# Computer Modelling Exercise 3 Group Report

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Due Thursday Week 11

In this exercise we were tasked with implementing a class in python to represent a particle in three dimensions. We were to use that class and implement two different time integration algorithms (Euler and Verlet) and use these to simulate vibrating oxygen and nitrogen molecules.

One weakness of discrete integrators is their susceptibility to large errors when the timestep is set too large. Below are two plots with timesteps $\Delta t = 0.1u$ and $\Delta t = 1u$ over the same time interval. Each u unit of time (for the timestep) corresponds to 10.8fs.
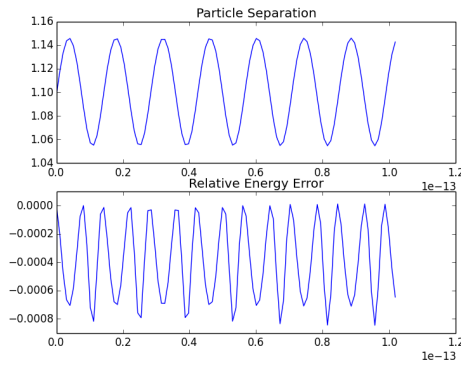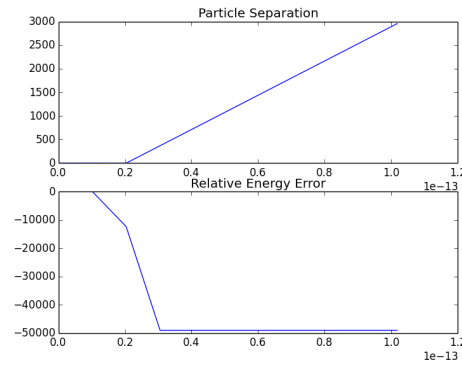
$\Delta t = 0.1 \times (10.8\text{fs})$ $\Delta t = 1 \times (10.8\text{fs})$

The left figure is clearly showing signs of inaccuracy and is rather jagged. The right figure is wildly inaccurate.

To determine the $dt_{\max}$ we have to find the largest possible dt such that the relative energy error has magnitude less than 10^{-3}. This will be different for each integrator. For the velocity Verlet integrator we find that $dt_{\max} \approx 0.1u$ For the symplectic Euler integrator we find that $dt_{\max} \approx 0.015u$, which is far smaller than the maximum

timestep for the Verlet integrator. This shows that the Verlet integrator is more accurate with a larger timestep.

When we run the Verlet integrator for a decent period of time with the timestep set to $dt_{\max}$. We can determine the frequency of oscillation using XMGrace. We determine the period of N_2 without spin to be $T = 1.40 \times 10^{-14}$s, so we determine $f = 1/T = 7.14 \times 10^{13}$Hz from which we derive the wavelength λ using $c = \lambda f$. We see that $\lambda = 4.20 \times 10^{-6} m$. To compute the inverse wavelength we take the inverse of this and see that $\nu(N_2) = 238260\text{m}^{-1}$ which corresponds to $\nu(N_2) = 2382\text{cm}^{-1}$ which is close to the experimental result of $\nu(N_2) = 2359 cm^{-1}$.

Following the same procedure we will tabulate the vibrational frequencies below.

	Calculated Frequency (cm^{-1})	Experimental Results (cm^{-1})
$\nu(N_2)$		
No spin	2382	2359
Spin	2197	–
$\nu(O_2)$		
No spin	1564	1580
Spin	1506	–

The frequencies for the oscillation decrease for the systems in which the atoms have spin. This is because they are

Below is a sample graph of the particle separations within the nitrogen with spin and the nitrogen without spin.
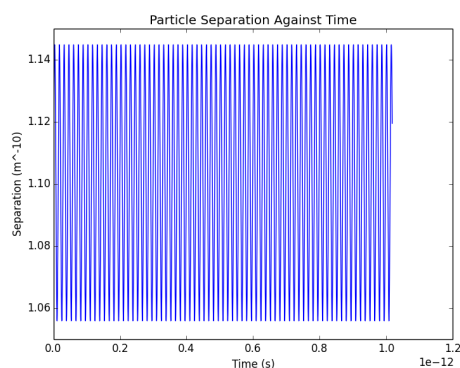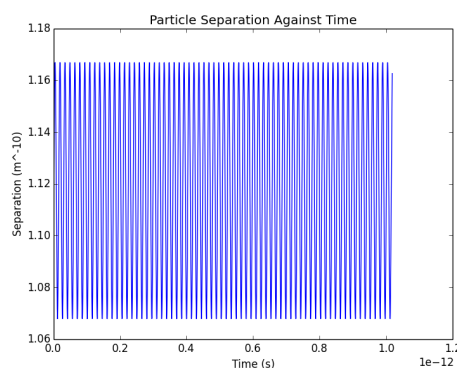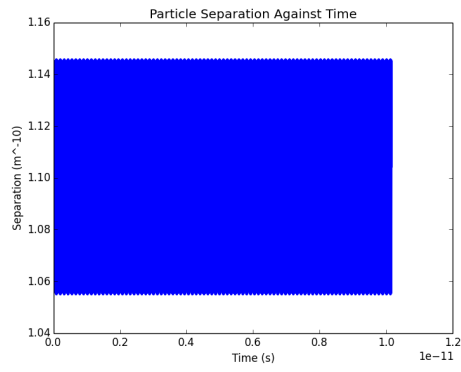

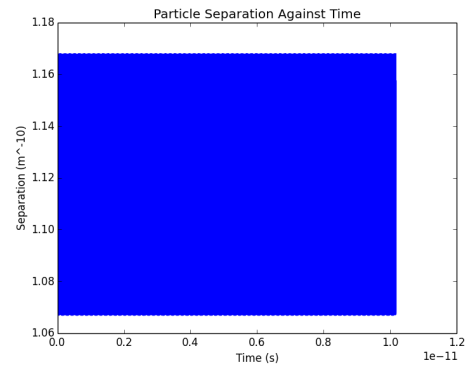N_2 particle separations without spin N_2 particle separations with spin

It can be seen that the graphs look very similar on small scales such as these. However if you run them over a longer period of time you can see the difference in

the envelope very clearly.

N_2 particle separations without spin N_2 particle separations with spin

You can see that the one without spin is more 'jagged', for lack of a better word.