Molecular Statistics, Week 1

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Programming?!

Motivation

Video

Executing Python

python first_program.py

```
print "Hello World"

for i in range(5):
    print 'i', i
```

Output

```
Hello  World
i 0
i 1
i 2
i 3
i 4
```

Programming in Python

- Variables and Datatypes
- Operators
- Comments
- Indentation
- Modules
- Looping
- If-else

Variables and Datatypes

- String
- Integer
- Float
- List

```
name = "Peter"      # String
age = 31            # Integer
height = 1.80       # Float

s = [2, 4, 8, 16] # List
```

i	0	1	2	3
$s(i)$	2	4	8	16

Operators

Operator	Description
+	Addition
-	Subtraction
*	Multiplication
/	Division
%	Modulus
**	Exponent (a^b)

```
print 5.0 + 5.0
print 5.0 - 5.0
print 5.0 / 5.0
print 5.0 % 5.0
print 5.0**5.0

print 3 / 2
print 3.0 / 2.0
```

Comments and Indentation

Python is indentation based
Indentation is **4 spaces**

```
a = 5
 a = 5 # Error , why ?
```

Comments are very usefull when
looking at previous code

```
# Line comment

"""
Multiline
comment
"""
```

Looping

```
my_list = [2.0, 4.0, 8.0]

for x in my_list:
    print x
```

```
for i in range(24):
    print 'i', i
```

```
x_list = [i**2 for i in range(10)]
```

Modules

Always in the top of the program
Use Python modules or local .py-files

```python
import random
import matplotlib.pyplot as plt
```

```python
import video   # imports video.py
```

Looping

$$K = \sum_{j=1}^{50} j^2$$

Looping

$$K = \sum_{j=1}^{50} j^2$$

```
j_list = range(1, 51)
K = 0

for j in my_list:
    K = K + j**2

print K
```

If and Else

Operator	Meaning
<	Is less than
<=	Is less than or equal to
>	Is greater than
>=	Is greater than or equal to
==	Is equal to
!=	Is not equal to

```
k = 1.0

if k == 5.0:
    print "The number is five"

if k < 5.0:
    print "Smaller than five"
```

First Exercise

```python
import random
import matplotlib.pyplot as plt

# initialize some variables
n_particles = 100
n_steps = 1
dt = 0.01

# create the x- and y-coordinates
pos_x = [random.random() for i in range(n_particles)]
pos_y = [random.random() for i in range(n_particles)]

# plot the x- and y-coordinates in a figure.
plt.plot(pos_x, pos_y, 'ro')
plt.axis((-1, 1, -1, 1))
plt.savefig('coordinates_start.png')
```

The End

Exercise time