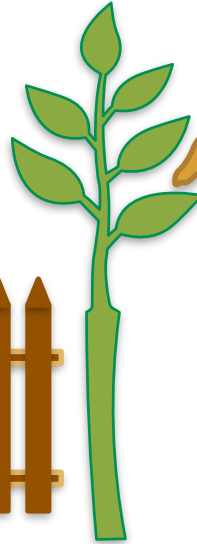
# Why environments?

## Project 1

= 1st year  
PhD project



pandas = 1.2.4



pandas = 1.3.0



## Project 2

= 2nd year  
PhD project

dependencies

# Breaking changes

- Ever ignored a one of these?

```
<stdin>:1: FutureWarning: In a future version of pandas all arguments of concat except for the argument 'objs' will be keyword-only
```

- This means that if you keep updating your python packages, you will run into issues at some point
  - code errors
  - unexpected results

*Previous behavior:*

```
In [1]: df.groupby('label1').rolling(1).sum()
Out[1]:
```

	a	b
label1		
idx1	1.0	2.0

*New behavior:*

```
In [61]: df.groupby('label1').rolling(1).sum()
Out[61]:
```

		a	b	
label1	label1	label2		
idx1	idx1	idx2	1.0	2.0

# Virtual Environments

What is a virtual environment?

- A semi-isolated python environment -> you cannot access packages (libraries and their dependencies) installed in other environments.
- packages are installed inside a project-specific virtual environment folder (not added to general python path)
- If you break something, you can delete those folders and start over

# Virtual Environments



- Create and activate a virtual environment following the directions in **Exercise 5 Virtual Environments.md**



- See what changed with regard to the Python interpreter and the installed packages

# Additional advantages

- If you package your code, in your `pyproject.toml` you will have a record of at least one working combination of the versions of your dependency packages

# Additional advantages

- If you package your code, in your pyproject.toml you will have a record of at least one working combination of the versions of your dependency packages





# Environment Managers

- **venv** - current standard recommended by Python
- **poetry** - super useful (if it works o.0).  
solves dependency conflicts, creates pyproject.toml for you,  
keeps record of all dependency versions in committable file
- **pyenv** - if you need different Python versions in different projects



?

readability

# Documentation

- Documenting your code provides a way of making you code **usable for future you and others**
  - **Comments** (#): describe what a line (or multiple lines of code do); notes to self
  - **Function/method docstring** (''' '''): purpose of function + params / return
  - **Module docstring** (''' '''): what's in this file

```
""" Module docstring """  
  
def add_points(house_points,  
               points=0):  
    """ Function docstring."""  
    # comment  
    points += 1000  
    return house_points + points
```

# NumPy style

- triple double quotes below declaration
- The first line should be a short description
- If more explanation is required, that text should be separated from the first line by a blank line
- Specify Parameters and Returns as  
    name : type  
        description  
(put a line of --- below sections)
- Each line should begin with a capital letter and end with a full stop
- access docs:  
    pydoc3 <module>.<object>

```
""" This module demonstrates docstrings. """

def add_points(house, house_points, points=0):
    """ Adds up points for house cup.

    If the house is Gryffindor, Dumbledore adds
    1000 points no matter what.

    Parameters
    -----
    house_points : int
        Current house cup score.
    points : int, optional
        New points to be added/ subtracted.

    Returns
    -----
    int
    """
    if house == "Gryffindor":
        points += 1000
    return house_points + points
```

# Typing

- you can declare the type of the function argument
- the package *mypy* checks whether the types make sense
- Be aware that this might be a pain to maintain if you change your functions often and pass complicated objects...  
`tuple[int, dict[str, str]]`

```
""" This module demonstrates docstrings. """

def add_points(house: str,
               house_points: int,
               points: int = 0)
    -> int:
    """ Adds up points for house cup.

    If the house is Gryffindor, Dumbledore adds
    1000 points no matter what.

    Parameters
    -----
    house_points : Current house cup score.
    points : optional; New points to be added
    """
    if house == "Gryffindor":
        points += 1000
    return house_points + points
```

# Variable names

- name your variables so that you can later go back and \*read\* what the code does (same principle as with module names)

```
x = 10
```

```
p = 10
```

```
poi = 10
```

```
points = 10
```

```
points_add = 10
```

```
points_to_be_added = 10
```

