Computational practicum Q2 Lecture 1 Advanced python programming

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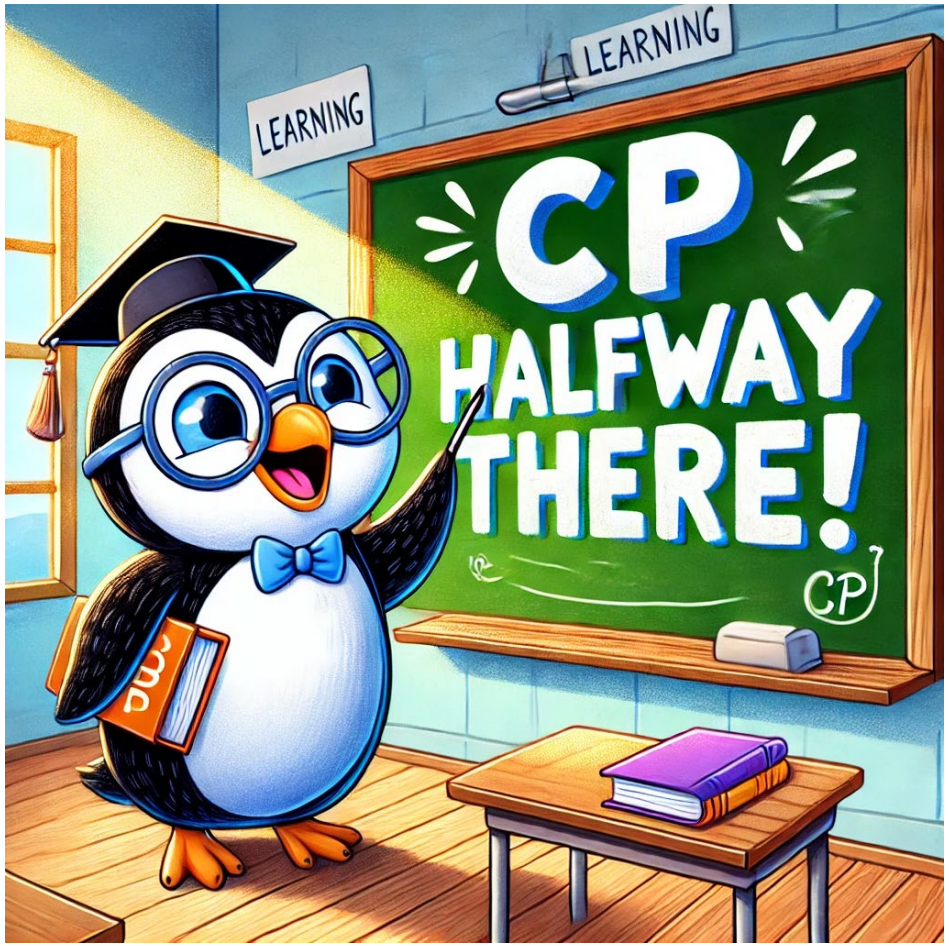
Welcome to Q2

- We hope you enjoyed the first half of the class so far!
- We also hope you had a successful Q1 exam!



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Lecture overview Q2

- Lecture 1: Advanced programming
- Lecture 2: Partial differential equations, finite difference method
- Lecture 3: Partial differential equations in multiple space dimensions and time
- Lecture 4: Optimization 1
- Lecture 5: Optimization 2
- Lecture 6: Regression, interpolation, least squares
- Lecture 7: Use of LLMs in Chemical Engineering

Agenda

- **Recap Q1**
- **Feedback Q1**
- **Advanced programming**
  - Some fundamental programming principles
  - Managing imports, packages, virtual environments
  - Managing multiple modules
  - Basic object-oriented programming
  - Unit testing

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Recap Q1

- In Q1, you learned:
  - The basics of Python programming, linear algebra, and calculus
  - Solving linear systems of equations
  - Solving nonlinear systems of equations
  - Numerical integration and differentiation
  - Solving initial value problems
  - Solving boundary value problems with the finite difference method
  - Solving boundary value problems with the shooting method

Learning goals of this lecture

After successfully completing this lecture, you are able to…

- explain basic programming principles.
- explain package management and why it is important.
- design a bigger coding project with multiple modules and packages of your own.
- apply object-oriented programming in your code.
- formulate simple test functions to ensure the functionality of your code.

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Advanced programming: motivation and challenge

- Coding is easy, but coding well is hard.
- Large programs become very complex fast.
  A model of a methanol plant can have
  > 2000 lines!!
- Big challenge with respect to:
  - Readability (others and yourself)
  - Maintainability
  - Reusability

