COSMOS 2022, Computational Lab 05, part one

More Molecular Dynamics

This Lab:

- More classical trajectories: mass on a spring.
- Plotting.

Coming up (countdown to quantum state transfer):

- LRC circuit analogies!
- More classical trajectories: projectile motion in 2D.
- More classical trajectories: Kepler problem???
- Math: Matrices! **(A lot here, will not give details $\cdots$).**
- Energy band of solids **(A lot here, will not give details $\cdots$).**
- Quantum State Transfer **(A lot here, will not give details $\cdots$).**

[01] Write a MD code for a mass on a spring. The force is given by Hooke's Law,

$$F = -k\,x$$

To do this, you can take your MD code for a ball thrown upwards, rename y to x, and replace the gravity force by Hooke's Law. You should probably use the for-loop version of your code.

[02] Run your code for initial $x = 0.02$ and initial $v = 0$. This corresponds physically to stretching the spring and releasing the mass from rest. Use $k = 100$ and $m = 0.1$. Since the period is $T = 2\pi\sqrt{m/k} \sim 0.2$ second, you should use $dt = 0.001$ so that dt is much smaller than T. If you use $N = 1000$ steps, the total elapsed simulation time $t = N\,dt = 1000(0.001) = 1$ second or about five periods.

Make plots of $x(t)$ and $v(t)$. Do you get about five periods?

If you want to check your code more accurately than just roughly looking at a plot, go into the data file and figure out exactly when x returns to its initial value of $x = 0.02$. This will allow you to read off the period by seeing what time it is. (The exact value is = 0.19869.) You will only be able to resolve the period to an accuracy of $dt = 0.001$.

What do you notice about $x(t)$ when $v(t) = 0$? Can you explain?

What do you notice about $v(t)$ when $x(t) = 0$? Can you explain?

[03] Run your code again, changing only the initial position to $x = 0.04$. Make a plot. How does $x(t)$ change? Does the period change?

[04] Run your code again, changing the initial position to $x = 0.00$, but using an initial velocity $v = 0.6$. Make a plot. Does the period change?

[05] Add friction to your code:

$$F = -k\,x - b\,v$$

Run with the same parameters as [02] but now also use $b = 0.1$

Make a plot of $x(t)$. How does it differ from $b = 0.0$ (no friction)? Is what you observe reasonable?

Your code is actually also simulating an 'LRC' circuit! We will discuss this further in a few days.