

Lecture 3: Lists, arrays, and optimisation with NumPy

Dr Benjamin J. Morgan¹ and Dr Andrew R. McCluskey^{1,2}

¹*Department of Chemistry, University of Bath, email: b.j.morgan@bath.ac.uk*

²*Diamond Light Source, email: andrew.mccluskey@diamond.ac.uk*

July 15, 2019

Aim

This lecture will introduce lists, arrays, and show how the NumPy library can be used to make your code faster.

1 Lists

The Python programming language natively includes the ability to group together a series of objects. These are `lists` and are one of the most powerful Python objects. A list is defined as follows,

```
# Making a list
```

```
elements = ["Hydrogen", "Helium", "Lithium", "Beryllium",  
            "Boron", "Carbon", "Nitrogen", "Oxygen"]
```

Having defined the list, it is then possible to select individual items of the list by using the following syntax,

```
# Printing some items
```

```
print(elements[0], elements[4], elements[-1])
```

Note, that Python starts counting from the number 0, and using the minus sign we can ask Python to count from the end. This means that the above code should print, "Hydrogen", "Boron", "Oxygen". This counting from 0 means that in the above list, the string "Hydrogen" would be referred to as the zeroth object in the list, while "Helium" would be the first.

In addition to making use of single objects from within a list, it is also possible to create sublists, for example,

```
# Just the first 4 elements
```

```
print(elements[0:4])
```

Note that above, the numbers on either side of the colon the list indices. However, rather strangely, the sublist created is **inclusive** of the first number and **exclusive** of the second. Additionally, it is possible to select non-consecutive objects from a list by placing commas between the indices,

```
# Just the gases
```

```
print(elements[0, 1, 6, 7])
```