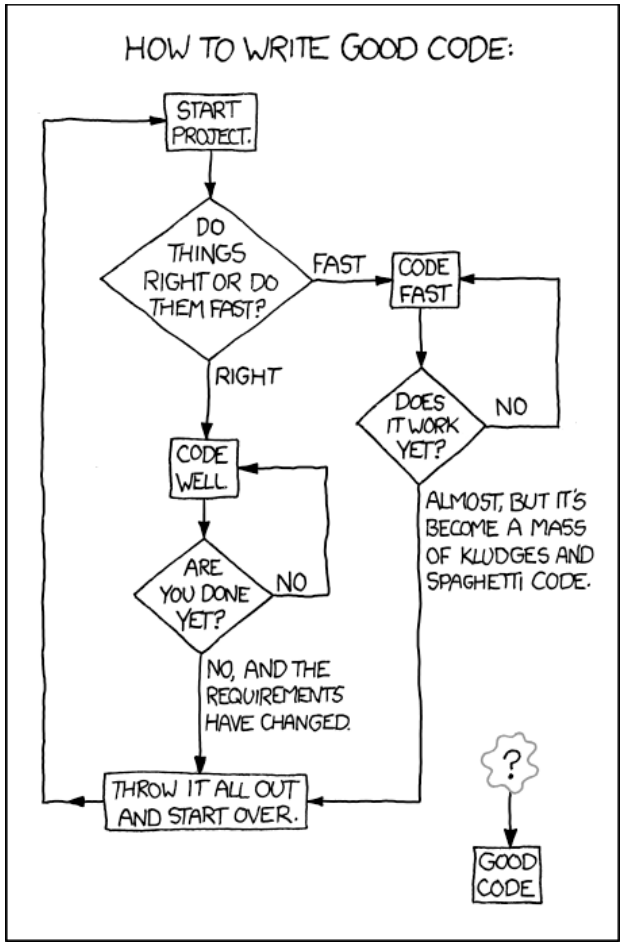
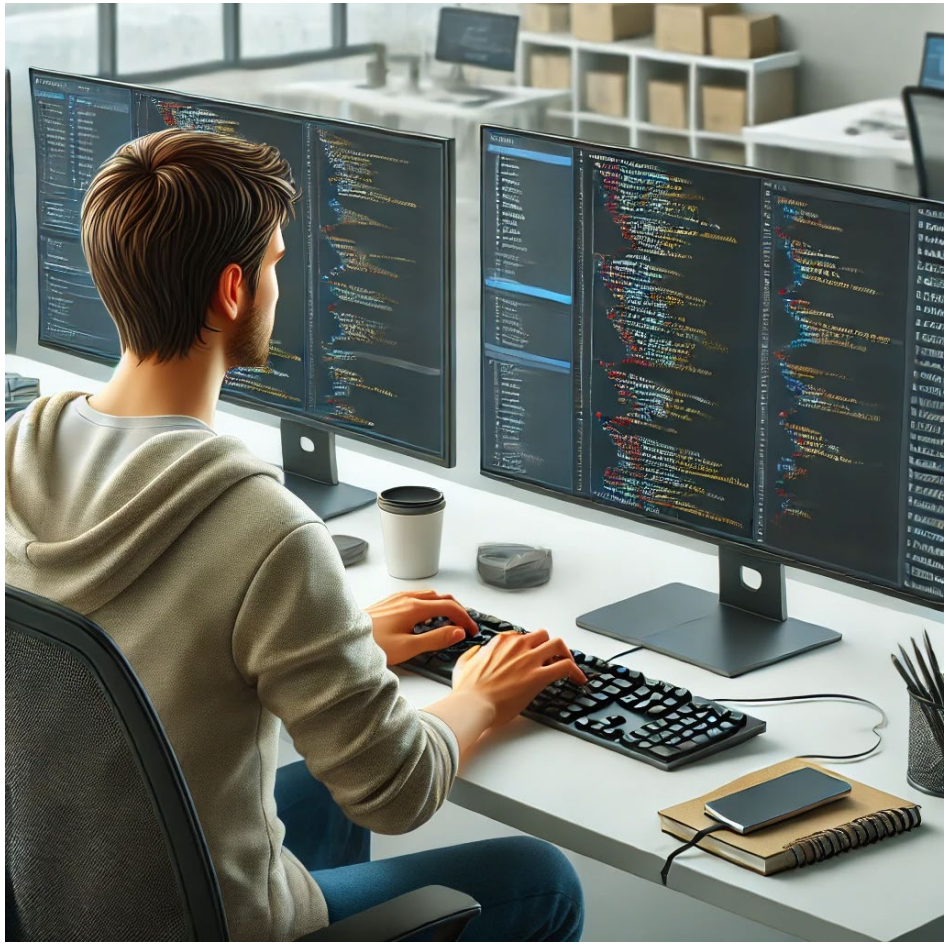


Image: https://xkcd.com/844/

Overview: Basic programming principles

- Single-responsibility principle (SRP)
- Don't repeat yourself (DRY)
- Separation of concerns (SoC)
- You aren't gonna need it (YAGNI)

- *There are (way) more, but we will focus on those! (e.g., https://github.com/webpro/programming-principles)*



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Single-responsibility principle (SRP) (1/2)

- A function (or a class, module) should be responsible for a single part of the functionality
- Otherwise, changes to one functionality can break the other

```python
import this
import numpy as np

def mean_and_variance(data: np.array):
    """This function has too many
    responsibilities."""
    mean = sum(data) / len(data)

    variance_sum = 0.
    for x in data:
        variance_sum += (x - mean) ** 2
    variance = variance_sum / len(data)

    return mean, variance
```

Single-responsibility principle (SRP) (2/2)

- A function (or a class, module) should be responsible for a single part of the functionality
- Otherwise, changes to one functionality can break the other

```python
import this
import numpy as np

def mean(data: np.ndarray) -> float:
    """This only calculates the mean."""
    mean = sum(data) / len(data)
    return mean

def variance(data: np.ndarray) -> float:
    """This only calculates the variance."""
    variance_sum = 0.
    data_mean = mean(data)
    for x in data:
        variance_sum += (x - data_mean) ** 2
    variance = variance_sum / len(data)
    return variance
```

Don’t repeat yourself (DRY)

- Code should not be duplicated.
- If you need code more than once, write a function.
- If you catch yourself copying code, that’s a warning sign!

