Molecular Statistics, Week 3

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Week 3, Overview

- Copy of lists
- More Python
- More Functions
- More Debugging
- LJ energy loop

Copy of lists

"To take a copy or not to take a copy"

```
a = 5.0
b = a # Copy
```

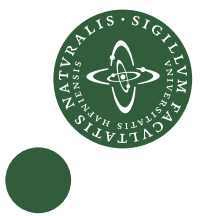
```
a = [1.0, 2.0, 3.0]
b = a # Not a copy
```

```
import copy
b = copy.copy(a) # a copy
```

Operator fun

```
c = 5.0

# Next two lines does exactly the same
c = c + 5.0
c += 5.0
```



Functions

Local vs Global variable

```
def f(x):
    b = 2.0 # local
    return x*b

a = 2.0 # global
print f(a)
print b # NameError: name 'b' is not defined
print a
```

More debugging fun

Double sum

Unique pair interaction

$$E_{ij} = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] \tag{1}$$

$$E_{Total} = \sum_{i} \sum_{j}^{i-1} E_{ij} = \sum_{i>j} E_{ij} \tag{2}$$

```
energy = 0.0
for i in range(n_particles):
    for j in range(n_particles):
        if i > j:
            rij = distance(xi, yi, xj, yj)
            energy = energy + lennard_jones(rij)
```