# Variable names

- name your variables so that you can later go back and \*read\* what the code does (same principle as with module names)

```
x = 10  -> terrible
```

```
p = 10  -> just as terrible
```

```
poi = 10  -> still terrible
```

```
points = 10  -> better, but potentially unspecific
```

```
points_add = 10  -> possibly better, possible worse than the one before
```

```
points_to_be_added = 10  # clear, but maybe a bit long
```

# Variable names



# Variable names

```
added_points = [10, 5, 1]
# -> variable names use underscores

def add_points(house, house_points, points=0):
    if house == "Gryffindor":
        points += 1000
    return house_points + points
# -> function names also use underscores

def ScoreKeeper():
    def __init__(self):
        self.house_points = 0
        self._secret_bonus = 5

    def add_points(self, house, points):
        if house == "Gryffindor":
            points += 1000
        return house_points + points
# -> Class names use CamelCase
# -> private variables (intended for use only within the class) prepend "_"
```

# Document your function



- Document the function you just wrote according to the instructions in **Exercise 4 Documentation**.
- Use the same Pull Request



# Publishing code

- **Github/Gitlab**

- perfectly fine for publishing publication code
- perfectly fine for hosting research group code

- **PyPI: Python Package Index**

- if you want others to use your analysis/model/... you should try to have it on PyPI to make it easier for others to download and use

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?

Summary

# Contents



usability features:

## 1) folder and file structure

- standard Python package structure

## 2) error-free importing and installation

- editable pip installation

## 3) isolated, protected code

- virtual environments

## 4) readability

- documentation, typing, naming

# Contents

usability features:

## 1) folder and file structure

- standard Python package structure

## 2) error-free importing and installation

- editable pip installation

## 3) isolated, protected code

- virtual environments

## 4) readability

- documentation, typing, naming





# Mischief Managed

Any questions?





?

Extra material

# Module structure

- constants
- functions
- ...

# Importing modules

- you can always import code from other modules (.py files) in your **current directory**
- generally:

1. `import module-name` + `module-name.object`

2. `import module-name as abbr` + `abbr.object`

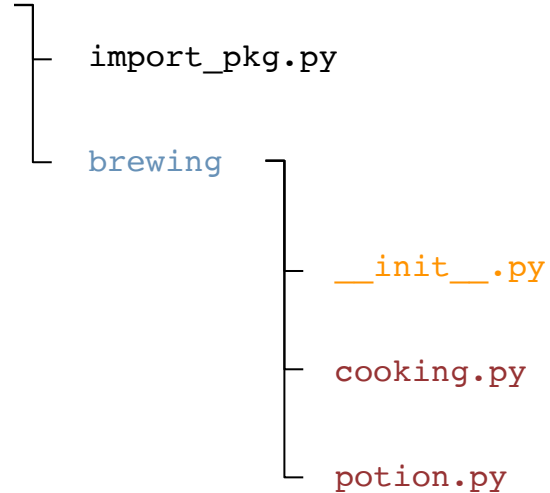
3. `from module-name import object` + `object`

4. ~~`from module-name import *`~~

# Order of execution

Terminal

```
> python3 import_pkg.py
```



# Order of execution

Terminal

```
> python3 import_pkg.py
```



import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

potion.py

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py  
import brewing
```



import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

potion.py

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py  
import brewing
```



import\_pkg.py

brewing

\_\_init\_\_.py

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# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py  
import brewing
```

import\_pkg.py

brewing



\_\_init\_\_.py

cooking.py

potion.py



# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py  
import brewing
```

import\_pkg.py

brewing



\_\_init\_\_.py

cooking.py

potion.py

```
# content of __init__.py
```

# Order of execution

Terminal

```
> python3 import_pkg.py
```



```
# content of import_pkg.py  
import brewing
```

import\_pkg.py

brewing

```
# content of __init__.py
```

`__init__.py`

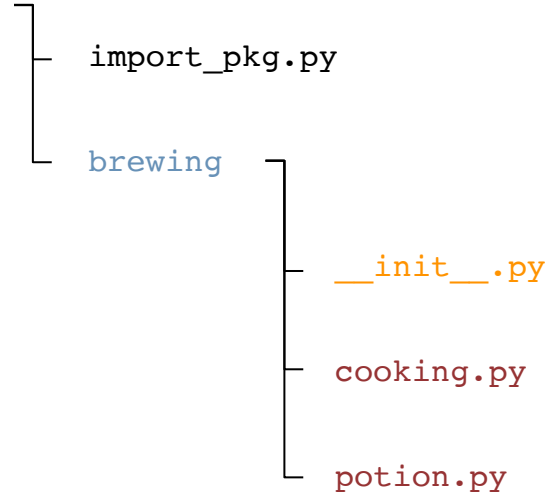
`cooking.py`

`potion.py`

# Order of execution

Terminal

```
> python3 import_pkg.py
```



# Order of execution

Terminal

```
> python3 import_pkg.py
```



import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

potion.py

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py  
import brewing.cooking
```



import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

potion.py

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py  
import brewing.cooking
```



