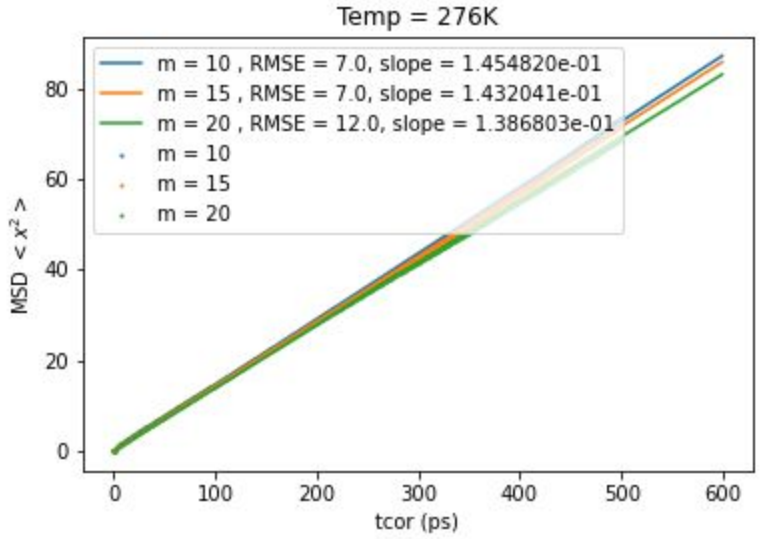
MSD_Assignment_Q1

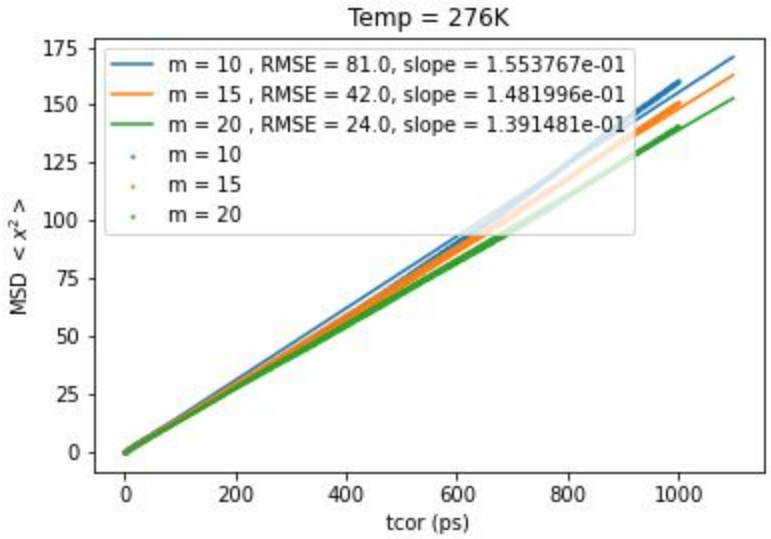
Name : Abhay Kshirsagar **ROll.No** : 19MS172

A . Calculate and plot the Mean Squared Displacement with two different values of the correlation time, and three sets of molecule numbers, for each temperature .

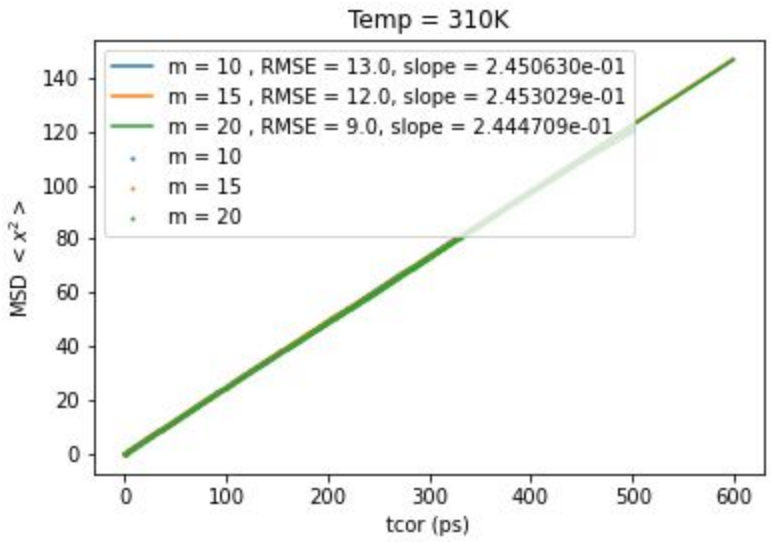
I have used the SciPy library of python for fitting the data. Below are the six plot two sets of the three different temperatures. For each temperature the top plot is plotted for correlation time 500s and the bottom one is for the 1000s. Each plot has been plotted for 10, 15 and 20 molecules. The time is in pico sec and

