Homework 10 Write-Up

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1. MOLECULAR DYNAMICS AND MODELING IN VMD

In this week's assignment, we get a better understanding of how to code the motion of atoms and molecular dynamics. We were provided with an MD Example code which produces and XYZ file for the 1D case, which can then be inputted to VMD to visual the motion. Our assignment was to convert the code to also account for 2D motion.

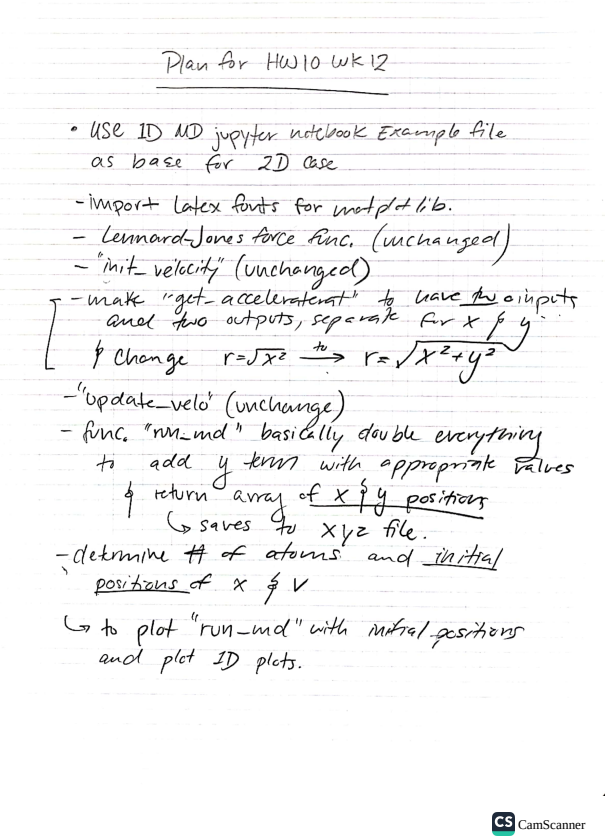

FIG. 1: Plan for HW 10.

The two functions in the example code that required the most altering was the function to calculate acceleration and the actual molecular dynamics simulation function which uses position, velocity, and acceleration to get the consecutive resulting positions. To add the y position, the y equivalent as added for all the terms in these functions.

Also, now that we are accounting for 2D motion, the total distance between two atoms (r) is seen in Equation 1.

$$r = \sqrt{x^2 + y^2} \tag{1}$$

Before plotting, an array for initial positions are determined for both x and y. To check that the updates 2D code still works in the one-dimension (1D), I set the y-velocity to zero and plot the x-positions. In Figure 2 you can see the x-position in 1D and that the code still works. The atoms start equally spaced and drift.

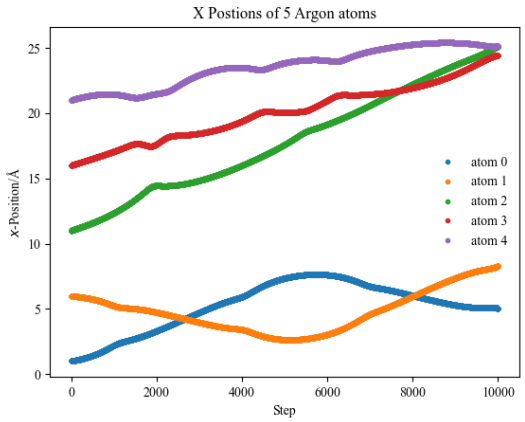

FIG. 2: X-position of Argon atoms.

In Figure 3, I also plotted the y-position in the 1D (which also works) and it can be see that initially there is no velocity, as expected.

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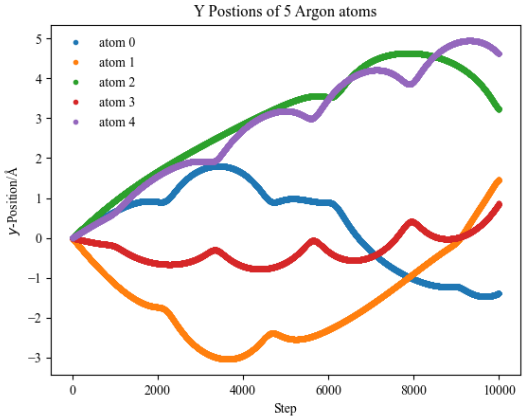

FIG. 3: Y-position of Argon atoms.

The output XYZ file from the MD simulation function can then be visualised in VMD (Visual Molecular Dynamics). Figure 4 shows the frames of the simulation as the atoms disperse in the XY plane.

2. SURVEY QUESTIONS

The homework this week took approximately 5 hours. This assignment was very fun and it was cool to be able to visualize the motion. I think it was a reasonable length. I'd be interested in using different atoms together.

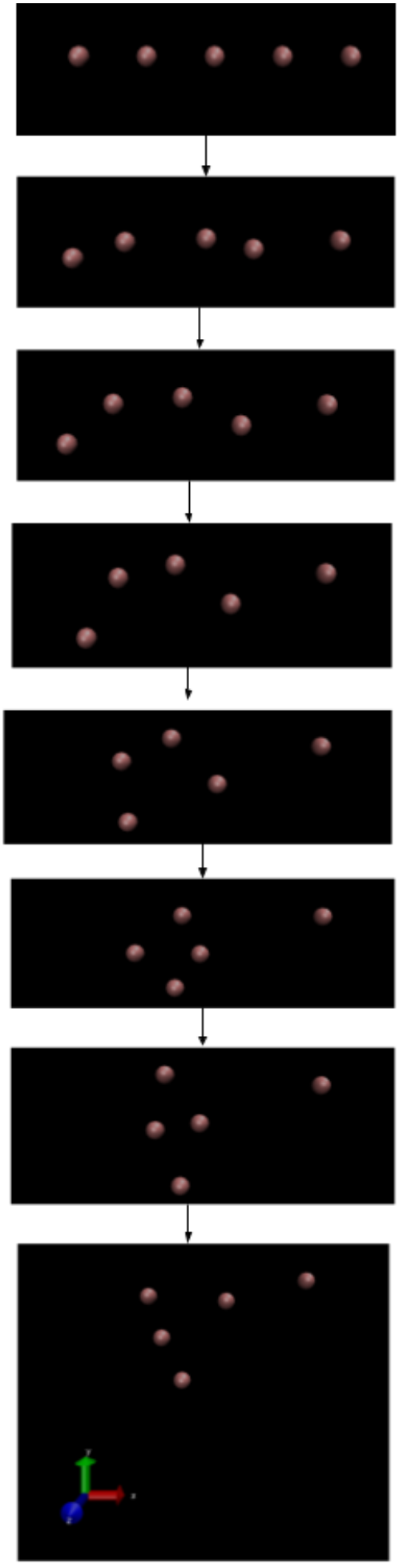

FIG. 4: Motion of 5 argon atoms in XY plane in VMD program.