import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

potion.py

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py  
import brewing.cooking
```

import\_pkg.py

brewing



\_\_init\_\_.py

cooking.py

potion.py

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py  
import brewing.cooking
```

import\_pkg.py

brewing



\_\_init\_\_.py

cooking.py

potion.py

```
# content of __init__.py
```



# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# content of import_pkg.py  
import brewing.cooking
```

import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

potion.py

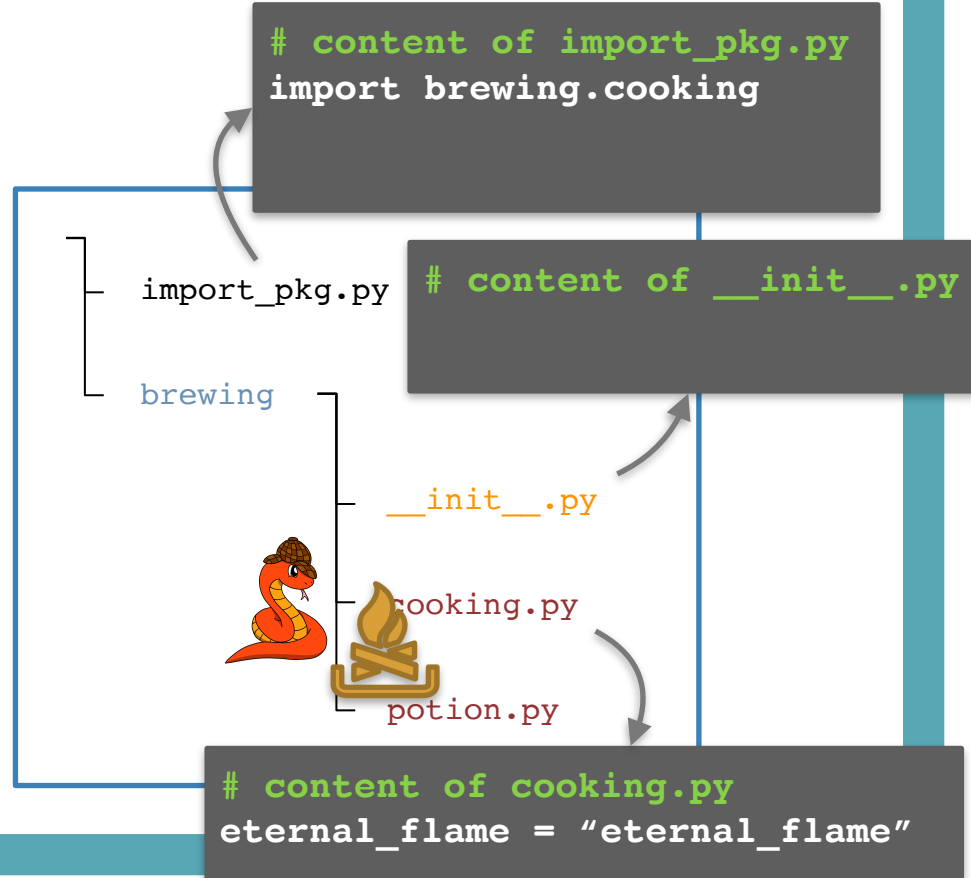


```
# content of __init__.py
```

# Order of execution

Terminal

```
> python3 import_pkg.py
```



# Order of execution

Terminal

```
> python3 import_pkg.py
```



```
# content of import_pkg.py  
import brewing.cooking
```

import\_pkg.py

brewing