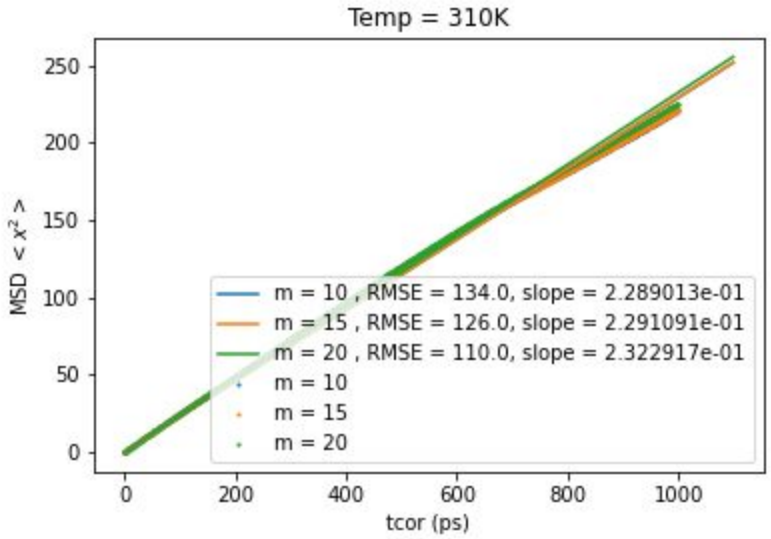
For the temperature 276K :



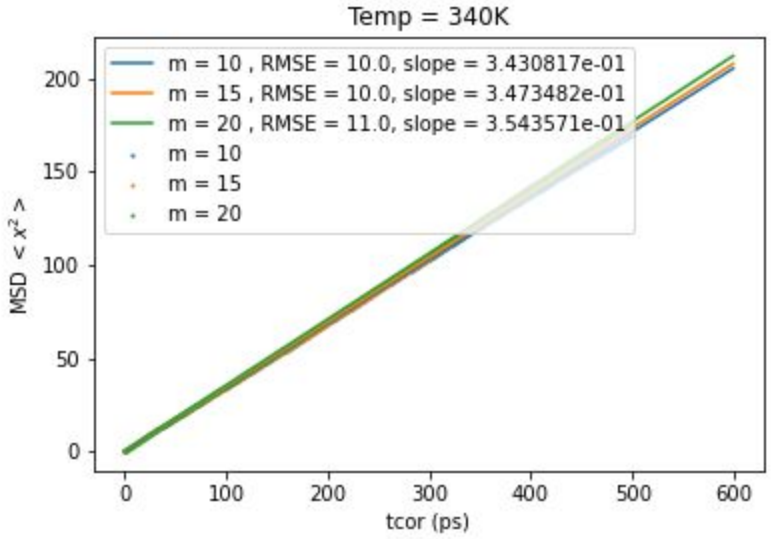


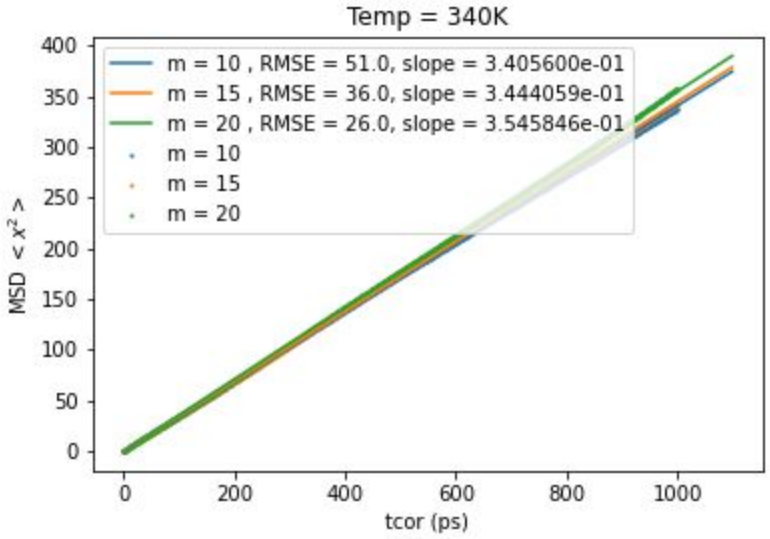
For the temperature 310K :





