NNSA HSAP Computational Laboratory 7 - 2026 Update

Goals: Molecular Dynamics in Python: Mass on a Spring

First we will discuss what motion (trajectory) we expect for a mass on a spring.

Next we will discuss the idea of Molecular Dynamics.

Finally we will implement Molecular Dynamics in python.

Below is version one of a Molecular Dynamics code for a mass on a spring (no damping) in python. One first has inputs for the number of time steps, mass, initial position, etc followed by the Molecular Dynamics loop which pushed the position and velocity forward in time. The positions and velocities are printed to the screen. Note the use of comment lines preceded by '#'.

```
# INPUTS
N =int(input('Enter N :  '))
dt=float(input('Enter dt:  '))
k =float(input('Enter k :  '))
m =float(input('Enter m :  '))
x =float(input('Enter x0:  '))
v =float(input('Enter v0:  '))

# DO THE MD AND PRINT EACH x,v
for i in range (1,N):
    t=dt*i
    x=x+v*dt
    v=v-k*x*dt/m
    print(t,x)
```

[EX 7-1] Type in this script. Call it something meaningful like "MDmassspring1.py".

[EX 7-2] Run your code for $N = 30, dt = 0.05, k = 8, m = 2, x0 = 5, v0 = 0$. We will discuss what your output is telling you., but first let's make it more readable!

[EX 7-3] Make a copy of your code:

```
cp MDmassspring1.py MDmassspring2.py
```

In the copy (version 2), replace the print statement with

```
    print(f"{t:8.3f}",f"{x:8.3f}")
```

Run your code again with the same parameters. It will now be a lot easier to read!

One **great** thing about python is you can plot things directly without having to use another piece of software. This is a huge advantage it has over languages like C and fortran! To do this we need to put the data into arrays. Alexandria has taught you a bit about this!

[EX 7-4] Start by copying your code again:

```
cp MDmassspring2.py MDmassspring3.py
```

Then edit your code to look like this:

```
# THIS IS NEEDED TO USE ARRAYS IN PYTHON:
from array import *

# THIS IS NEEDED TO MAKE PLOTS IN PYTHON:
import matplotlib.pyplot as plt

# INPUTS
N =int(input('Enter N :  \n'))
dt=float(input('Enter dt:  \n'))
k =float(input('Enter k :  \n'))
m =float(input('Enter m :  \n'))
x =float(input('Enter x0:  \n'))
v =float(input('Enter v0:  \n'))

# START OFF TIME, POSITION, VELOCITY ARRAYS
time =array('f', [0.])
xsave=array('f',[x])
vsave=array('f',[v])

# DO THE MD AND APPEND EACH NEW TIME, POSITION, VELOCITY TO ITS ARRAY
for i in range (1,N):
    t=dt*i
    x=x+v*dt
    v=v-k*x*dt/m
    time.append(t)
    xsave.append(x)
    vsave.append(v)

# MAKE A PLOT
plt.plot(time, xsave)
plt.xlabel('t')
plt.ylabel('x')
plt.show()
```

You will have to be careful to identify the new lines and insert them accurately! Also remove lines no longer needed...

Let's discuss some physics now that we can make nice plots!

[**EX 7-5**] Run your code for $N = 1000, dt = 0.01, k = 8, m = 2, x0 = 5, v0 = 0$.

Let's look carefully at your plot of position x versus time t and see if it is looking as we expect.

- What is x at $t = 0$?
- Does x get bigger or smaller as t increases from $t = 0$? Is the behavior what you expect?
- Is the general shape of x what you expect for a mass on a spring?
- What are we leaving out?

Those are all qualitative things to think about and check, but we can also get precise numbers. The period of the motion is how much time it takes to repeat.

[**EX 7-6**] Estimate the period from your graph.

The usual symbol for the period is T. There is a formula for T:

$$T = 2\pi\sqrt{\frac{m}{k}}$$

[**EX 7-7**] What do you get for T when $m = 2$ and $k = 8$? Does it agree with your graph?

[**EX 7-8**] Run your code for $N = 500, dt = 0.01, k = 8, m = 2, x0 = 5, v0 = 10$.

- How is the general shape of x different from previously when $v0 = 0$?
- Can you explain why?
- What is the period? Has it changed from $v0 = 0$?

[**EX 7-9**] To do on your own if you are interested:
Run your code for $N = 500, dt = 0.01, k = 8, m = 2, x0 = 5, v0 = 10$. Look at the graph of $x(t)$ and see what the largest value of x is. This is called the 'amplitude' A. There is a formula for A:

$$A = \sqrt{x_0^2 + m\,v_0^2/k}$$

Does your plot agree with this formula?

[**EX 7-10**] To do on your own if you are interested:
Change your code to plot velocity as a function of time instead of position.

[**EX 7-11**] To do on your own if you are interested:
Look at your plot of $v(t)$ and get the maximum velocity $v_{\max}$. Does it agree with the formula:

$$v_{\max} = \sqrt{v_0^2 + k\,x_0^2/m}$$

In these exercises you are learning about a very important principle of physics called the conservation of energy.