```
# content of __init__.py
```

`__init__.py`

`cooking.py`

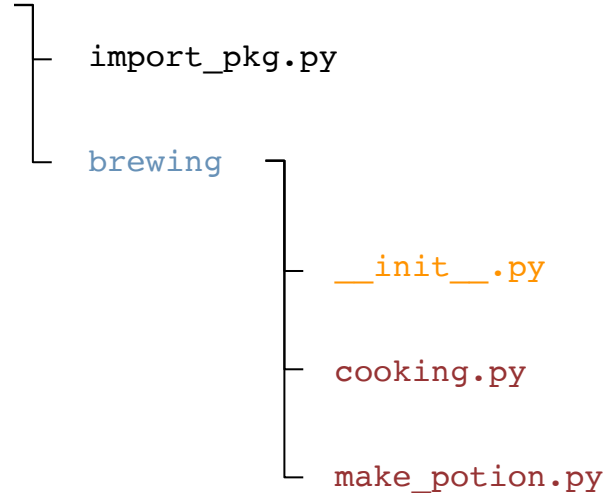
`potion.py`

```
# content of cooking.py  
eternal_flame = "eternal_flame"
```

# Order of execution

Terminal

```
> python3 import_pkg.py
```



# Order of execution

Terminal

```
> python3 import_pkg.py
```



import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

make\_potion.py

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# import_pkg.py  
import brewing.make_potion
```



import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

make\_potion.py

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# import_pkg.py  
import brewing.make_potion
```



import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

make\_potion.py

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# import_pkg.py  
import brewing.make_potion
```

import\_pkg.py

brewing



\_\_init\_\_.py

cooking.py

make\_potion.py



# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# import_pkg.py  
import brewing.make_potion
```

import\_pkg.py

brewing



\_\_init\_\_.py

cooking.py

make\_potion.py

```
# __init__.py
```

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# import_pkg.py  
import brewing.make_potion
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import\_pkg.py

brewing

\_\_init\_\_.py

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```
# __init__.py
```

# Order of execution

Terminal

```
> python3 import_pkg.py
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```
# import_pkg.py  
import brewing.make_potion
```

import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

make\_potion.py



```
# __init__.py
```

```
# make_potion.py  
import cooking  
stuff
```

# Order of execution

Terminal

```
> python3 import_pkg.py
```

```
# import_pkg.py  
import brewing.make_potion
```

import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

make\_potion.py



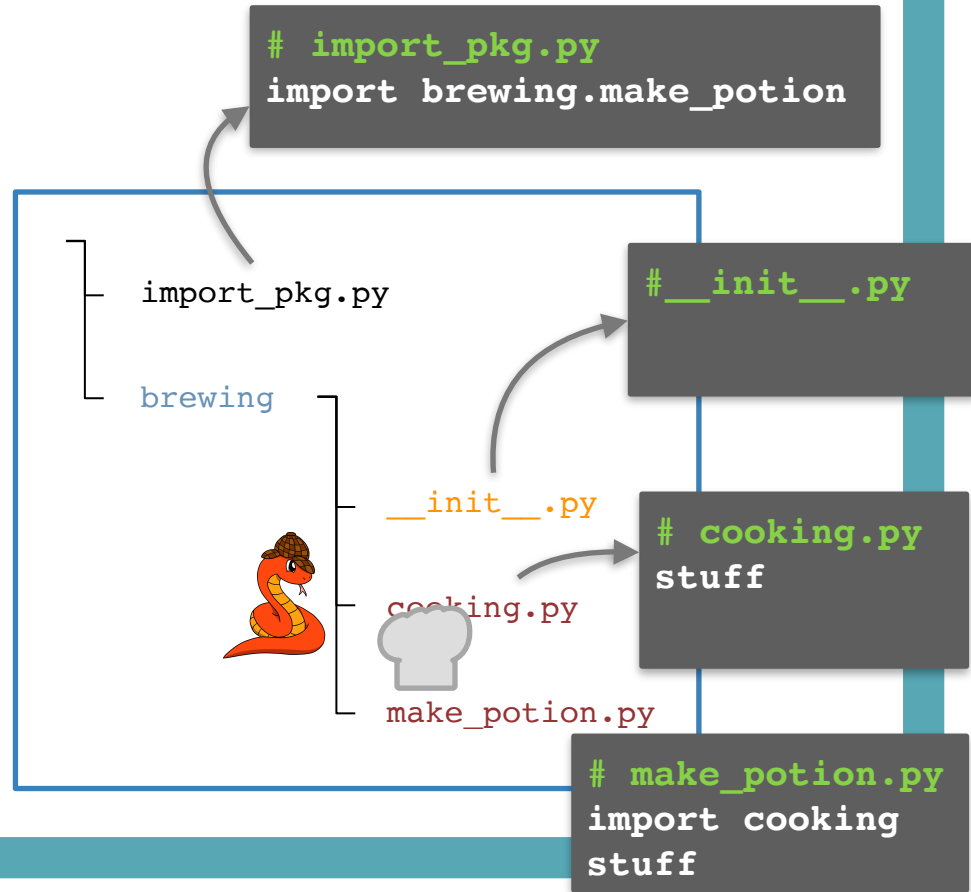
```
# __init__.py
```

```
# make_potion.py  
import cooking  
stuff
```

