

CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

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# INTRODUCTION TO PYTHON

# INTRODUCTION

- ▶ Aim is to give experience with computer programming in Python for computational chemistry applications
- ▶ Will build on the first and second year Python labs
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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

**NO INTERNET  
MAY BE USED**

▶ x Dec: xx:xx M

▶ MCQs cover

▶ Error spotting

▶ Do not spe

▶ x Dec: xx:xx F

▶ Up to 3 hours

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

## 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

## 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**

## 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

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