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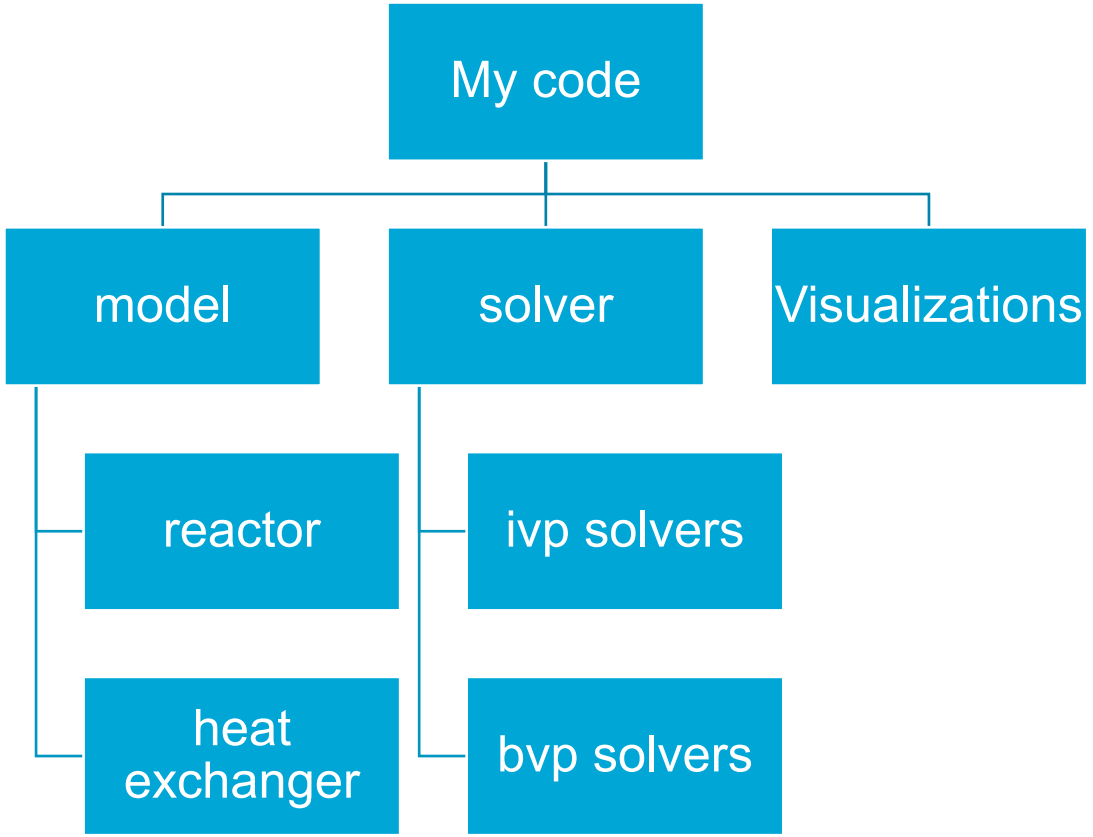
Separation of Concerns (SoC)

- Each part of your program should focus on a single aspect or concern of the system.
- Different parts of the program should only be coupled loosely.
- SoC is similar to single responsibility, but focusses on a higher, architectural level.



You aren’t gonna need it (YAGNI)

- Don’t write code for hypothetical requirements
- Focus on current requirements
- Add features to code when they are needed

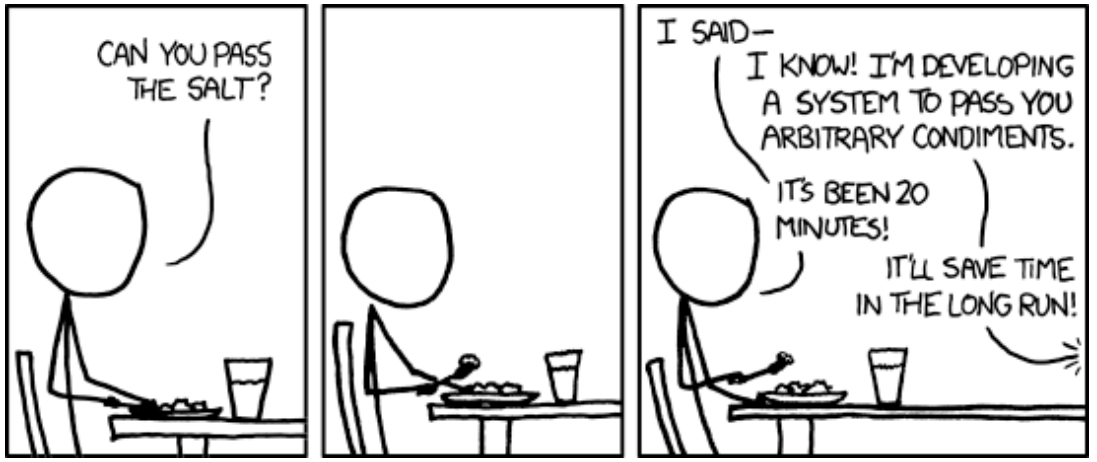


Image: https://xkcd.com/974/

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Managing imports, packages, virtual environments

- Last quarter, we have already been importing several packages:
- Where are we actually importing *from*?
- There are three main sources:
  - 1) Python standard library.
  - 2) External packages managed via the Python package installer.
  - 3) Our own packages or modules.

```
import numpy as np
import scipy
from math import sqrt, pi
```

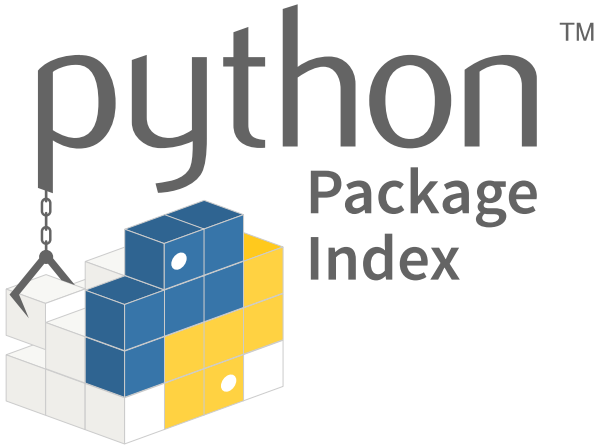
Python standard library

- Some packages come with the installation of python itself. They are part of the **Python standard library.**
- These packages usually contain very basic functionality, e.g.:
  - **os:** package for miscellaneous operating system interfaces, e.g., accessing, creating, deleting folders.
  - **math:** basic mathematical functions like square root or factorial.

- Packages can simply be imported via `import` without other action.
- Why do I have to import these modules even though they are part of the Python installation?
  ➔ The less commands Python has to keep track of, the faster it is!

