

Computational Science and Scientific Computing Workshop

Data Programming - Python as a scientific computing tool

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October 14, 2025

data storage, loops, len and range, if statements

Interpreter - List, Tuples and Dictionaries

```
1 >>> x = ["Hey", "you", 5, 8.7]
2 >>> y = ("hello", "hi", "you")
3 >>> w = {"foo": 1.0, "bar": 2.0 }
4 >>> print(type(x))
5 >>> <class 'list'>
6 >>> print(type(y))
7 >>> <class 'tuple'>
8 >>> print(type(w))
9 >>> <class 'dict'>
10
```

Empty list:

```
1 >>> x = []
2 >>> x
3 [ ]
4
```

Interpreter - List, Tuples and Dictionaries

Indexing and memory location:

Memory locations for storing data in list and tuples are indexed so that one could access data stored in a specific memory locations.

NB: By default, index locations begin from zero (0).

```
1 >>> z = [2, 3, 4, 5]
2 >>> num0 = z[0]
3 >>> print(num0)
4 2
5
```

Interpreter - If Statements

if...

```
1 >>> if(condition):  
2 ...     statement_1  
3 ...     statement_2  
4
```

if...else

```
1 >>> if(condition):  
2 ...     statement_1  
3 ...     statement_2  
4 ... else:  
5 ...     statement_3  
6 ...     statement_4
```

Interpreter - If Statements

if...else if

```
1 >>> if(condition_1):  
2 ...     statement_1a  
3 ...     statement_2a  
4 ... else if(condition_2):  
5 ...     statement_1b  
6 ...     statement_2b  
7
```

if...else if...else

```
1 >>> if(condition_1):  
2 ...     statement_1a  
3 ...     statement_2a  
4 ... else if(condition_2):  
5 ...     statement_1b  
6 ...     statement_2b  
7 ... else if(condition_3):  
8 ...     statement_1c  
9 ...     statement_2c  
10 ... else:  
11 ...     statement_1d
```

Interpreter - If Statements

Nested if

```
1 >>> if(condition_1):
2 ...     if(condition_1A):
3 ...         statement_1A_a
4 ...         statement_2A_a
5 ...     else:
6 ...         statement_1A_b
7 ...         statement_2A_b
8 ... else:
9 ...     if(condition_2A):
10 ...         statement_2A_a
11 ...         statement_2A_b
12
```

Interpreter - List, Tuples and Loops

for loop and range:

```
1 >>> for i in z:  
2     ...     print(i)  
3     ...  
4
```

```
1 2  
2 3  
3 4  
4 5  
5
```

range & len intrinsic functions

```
1 >>> range(4)  
2 range(0,4)  
3 >>> len(z)  
4 4  
5
```

0 = Starting index

4 = Total no. of numbers

4 = Number of elements in list z.

Interpreter - List, Tuples and Loops

range and **len** can be combined and used in loops:

```
1 >>> for i in range(len(z)):  
2     ...     print(i)  
3     ...  
4  
5
```

```
1 0  
2 1  
3 2  
4 3  
5
```

len gives length of list z, that is, 4.

range gives 4 integers used as indexes starting from index 0.

Interpreter - While loops and Boolean

while loops and **boolean**

```
1 >>> a = True:
2 >>> print(a)
3 True
4 >>> res = 0
5 >>> while (a):
6 ...     res += 1
7 ...     print(res)
8 ...     if (res >= 10):
9 ...         a = False
10
11
```

```
1 1
2 2
3 3
4 4
5 ...
6
```

boolean **a** changes to False and it is used to terminate loop in the condition test section

Exercises 2 - Algorithm Development

Exercise A: Multiples of 3 & 5

If we list all the natural numbers below 10 that are multiples of 3 or 5, we get 3, 5, 6 and 9. The sum of these multiples is 23.

Implement an algorithm, with Python, to find the sum of all the multiples of 3 or 5 below 1000.

Exercise B: Fibonacci sequence

Each new term of the Fibonacci sequence is generated by adding the previous two terms. By starting with 1 and 2, the first 10 terms will be:

1, 2, 3, 5, 8, 13, 21, 34, 55, 89, ...

By considering the terms of the Fibonacci sequence whose values do not exceed four million, find the sum of the even-valued terms.