For the temperature 340K :





B . Tabulate your data

Now we know that

$$< x^2 > \; = \; 6 \, D \, t$$

This transforms to

$$slope \; = \; 6 \, D$$

Thus

$$D \; = \; slope \, / \, 6$$

We will divide the values of D" by 1000 to convert it to $cm^2 \, s^{-1}$
For temperature 276 K :

Molecules	**Corr Time**	**Slope**	**RMSE**	**D($cm^2 \, s^{-1}$)**
10	500	0.14548201	6.817272467	2.42E-05
15	500	0.14320409	7.226112632	2.39E-05
20	500	0.13868026	12.46797952	2.31E-05
10	1000	0.15537675	81.19701834	2.59E-05
15	1000	0.14819963	42.37211226	2.47E-05
20	1000	0.13914811	23.84978341	2.32E-05

The mean D for each time correlation can be calculated as follows

Mean 500	2.37E-05
Mean 1000	2.46E-05

For temperature 310 K :

Molecules	Corr Time	Slope	RMSE	D($cm^2\ s^{-1}$)
10	500	0.24506301	12.72308366	4.08E-05
15	500	0.24530291	11.58193403	4.09E-05
20	500	0.24447089	8.556737168	4.07E-05
10	1000	0.2289013	134.2174983	3.82E-05
15	1000	0.22910905	126.3140433	3.82E-05
20	1000	0.23229174	110.0511037	3.87E-05

The mean D for each time correlation can be calculated as follows

Mean 500	4.08E-05
Mean 1000	3.84E-05

For temperature 340 K :

Molecules	Corr Time	Slope	RMSE	D($cm^2\ s^{-1}$)
10	500	0.34308173	9.622266628	5.72E-05
15	500	0.34734819	9.931105238	5.79E-05
20	500	0.35435713	10.92348059	5.91E-05
10	1000	0.34056005	50.99607238	5.68E-05
15	1000	0.34440589	36.37734395	5.74E-05
20	1000	0.35458461	25.81283598	5.91E-05

The mean D for each time correlation can be calculated as follows

Mean 500	5.80E-05
Mean 1000	5.78E-05

C . Estimate the the values of the slopes and the corresponding D

Solved in B

D . Comment on which one you consider the most appropriate estimate, providing your reasons.

Answer :

The most appropriate estimate for each temperature is given below

Temperature (K)	**Estimate of D($cm^2\ s^{-1}$)**
276	2.46E-05
310	3.84E-05
340	5.78E-05

We take approximately ⅛ th of 8000 ps thus the time corresponding to this value is 1000. The graph is also comparatively linear thus. Another reason for choosing this value is that the error is considerably within the acceptable range. We can also see that the value of D increases with temperature.