The Package Installer for Python (pip)

- Use **package installer for Python (pip)** to install further packages from the Python Package Index (PyPI).
- That way, you can **customize what your Python can do** without downloading the vast number of packages.
- Basic pip commands you will need:
  - **“pip install <package>”:** Install a package
  - **“pip install <package>==<version>”:** Install a specific version of a package
  - **“pip list”:** List installed packages

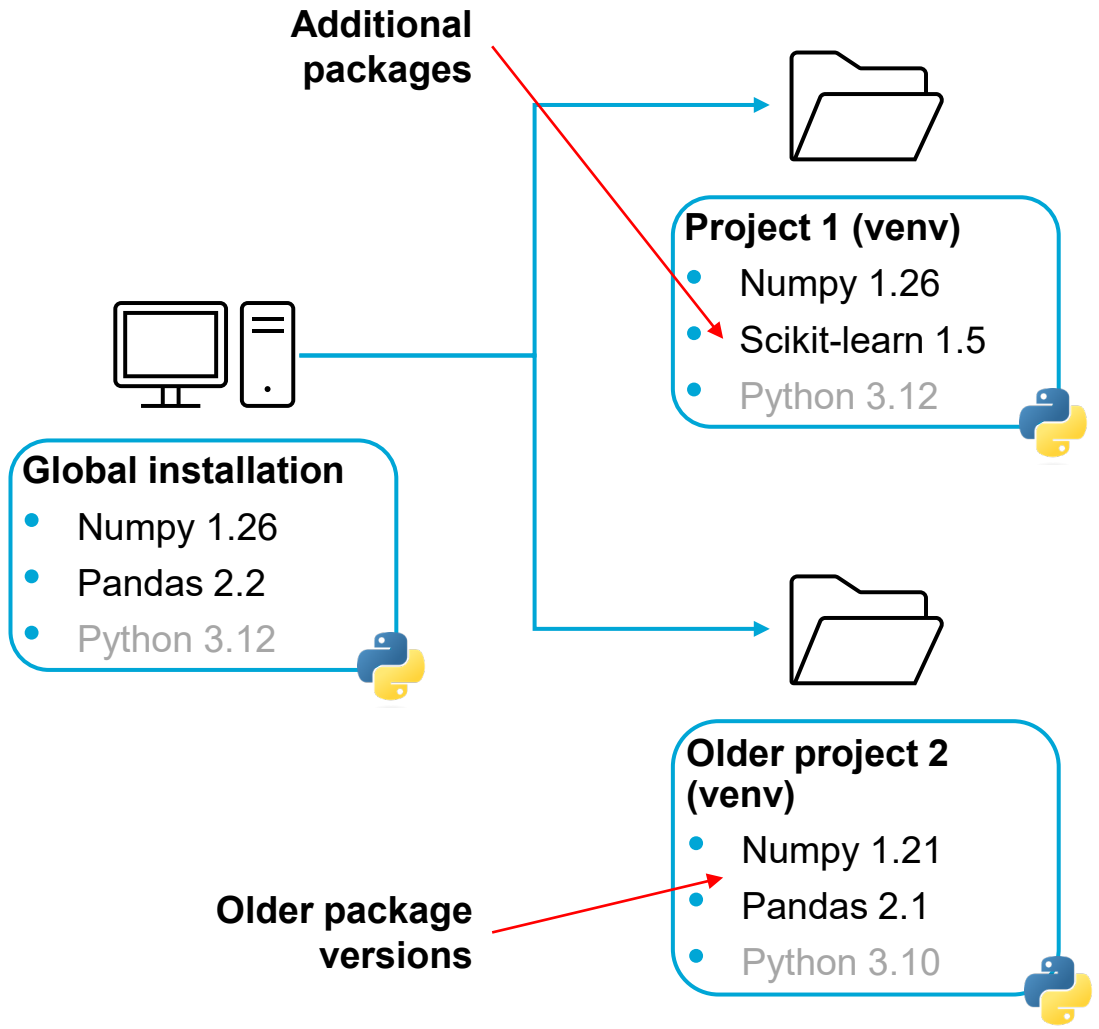



```
>> pip install pytorch
>> pip install numpy==1.19.5
>> pip list
```

But I have different projects with different, conflicting package requirements. How do I manage that that?

Virtual environments

- **Virtual environments** are **isolated Python environments** that allow separate management of package dependencies.
- Having separate environments for each project **avoids package conflicts** and ensures consistency.
- There are several frameworks for virtual environments. The **venv module** comes with the Python standard library.



Setting up a virtual environment

- Managing the virtual environment happens in the console.
- Typical steps in setting up and using your virtual environment:
  1. Creating the environment and giving it a name (typically ".venv" or "venv")
  2. Activate the environment
  3. Use pip in the environment
  4. Deactivate the environment

```
>> python -m venv .venv
>> .venv/Scripts/activate
(.venv)>> pip install numpy
(.venv)>> pip install -r requirements.txt
(.venv)>> deactivate
>>
```

```
>> python -m venv .venv
>> source .venv/bin/activate
(.venv)>> pip install numpy
(.venv)>> pip install -r requirements.txt
(.venv)>> deactivate
>>
```

