Computer Modelling: Exercise 3

Sam Hanson

November 18, 2023

1 Introduction

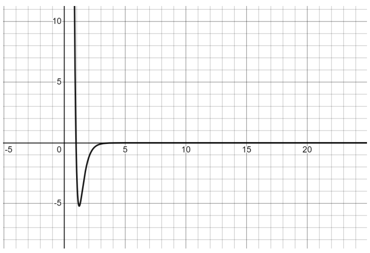


Figure 1: Desmos plot of Morse potential for O_2 parameters.

Exercise 3 asks to simulate 2 oscillating particles using the Morse potential (see equation 1) and the force on the particles $\mathbf{F} = -\nabla U_M$.

$$U_M(\mathbf{r_1}, \mathbf{r_2}) = D_e([1 - e^{-\alpha(r_{12} - r_e}]^2 - 1) \tag{1}$$

$$\mathbf{F_1}(\mathbf{r_1}, \mathbf{r_2}) = 2\alpha D_e[1 - e^{-\alpha(r_{12} - r_e)}]^2 e^{-\alpha(r_{12} - r_e)} \hat{\mathbf{r_{12}}} \tag{2}$$

Where $r_{12} = \mid \mathbf{r_2} - \mathbf{r_1} \mid$, $\hat{\mathbf{r_{12}}} = \frac{\mathbf{r_{12}}}{r_{12}}$ and $\mathbf{F_1} = -\mathbf{F_2}$ due to Newton's third law. α, D_e and r_e control the depth and curvature of the potential minimum, shown in figure 1 [1].

As the code simulates atoms, for the code to be sensible we use incredibly small units, like eV, Å and amu. The time units in the code are not seconds but are shown in equation 3, giving a value of $T = 1.02 \times 10^{-14}\ s$.

$$T = \text{Å}\sqrt{\frac{amu}{eV}} \tag{3}$$

In this code we are measuring the wavenumber of oscillation of the particles and the energy variation of the simulation. Wavenumber is related to period by $\bar{v} = \frac{v}{c} = \frac{1}{Tc}$, similar to $k = \frac{2\pi}{Tc}$. Energy variation increases with time-step (seen in figure 2b) and oscillates along with position.

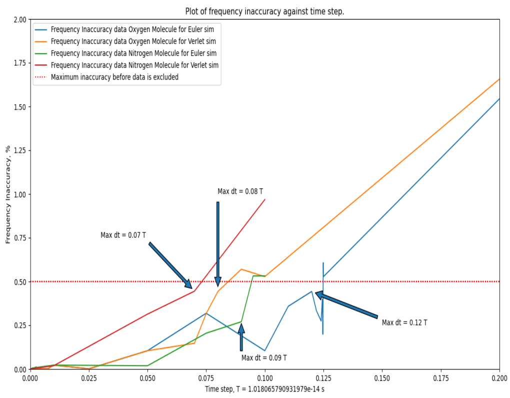
2 Calculating Maximum Time-Step

Table 1 shows the maximum time-step for each simulation. These values are also shown in figure 2. The values were calculated by comparing the frequency of each simulation to the same simulation at a time step, $dt = 10^{-5}T$. Equation 4 shows the calculation for the frequency inaccuracy, where v_0 is the frequency at $dt = 10^{-5}T$.

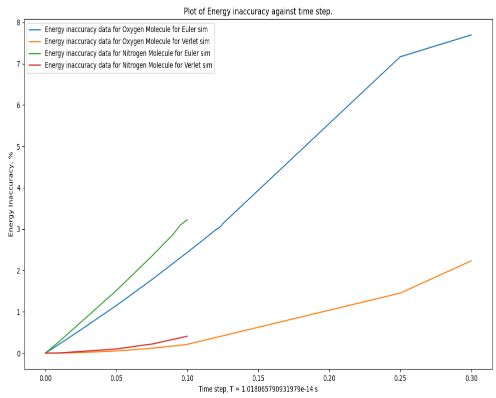
$$\frac{\Delta v}{v_0} \equiv \frac{\mid v - v_0 \mid}{v_0} \tag{4}$$

Table 1: Table showing maximum time-steps for each simulation method and molecule simulated. Units given in Figure 2.

Simulation	Molecule	Maximum Time-step (T)
Symplectic Euler	Oxygen	0.12
Symplectic Euler	Nitrogen	0.09
Velocity Verlet	Oxygen	0.08
Velocity Verlet	Nitrogen	0.07



(a) Plot of frequency inaccuracy against time-step for O_2.



