CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

LISTS, ARRAYS AND NUMPY

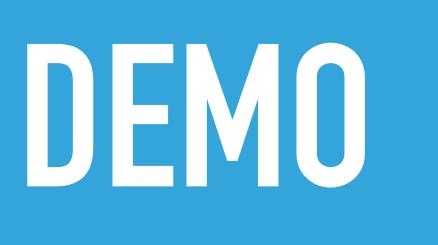
LISTS

- In week I, we met different variable types
- Now we will see how to create batches of these types
- The list object is native to Python and sorts and ordered set of objects that can be of any type

LISTS

- Once defined, it is possible to take a all, one or many values from a list
- We can even loop through the list, as we did last week with the range function
- The items within the list do **not** need to be of the same type

LISTS



NUMPY

- NumPy is an open source Python library
 - Open source means that the code used to create the library is available for free
- A library contains a large number of functions and tools that can be used by a Python code
- However, in order to harness a library, first we must import it

IMPORTING LIBRARIES

- Through this course you will import a lot of libraries
- To import a library is to ask the Python interpreter to go and find the code present in the library so that you can make use of it
- When a library is imported we can import the whole thing, or just a single (or a few) element(s) from it

IMPORTING LIBRARIES



NUMPY ARRAYS

- Now that we have NumPy imported, we can harness one of its most powerful tools, the np.array
- The NumPy array is similar in many ways to the lists introduced previously
- However, they can only hold numerical data

```
my_array = np.array([1, 2, 3, 4])
```

NUMPY ARRAYS



NUMPY ARRAYS

- NumPy arrays can undergo mathematical operations, just like other Pythonic numerical types
- NumPy array has additional functionality from the NumPy library; typically matrix operations and linear regression mathematics

LINEAR REGRESSION



CODE OPTIMISATION WITH NUMPY

- Large NumPy arrays are able to perform mathematical operations a lot faster than large numerical lists
- This is due to the reduced overhead on a NumPy array
- We must harness this as for very large arrays, this can be the difference between an intensive code running for days or minutes

CODE OPTIMISATION WITH NUMPY



A WARNING ABOUT DUPLICATION

- It is important to be aware that if you assign a list or an array to a new variable, this variable is essentially just an alias for the original array
- This means that changes to the new list or array will also occur to the old list or array
- Therefore, if you want to duplicate a list or array it is necessary to use the appropriate Copy function

A WARNING ABOUT DUPLICATION



PROBLEM

- Look back at the code written to calculate interatomic distances last week
- Try and use NumPy arrays to improve the efficiency of the code
 - Be aware that with the triatomic molecule is will not be possible to tell the difference
- Remember to determine the *new* algorithm before you write any code!