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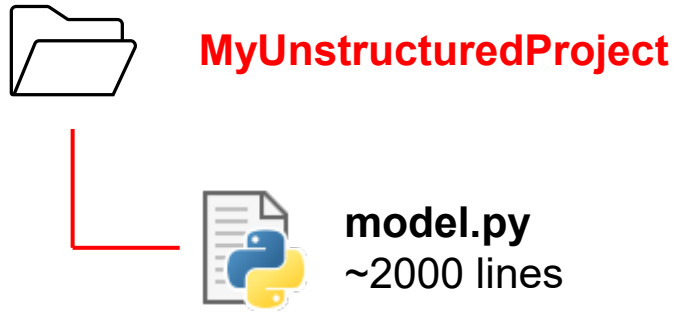
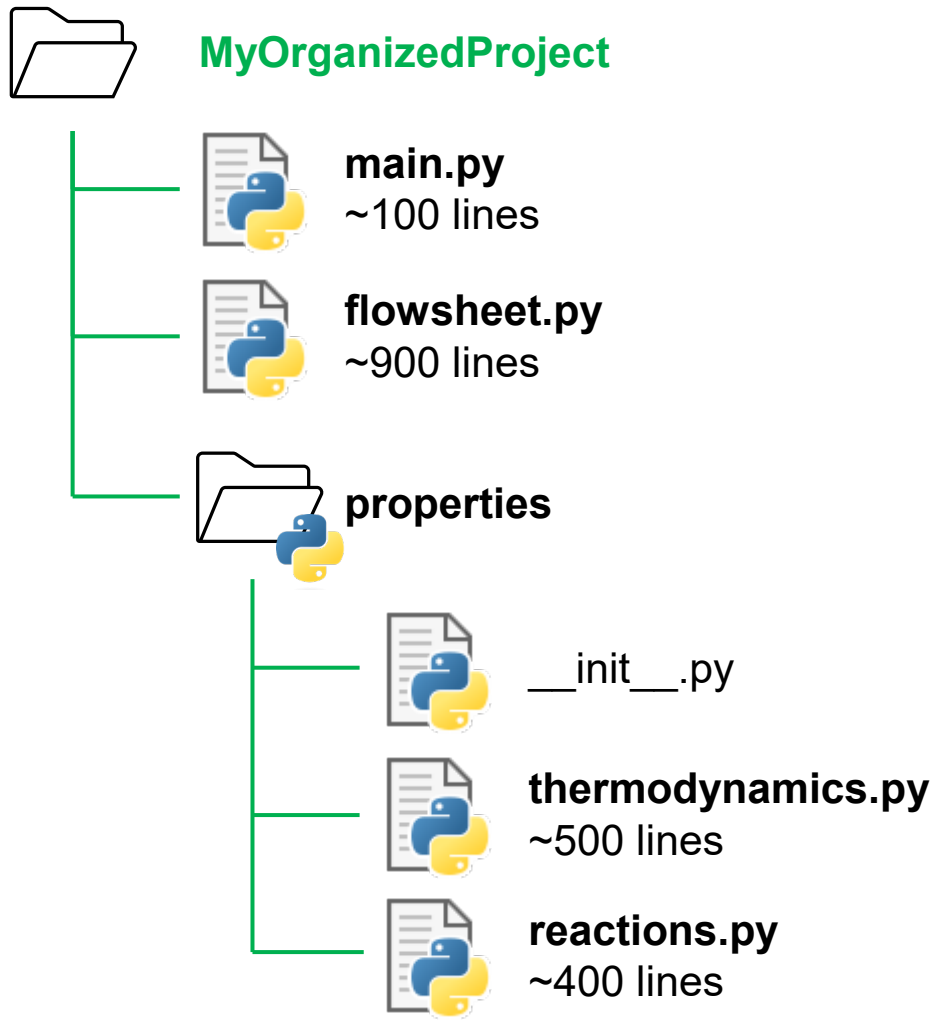
Managing projects with many modules and packages

- Project become big very fast
- Challenges arise for code management:
  - Readability (others and **yourself**)
  - Maintainability
  - Reusability
  - Namespace management
  - …



Managing projects with many modules and packages

- Organize your project into
  - Modules (python files)
  - Packages (python folders, i.e. folders with an __init__.py file)
- Deciding what to put in a module/package requires practice and experience
- The importing syntax is like importing from standard library or PyPI packages.



Importing my modules and packages

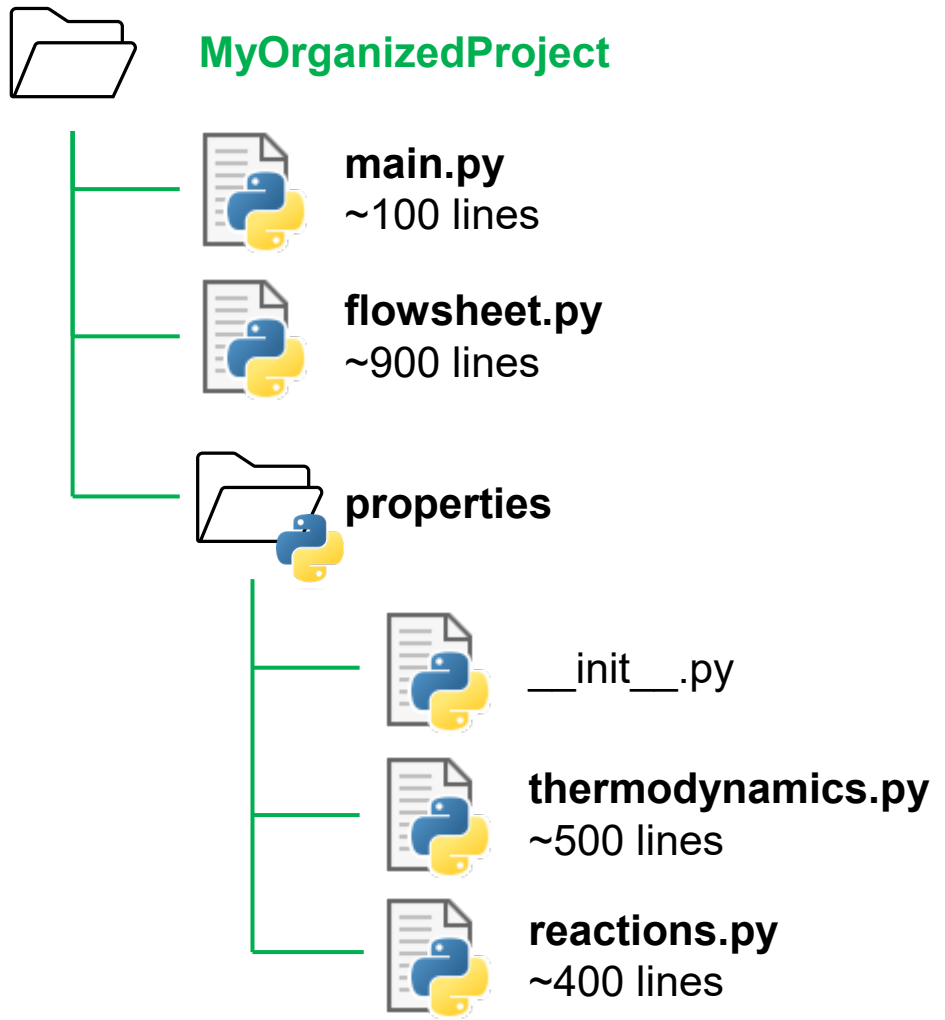
```python
# In module "main.py"
import flowsheet
import properties.thermodynamics
from properties.reactions import WGShift,
                                 Syngas2Methanol

# Class MyFlowsheet in flowsheet
print(flowsheet.MyFlowsheet)

# Function ideal_gas_law in thermodynamics
print(properties.thermodynamics.ideal_gas_law)

# Classes WGShift and Syngas2Methanol in reactions
print(WGShift)
print(Syngas2Methanol)
```

```
>> <class 'flowsheet.MyFlowsheet'>
>> <function ideal_gas_law at 0x000001D7B5A4A520>
>> <class 'properties.reactions.WGShift'>
>> <class 'properties.reactions.Syngas2Methanol'>
```