(b) Plot of energy inaccuracy against time-step for O_2.

Figure 2: Plots showing inaccuracy of frequency and energy as time-step increases for the Euler and Verlet simulation of O_2 and N_2.

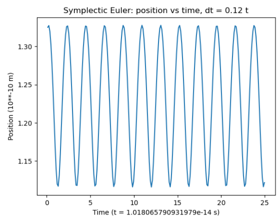
3 Results

Table 2 shows the wavenumber measurements for all simulations with the maximum time-step for each simulation. These values are an underestimate on the experimental values. The spinned simulations (2D velocity) show this significantly more than the 1D oscillations. Other than that both simulation methods (Euler and Verlet) agree with each other so a place where the simulations go wrong could be initialising the particles or calculations of the force. The code is a good simulator for the Morse potential between 2 particles. Symplectic Euler simulation plots can be seen in figure 3, Verlet simulations are in figure 4. The code measures the position as the distance between particle 1 and particle 2. Applying a spin to both particles produces rotational frequency on top of the vibrational frequency, complicating the period analysis, thus giving an inaccurate wavenumber measurement. The code could be improved to find the distance between each particle and a common center.

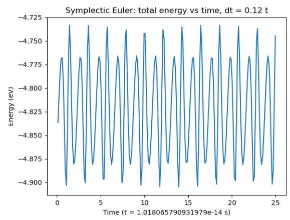
Velocity Verlet integration method is much better at keeping energy constant which can be seen in figure 2b as the Verlet lines have a smaller gradient than the Euler lines. However, in the way that Verlet is better at keeping energy constant, the Euler method produces more accurate frequencies, as shown in table 1 and figure 2a, as Euler simulations have a higher maximum time-step and generally lower frequency inaccuracies than Verlet simulations.

Table 2: Table of wavenumbers for all simulations Including experimental values for O_2 and N_2 from [1].

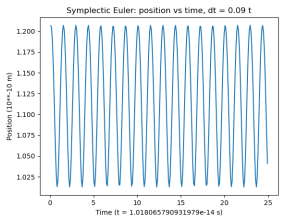
Simulation	Wavenumber Measured cm^{-1}
1D Symplectic Euler O_2	1532
2D Symplectic Euler O_2	1386
1D Velocity Verlet O_2	1532
2D Velocity Verlet O_2	1384
Experimental O_2	1580
1D Symplectic Euler N_2	2293
2D Symplectic Euler N_2	2198
1D Velocity Verlet N_2	2297
2D Velocity Verlet N_2	2201
Experimental N_2	2359



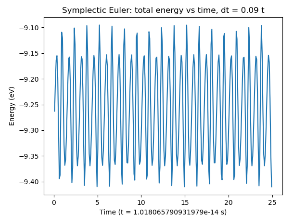
(a) Position plot for O_2.



(b) Energy plot for O_2.



(c) Position plot for N_2.

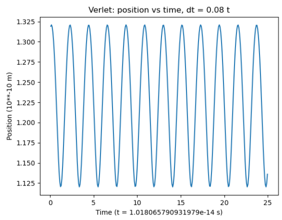


(d) Energy plot for N_2.

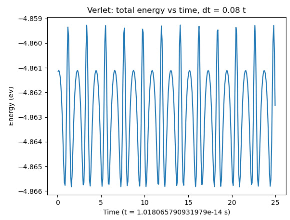
Figure 3: Plots of Symplectic Euler simulation.

References

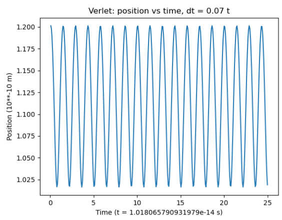
1. Zuntz, J. *Computer Modelling Exercise 3* `https://www.learn.ed.ac.uk/ultra/courses/_111189_1/outline/file/_9269517_1` (Nov. 7, 2023).



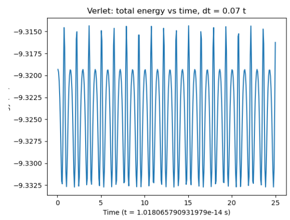
(a) Position plot for O_2.



(b) Energy plot for O_2.



(c) Position plot for N_2.



(d) Energy plot for N_2.

Figure 4: Plots of Velocity Verlet simulation.