

CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

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