Live coding: Managing multiple modules

- Open Colab: Managing modules and packages

- Find more in the Github repository of the course: https://github.com/process-intelligence-research/computational_practicum_lecture_coding/tree/main

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Basics of object-oriented programming: Motivation

- Sometimes, organizing loose functions into modules is not enough.
  - Data and corresponding functionality are separated.
  - Changes in one part of the code impacts the rest of the program.
- **Object oriented programming (OOP):** A programming paradigm based on the concept of “objects”.

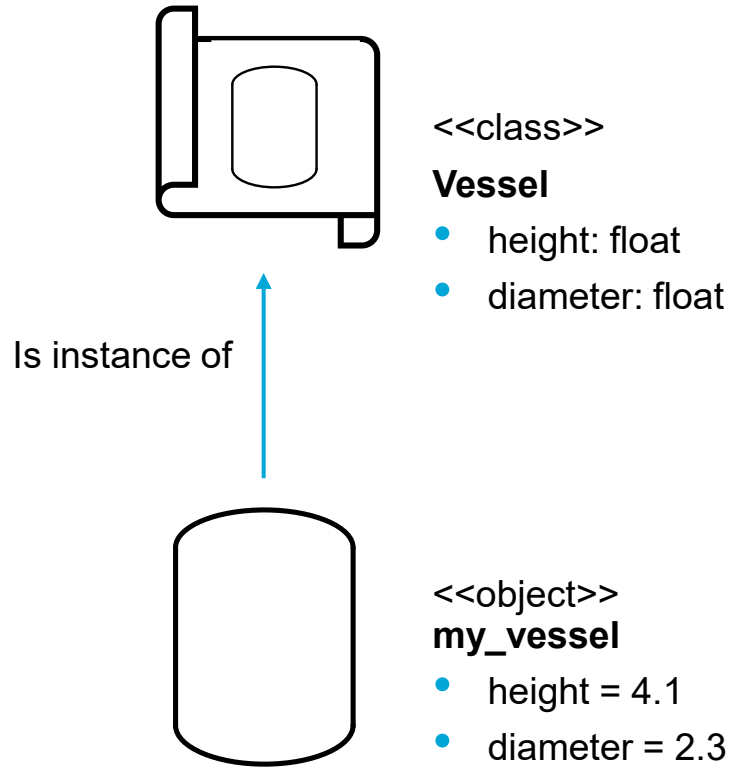
An Object in object oriented programming (OOP)

- An **object** is a programming concept, which
  - **“Is something”:** Has a predefined conceptual data and behavioural structure **(class).**
  - **“Has something”:** Contains and encapsulates data related to its meaning **(attributes).**
  - **“Does something”:** Has associated functionality operating on its data **(methods).**
- **Example**: The *silver reaction vessel (on the right)*
  - Is a vessel *(<<class>>)*
  - Has a volume of 10,000 L *(attribute)*
  - Can be filled *(method)*

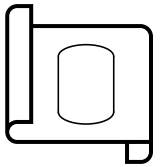
Figure: https://www.ssengindia.com/chemical-vessel.html

Core concepts of OOP: classes and objects

- **Class**: A blueprint for creating objects. Defines:
  - Attributes (data)
  - Methods (functions)
- **Object**: An instance of a class. Contains actual data and can use methods defined in the class.
- **Note**: An object can have other objects as attributes.



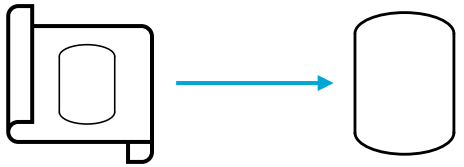
Defining a class



- Define a class using the **“class”** command.
- Define a constructor to your class with the **“__init__”.** It
  - sets the attributes to an initial value.
  - defines further instructions for the instantiation of a new class.
- **“self”** is a reference to the object itself used to retrieve attributes and other methods.
- Add **methods** to give your class functionality. They look like functions.
- Describe your class, its attributes and methods in a class docstring (optional, but recommended).
- Mind the **colons** and **indentations.**

```python
class Vessel:
    """
    A class to represent a cylindrical vessel and calculate
    its volume.

    Attributes:
        height (float): The height of the vessel.
        diameter (float): The diameter of the vessel.

    Methods:
        calculate_volume: Calculates vessel volume.
    """

    def __init__(self, height:float, diameter:float):
        """The constructor with instructions for creating a
        class."""
        self.diameter = diameter
        self.height = height

    def calculate_volume(self) -> float:
        """Also add docstrings to methods."""
        volume = self.height* self.diameter**2 *math.pi/4
        return volume
```