# Order of execution

Terminal

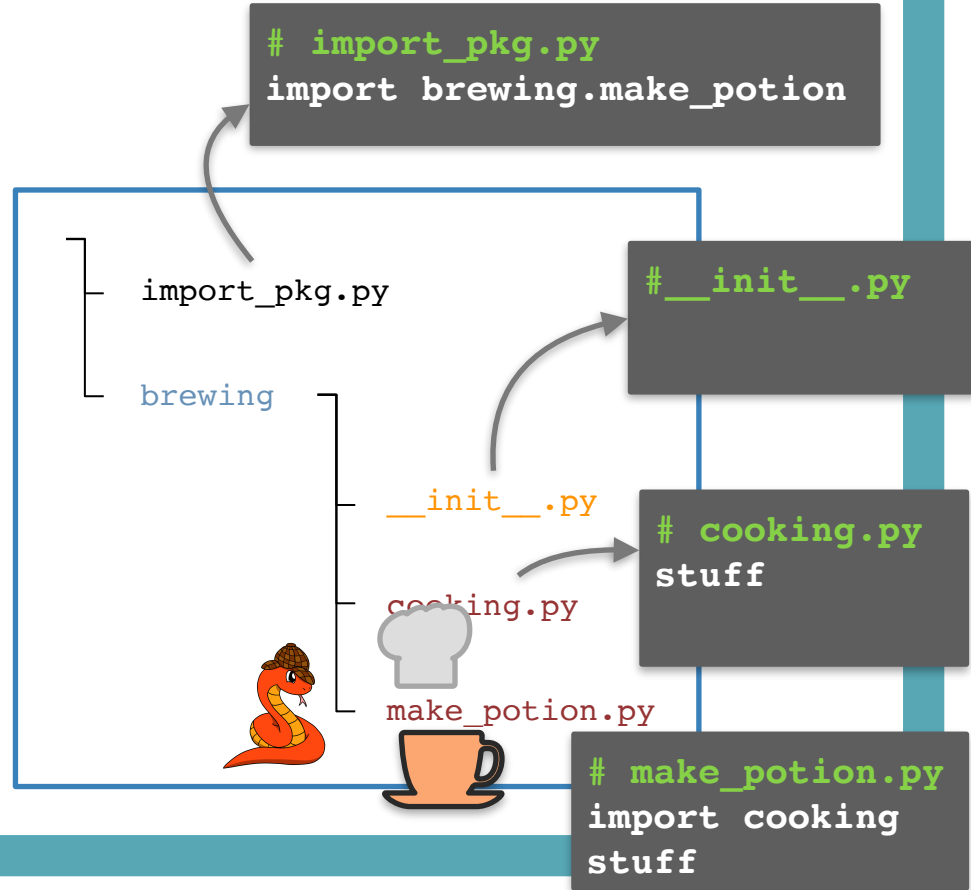
```
> python3 import_pkg.py
```



# Order of execution

Terminal

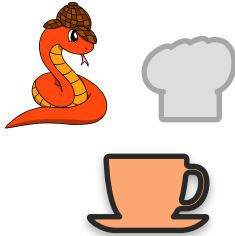
```
> python3 import_pkg.py
```



# Order of execution

Terminal

```
> python3 import_pkg.py
```



```
# import_pkg.py  
import brewing.make_potion
```

import\_pkg.py

brewing

\_\_init\_\_.py

cooking.py

make\_potion.py

```
# __init__.py
```

```
# cooking.py  
stuff
```

```
# make_potion.py  
import cooking  
stuff
```

# Keeping track of docstrings

- Most commonly used hosting websites: facilitate building, versioning, and hosting
  - [github.io](https://github.io)
  - [readthedocs.org](https://readthedocs.org)
- Automate documentation
  - [Sphinx](#): a package to collect docstrings and create a nicely formatted documentation website