38 + 5 = 43

43/61

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.

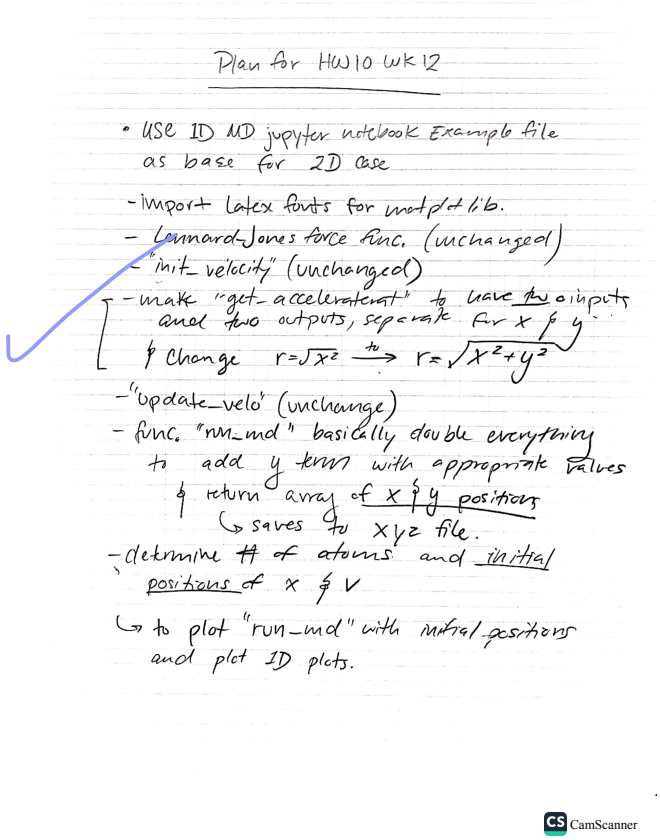

FIG. 1: Plan for HW 10.

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.

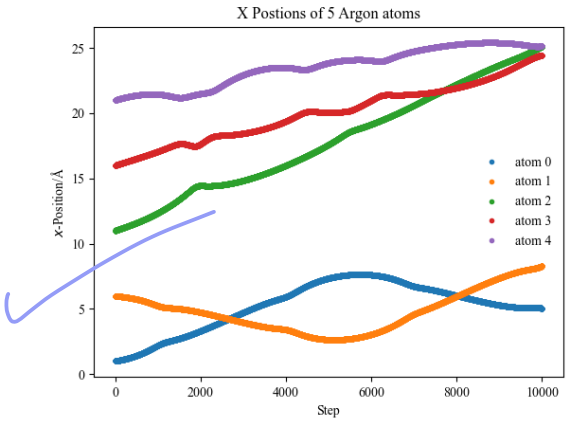

FIG. 2: X-position of Argon atoms.

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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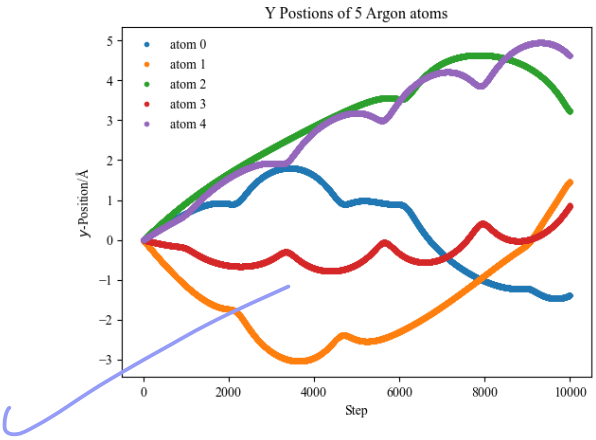

FIG. 3: Y-position of Argon atoms.

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.

