

CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

PYTHONIC LOGIC AND LOOPS

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



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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



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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

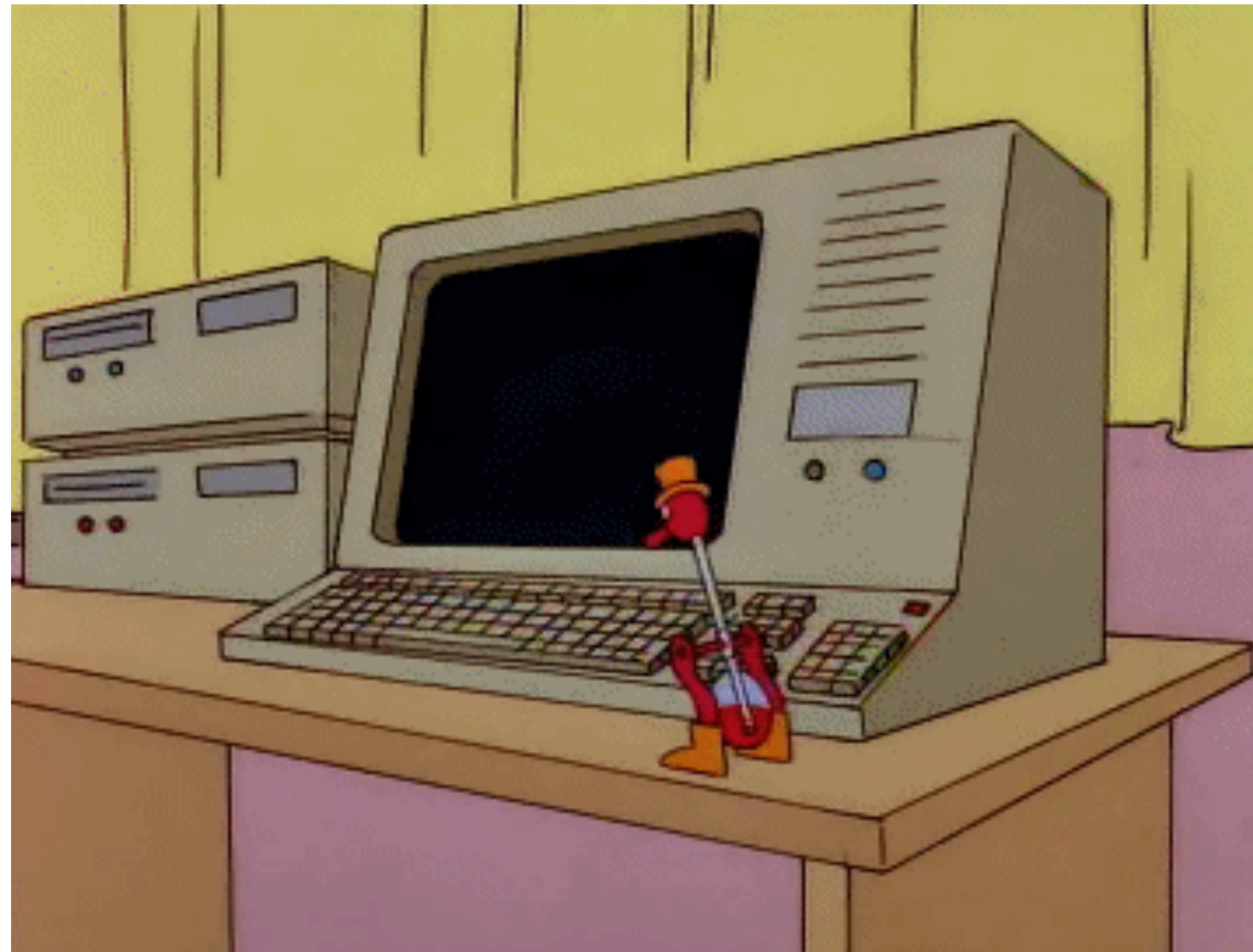
MORE LOGICAL OPERATORS



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LOOPS

- ▶ One of the most powerful tools of a computer is to perform repetitive tasks



LOOPS

- ▶ Loops allow us to ask the computer to perform the same (or a very similar) task multiple times over
- ▶ Python has two types of loop
 - ▶ `for` loops iterate over a given list
 - ▶ `while` loops repeat as long as a logical operation is `True`
- ▶ Generally it is safer to use a `for` loop than a `while` loop; with the `while` loop it is more easy to cause an infinite loop
- ▶ It may be desirable to escape from a loop, or to skip to the next iteration; for this there are the `break` and `continue` commands

LOOPS



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PROBLEMS

- ▶ There are two problems to tackle this week, which can be found on the handout
- ▶ **Remember** to first determine the algorithm that you will use (ideally write it down)
- ▶ Only once you have an algorithm in mind (or on paper), should you start to code