Instantiate your class



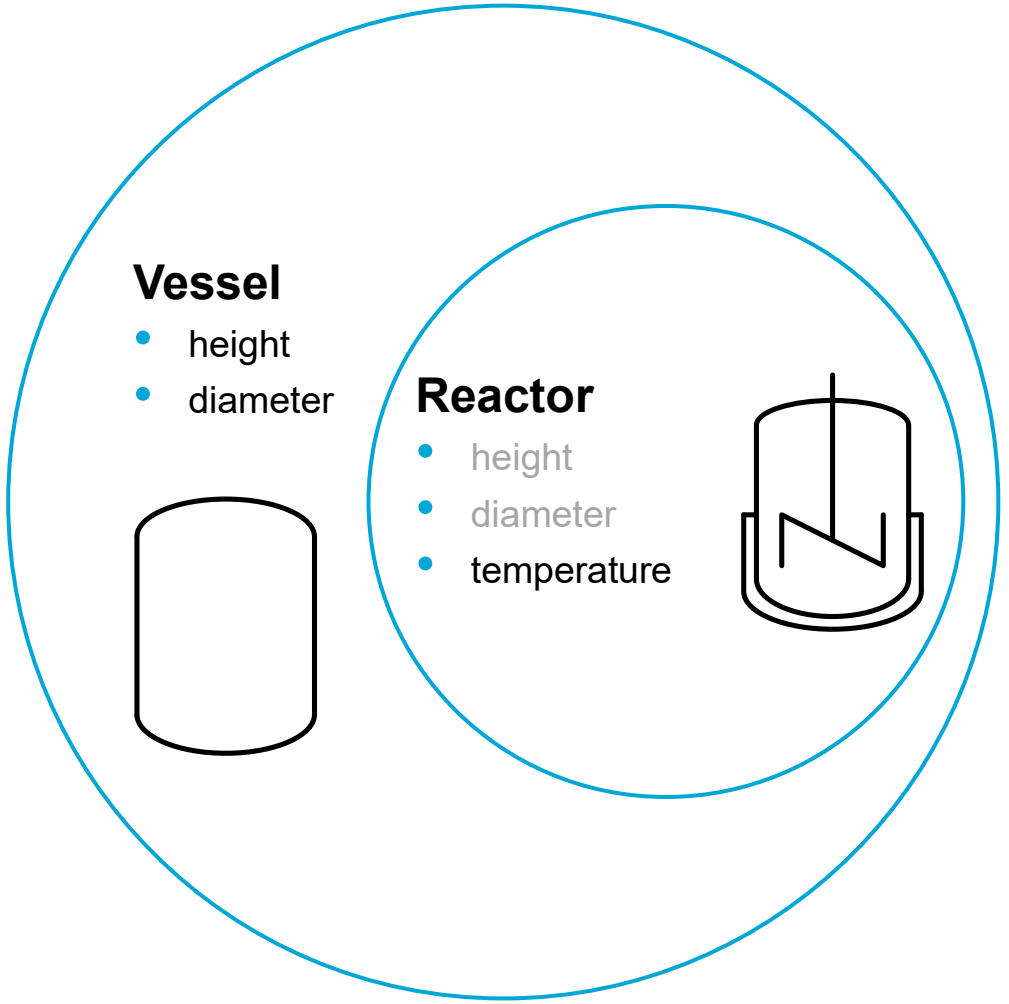
- Instantiate your class by calling the **constructor** of the class.
- To call the constructor, call the class name like a function with arguments.
- Store a reference to the new object like a variable.
- To access attributes or call methods, use the following dot-notation: **“<object>.<method_or_attribute>”**
- Note that the “self” argument is not explicitly specified.

```
# Instantiate the class
# For this, call the class name (Vessel). This
# invokes the constructor. Add the required
# arguments (height, diameter).
# Store the new Vessel object in my_vessel
my_vessel = Vessel(1.2, 3.5)
print(my_vessel)

# Retrieve the diameter of my_vessel
# For this, use the dot notation
# <object>.<attribute>
print(my_vessel.diameter)

# Call the calculate_volume method
# For this, use the dot notation
# <object>.<method>
print(my_vessel.calculate_volume())
```

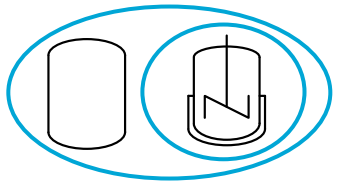
```
>> <__main__.Vessel object at 0x0000020F75510B50>
>> 3.5
>> 11.54535300194249
```

Class inheritance

- **Inheritance** allows a class (child) to **share** a parent-class attributes and methods while **extending** and **modifying** its functionality.
- Inheritance further improves:
  - Reusability
  - Modularity
  - Extendibility
- E.g.: A **reactor is a vessel**, that also has a specified content **temperature**.



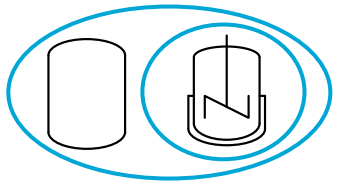
Defining a child class



- A child class is created with the **“class”** keyword as before.
- Name of parent after the class name indicates inheritance.
- In new constructor, first call parent constructor by referencing parent with **“super()”.**
- Then, add further functionality.
- Change the functionality of parent methods (overriding) or define new methods.

```python
class Reactor(Vessel):
    """Reactor class that is a vessel and also
    stores temperature."""

    def __init__(self,
                 height:float,
                 diameter:float,
                 temperature:float):
        """Constructor of reactor."""
        super().__init__(height, diameter)
        self.temperature = temperature

    def get_temperature(self):
        """Return reactor temperature"""
        return self.temperature
```

How does my child class behave?



- Instantiate your child class just like a normal class.
- Notice: a reactor still behaves like a vessel.
- But it also has its additional functionality!

```
# Instantiate the class
my_reactor = Reactor(1.2, 3.5, 350)
print(my_reactor)

# A reactor is a vessel. The functionality of the
# parent class is preserved.
print(my_reactor.diameter)
print(my_reactor.calculate_volume())

# But also use your new attributes and methods
print(my_reactor.temperature)
print(my_reactor.get_temperature())
```

```
>> <__main__.Reactor object at 0x0000020F75510B50>
>> 3.5
>> 11.54535300194249
>> 350
>> 350
```