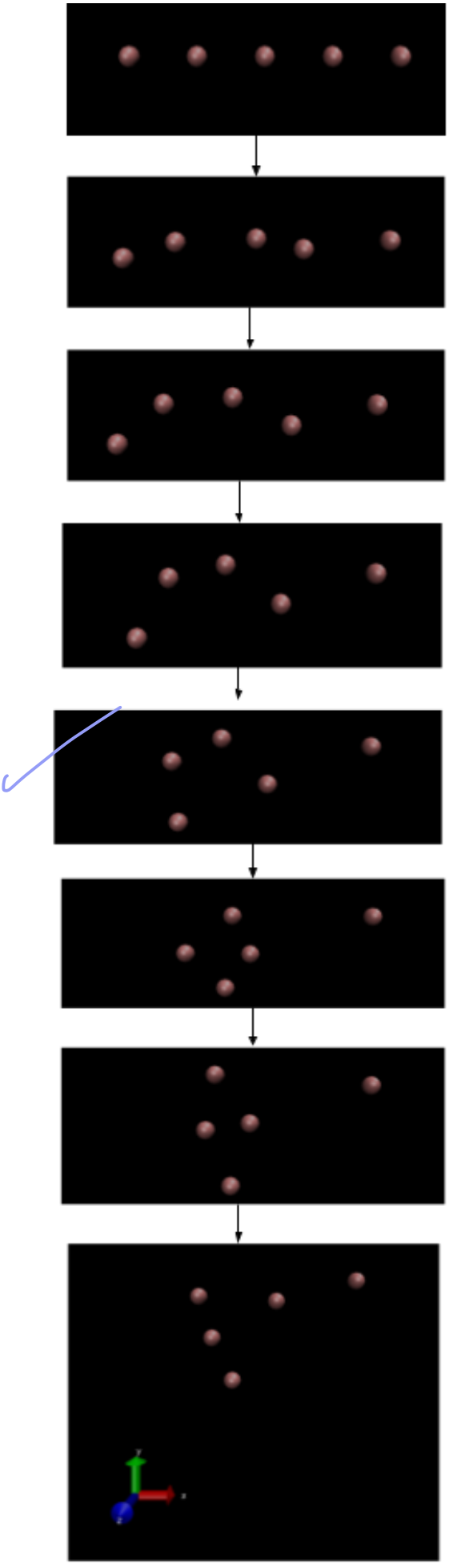

FIG. 4: Motion of 5 argon atoms in XY plane in VMD program.

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.

38/56 (half credit on code)

Computational Physics/Astrophysics, Winter 2024:

Grading Rubrics [1]

Haverford College, Prof. Daniel Grin

For coding assignments, roughly 56 points will be available per problem. Partial credit available on all non-1 items.

4 1. Does the program complete without crashing in a reasonable time frame? (+4 points)

2 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? (+2 points)

3 3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) (+3 points)

5 4. Is the algorithm appropriate for the problem? If a specific algorithm was requested in the prompt, was it used? (+5 points)

4 5. If relevant, were proper parameters/choices made for a numerically converged answer? (+4 points)

4 6. Is the output answer correct? (+4 points).

3 7. Is the code readable? (+3 points)

. 5.1. Are variables named reasonably?

. 5.2. Are the user-functions and imports used?

[1] Inspired by rubric of D. Narayanan, U. Florida, and C. Cooksey, U. Hawaii

. 5.3. Are units explained (if necessary)?

. 5.4. Are algorithms found on the internet/book/etc. properly attributed?

3 8. Is the code well documented? (+3 points)

. 6.1. Is the code author named?

. 6.2. Are the functions described and ambiguous variables defined?

. 6.3. Is the code functionality (i.e. can I run it easily enough?) documented?

9. Write-up (up to 28 points)

5 . Is the problem-solving approach clearly indicated through a flow-chart, pseudo-code, or other appropriate schematic? (+5 points)

✓ . Is a clear, legible LaTeX type-set write up handed in?

3 . Are key figures and numbers from the problem given? (+ 3 points)

4 . Do figures and or tables have captions/legends/units clearly indicated. (+ 4 points)

3 . Do figures have a sufficient number of points to infer the claimed/desired trends? (+ 3 points)

0 . Is a brief explanation of physical context given? (+2 points)

Explain your results and describe the physical interactions between particles −2

1 . If relevant, are helpful analytic scalings or known solutions given? (+1 point)

3 . Is the algorithm used explicitly stated and justified? (+3 points)

2 . When relevant, are numerical errors/convergence justified/shown/explained? (+2 points)

0 . Are 3-4 key equations listed (preferably the ones solved in the programming assignment) and algorithms named? (+2 points)

1 . Are collaborators clearly acknowledged? (+1 point)

2 . Are any outside references appropriately cited? (+2 point)

need more eqs for position & velocity −2