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

▸ Dr Benjamin Morgan

  ▸ Office: 1S 0.12; Email: b.j.morgan@bath.ac.uk

▸ Dr Andrew McCluskey

  ▸ Office: 1S 0.15 (Wednesdays Only); Email: andrew.mccluskey@diamond.ac.uk

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.

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    ▸ MCQs cove

    ▸ Error spotti

    ▸ Do not spe

▸ 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

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/