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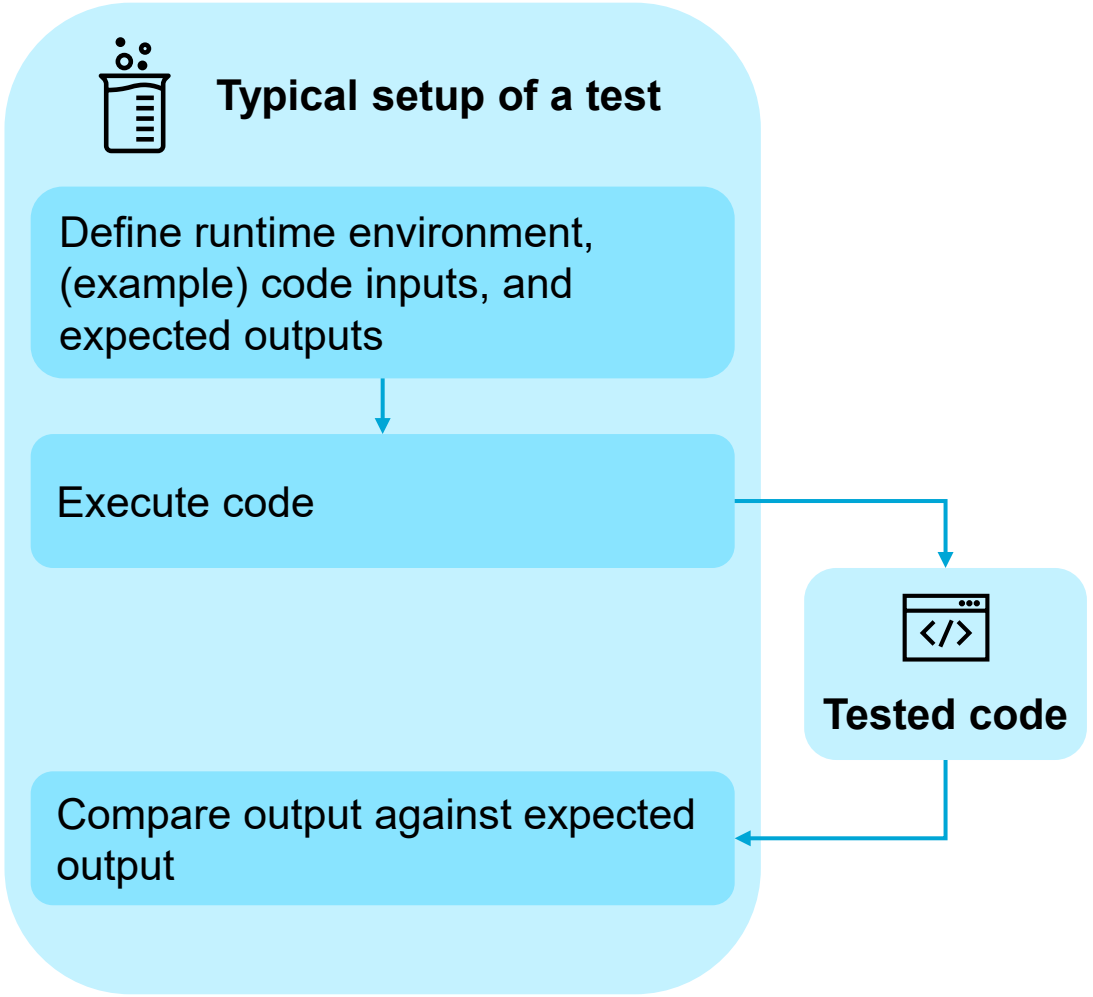
Testing code with unit tests

- Unit tests run other functions, check if they work as expected.
- Method to check if code works as intended.
- Ensures that code works after changes are made.
- A structured way of collecting code requirements.



Testing a function

- This function calculates the Reynolds number for a flow in a pipe.
- Does it work?
- Let's write a test with some example parameters and outputs!

```python
def reynolds_number(diam: float, vel: float,
                    dens: float, visc: float
                    ) -> float:
    """
    Calculates the Reynolds number for flow in a
    pipe.

    Args:
        diam (float): Pipe diameter in m.
        vel (float):  Fluid velocity in m/s.
        dens (float): Fluid density in kg/m^3.
        visc (float): (Dynamic) fluid viscosity in
                      Pa·s.

    Returns:
        float: Reynolds number (dimensionless).
    """
    return (diam * vel * dens) / visc
```

Testing a function

- A test function is a normal function with a function header.
- The test calls tested function with example parameters.
- `assert` compares output against expected output.
- `assert` does nothing if condition holds, otherwise, throws an AssertionError with this error message.
- A test can have multiple assert-statements to test for several cases.
- However, it is best to separate meaningful test cases into separate functions.

```python
def test_reynolds_number():
    """Simple test to see if reynolds number is
    calculated correctly"""
    # Typical values for water flow in a pipe
    res = reynolds_number(0.05, 1.5, 1000, 0.001)
    exp_res = 75000
    assert abs(res - exp_res) < 1e-6, \
           "Basic validation case failed“

    res = reynolds_number(0.05, 3, 1000, 0.001)
    exp_res = 150000
    assert abs(res - exp_res) < 1e-6, \
           "Basic validation case failed"

def test_reynolds_number_zero_velocity():
    """Test Reynolds number for zero velocity."""

    res = reynolds_number(0.05, 0, 1000, 0.001)
    exp_res = 0
    assert res == exp_res, \
           "Zero velocity edge case failed"
```

Where do I put my tests?

- Common convention: test directory with the same structure.
- Module names are the same with “test_”.
- Each function or class method has at least one (typically more) corresponding test function.

```
project
├── project_code
│   ├── models.py
│   ├── scripts.py
│   └── utils.py
└── tests
    ├── test_models.py
    ├── test_scripts.py
    └── test_utils.py
```

Testing with pytest

- pytest is a testing framework for Python
- Automatically finds testing functions, helps to organize and run them
  - In the command line, running pytest runs all tests in the project

```
>> pytest
```

  - Run tests in a specific module by running

```
>> pytest tests/test_reynolds_number.py
```

- Additional functionality to set up complex runtime environments and parametrize tests
- Find the documentation of pytest here: https://docs.pytest.org/en/stable/

Image and further reading: https://docs.pytest.org/en/stable/

Live coding: Unit testing

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Thank you very much for your attention!