

CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

INTRODUCTION TO PYTHON

INTRODUCTION

- ▶ Aim is to give experience with computer programming in Python for computational chemistry applications
- ▶ You may remember some of it from First and Second Year Labs
 - ▶ But we will go over everything again, so don't worry
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ASSESSMENT

- ▶ x Dec: xx:xx Multiple Choice Questions and Error Spotting exercise
 - ▶ MCQs cover all of the material up to that date
 - ▶ Error spotting should be familiar from earlier work
 - ▶ Do not spend more than 30 minutes on either
- ▶ x Dec: xx:xx Programming test
 - ▶ Up to 3 hours
- ▶ Both parts are “open book” assessments; you may consult lecture notes, etc.

ASSESSMENT

▶ x Dec: xx:xx M

▶ MCQs cover

▶ Error spotting

▶ Do not spend

▶ x Dec: xx:xx P

▶ Up to 3 hours

▶ Both parts are “open book” assessments; you may consult lecture notes, etc.

**NO INTERNET
MAY BE USED**

FIRST AND SECOND YEAR PYTHON

- ▶ Much of the first few weeks will feel like revision from first and second year
- ▶ More details and more opportunity for programming
 - ▶ Rather than filling in blanks
- ▶ If you would like to revise first or second year material, this should be available on moodle
- ▶ However, we will cover everything from those labs incase you didn't do them!

JUPYTER NOTEBOOK

- ▶ As with the first and second year labs, we will be using Jupyter Notebooks to interact with the Python programming language
- ▶ Create a folder on your H: drive named “CH40208” then visit the JupyterHub and navigate to this folder

<https://chsv-jupyter.bath.ac.uk/>

VARIABLE TYPES

- ▶ *Variables* are containers used to store data
- ▶ Different types of variables exist, and define the operations that can be performed
 - ▶ Integers: whole numbers (`int`)
 - ▶ Floats: numbers with decimal points (`float`)
 - ▶ Complex: complex number (`complex`)
 - ▶ String: some text (`str`)
 - ▶ Boolean: logical information, True or False (`bool`)

VARIABLE ASSIGNMENT

- ▶ The *assignment* of the variable define the value that the container holds
- ▶ This links the variable name with some location in computer memory, and places the value there.
- ▶ This means we can then use that variable in other parts of the code

VARIABLES



DEMO

ARITHMETIC

- ▶ Python *natively* can do basic mathematical operations
 - ▶ Addition: $(a + b)$
 - ▶ Subtraction: $(a - b)$
 - ▶ Multiplication: $(a * b)$
 - ▶ Division: (a / b)
 - ▶ Exponent: $(a ** b)$

ARITHMETIC

- ▶ Python will follow the *order of operations* that should be familiar from mathematics
 - ▶ BODMAS/BIDMAS/PIMDAS/POMDAS
 - ▶ **B**rackets
 - ▶ **O**rder
 - ▶ **D**ivide/**M**ultiply
 - ▶ **A**ddition/**S**ubtraction

ARITHMETIC



DEMO

MIXED MODE OPERATIONS

- ▶ As mentioned previously, not all variables are the same
- ▶ What happens when a mathematical operation is performed on variables of different types
 - ▶ `int` and `float`
 - ▶ `float` and `complex`
 - ▶ `float` and `str`?

MIXED MODE OPERATIONS



DEMO

OUTPUT

- ▶ Currently we are using the intrinsic functionality of the Jupyter Notebook to print the output from the last line in a given cell
- ▶ For printing not at the end of a cell, or from within a script the `print` function is necessary
- ▶ Print formatting is a useful tool in Python to make the print statements that you create easier to understand

INPUT

- ▶ In addition to the output of information, it is also of interest to read information from the user
- ▶ Python has multiple ways to receive information in (some of which will be introduced in the following weeks)
- ▶ The first is the `input` function

INPUT/OUTPUT



DEMO

LOGICAL OPERATORS

- ▶ Python and Jupiter Notebook can be used as a simple calculator
- ▶ Let's make our code more intelligent!
- ▶ To do this we can use *Boolean logic*; True or False questions
- ▶ Python is able to assess the truth of a particular operation

LOGICAL OPERATORS

Some logical operators

Name	Equals	Less than	Less than or equal	Greater than	Greater than or equal	Not equal
Operator	==	<	<=	>	>=	!=

LOGICAL OPERATORS



DEMO

FLOW CONTROL

- ▶ We are then able to use this Boolean logic to *control* the path that the code will follow
- ▶ To do this we use `if` statements; these ask `if x is True?`
 - ▶ Note the `is True` part is often implicit
- ▶ The `if` statement is often accompanied by an `else`; which is the path taken when `x is False`
- ▶ The third modifier in an `if` statement is the `elif` (short for else if); this offers an alternate path to follow

FLOW CONTROL



DEMO

MORE LOGICAL OPERATORS

- ▶ Logical operators can be extended to include those which link two statements
- ▶ These are the AND and OR operators; which are foundational to computational logic

The results of an AND operation

Input A	Input B	Logic	Output
True	False	AND	False
True	True	AND	True
False	False	AND	False

The results of an OR operation

Input A	Input B	Logic	Output
True	False	OR	True
True	True	OR	True
False	False	OR	False

MORE LOGICAL OPERATORS



DEMO

HOW TO WRITE GOOD CODE

- ▶ A lot of computer programming is about approaching the problem in the most constructive way
- ▶ In all of the exercises in this course, you will be given a *spec*; this is a description in plain English of what the code should perform
- ▶ To produce the best code, you should try and translate this into an *algorithm*; a step by step route (although not computer code) to complete the goals outlined in the spec
- ▶ The final step is then to take the algorithm and translate each individual step into the appropriate Python

PROBLEM

- ▶ In a *single* Jupyter Notebook cell, write a tool to convert from temperature in Fahrenheit to temperature in Celsius
- ▶ Consider the *algorithm* that you should employ to create useful code, **before** you start to code

$$T(^{\circ}\text{C}) = \frac{5(T(^{\circ}\text{F}) - 32)}{9}$$

PROBLEM

- ▶ The second problem this week involves calculating the equilibrium constant
- ▶ You need to use the logical expressions that have been introduced to control the flow of the program such that it can deal with multiple different units

$$K = \exp \left(\frac{-\Delta G}{RT} \right) = \exp \left(\frac{-\Delta g}{k_B T} \right)$$