# Practical 0 – Python and Newton

*Instruction*

The aim this practical is to get some familiarity with basic aspects of computer simulations:

-basic programming (we use Python)
-using the commandline rather than graphical user interfaces
-understanding the basic structure of a computer simulation program.

We do so by writing a very simple simulation program (a Python script, lets call it newton.py), that simulates a particle of mass M on a spring with spring constant k. The program should be called from the commandline as follows:

```
C:\mydir>python.exe  newton.py input.csv output1.csv output2.xyz
```

The input file input.csv has the initial position and velocity of the particle. All other (input) parameters are specified in the script and can be changed from within the script. Kinetic and Potential energies during the simulation run are written to output1.csv (to be opened with Excel). If your program works as it should, the total energy (kinetic+potential) should be conserved (it is determined by the initial speed). Finally, the program should write the coordinate of the particle during the simulation to the file output2.xyz (to be opened with the .xyz viewer Ovito).

You can do the work alone or in pairs, at the end of week 1 (Friday), I expect a completed "newton" script, an example input file and the corresponding output files (.csv and .xyz). By handing in the assigment you can get a "Pass" if it is adequate. You need a pass to get the grade for the Practical.

*Preparation Excercises*

1. Write down the potential energy $U_{pot}(\mathbf{r})$of a spring attached to the origin when the particle at the other end of the spring is at vector position **r**. From the potential energy, get the force $\mathbf{F}(\mathbf{r})$ by calculating the gradient. Also write down the kinetic energy $U_{kin}(\mathbf{v})$ of the particle when it has a vector speed **v**. You will need all of this information for the final assignment.

2. Using r(t+Dt) ≈r(t) + v(t)Dt and a(t) ≈(v(t+Dt)-v(t))/Dt, Newtons equation, and the expression for **F** from exercise 1, derive the update equations for r and v.

*Running Python from Commandline & using IDLE*

Arrange for a link to an MSDOS terminal on your desktop, and in its properties (right click) set the starting directory to be the directory where you have the python scripts. Type "python.exe", now your are in the interactive mode of python. Try for example using it as a calculator. Type quit() to return to the commandline. To run a python script, we will use:

```
C:\mydir> python.exe myscript.py
```

Scripts will be edited in the standard Python editor called IDLE.

*Python Crashcourse*

-Read the scripts for the crashcourse and finish the corresponding test scripts (instructions in test scripts).
-If neccesary, check the web for Python help on statements you do not understand, or browse through the Python Tutorial on Python.org. Or ask the teacher…
-For those of you already familiar with Python I expect this stuff can go quite quickly, only do those tests which are not immediately obvious to you…

order of the scripts:

a) basics.py / basics_test.py
b) functions.py /functions_test.py
c) commandlinearguments.py / commandlinearguments_test.py
d) writefile.py / writefile_test1.py & writefile_test2.py
e) readfile.py / readfile_test.py

*Assigment*

Now you are ready to start working on the asignment, which is to complete one of the incomplete newton.py scripts. I have three levels:

EASY
- write part of energy functions
- write part of update equation

INTERMEDIATE
- write complete energy functions
- write complete update equation
- write input section (parse inputfile)

ADVANCED
- write complete energy functions
- write complete update equation
- write input
- write output

If advanced is still to easy you may consider doing an MD program eg for three spheres on two springs that can also interact with each other.