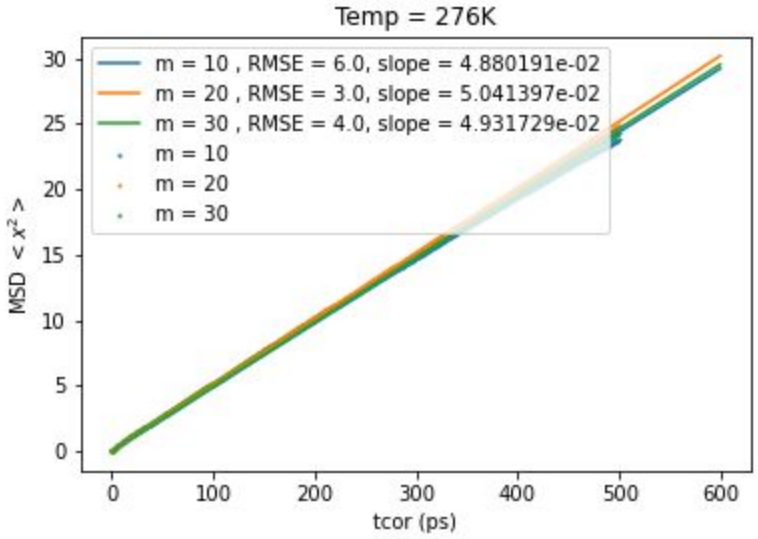
MSD_Assignment_Q2

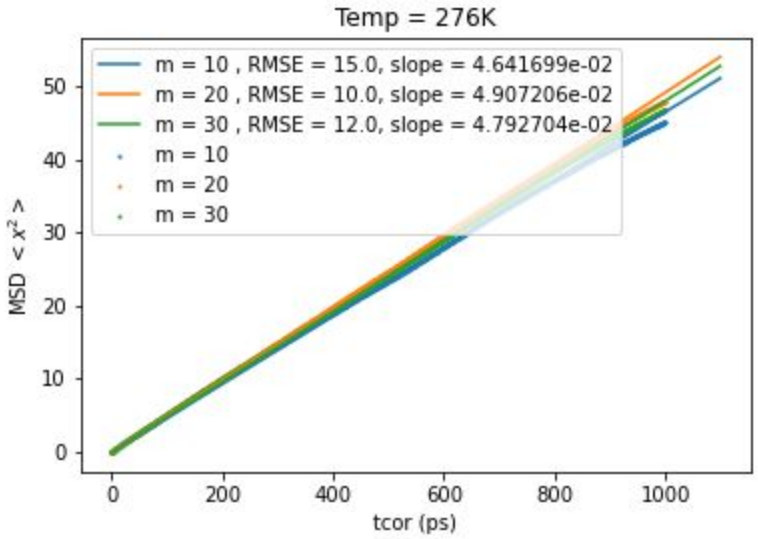
Name : Abhay Kshirsagar **ROll.No** : 19MS172

A . Calculate and plot the Mean Squared Displacement with two different values of the correlation time, and three sets of molecule numbers, for each temperature .

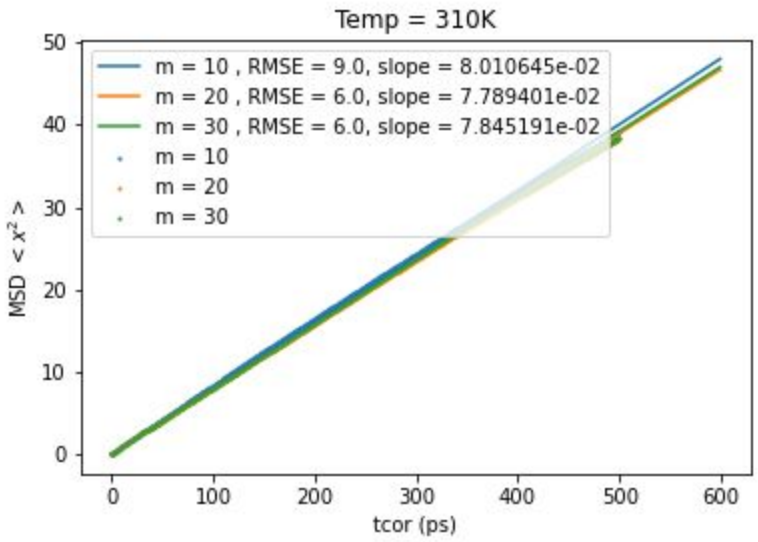
I have used the SciPy library of python for fitting the data. Below are the six plot two sets of the three different temperatures. For each temperature the top plot is plotted for correlation time 500s and the bottom one is for the 1000s. Each plot has been plotted for 10, 15 and 20 molecules.

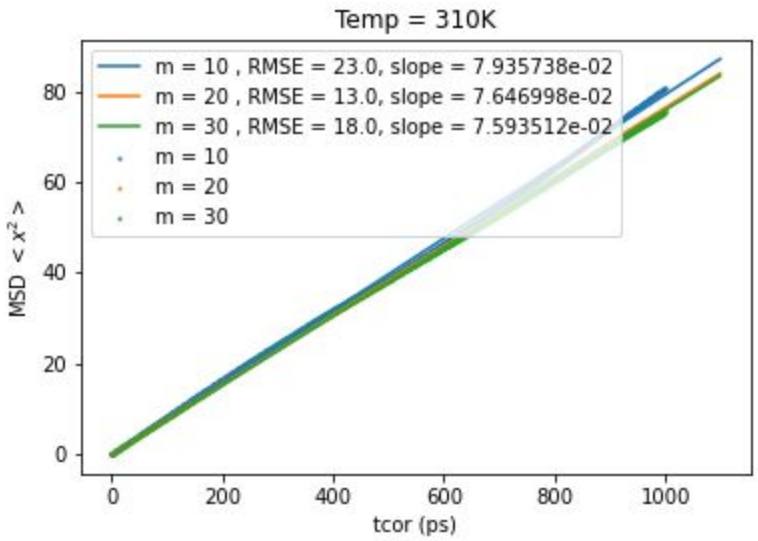
For the temperature 276K :



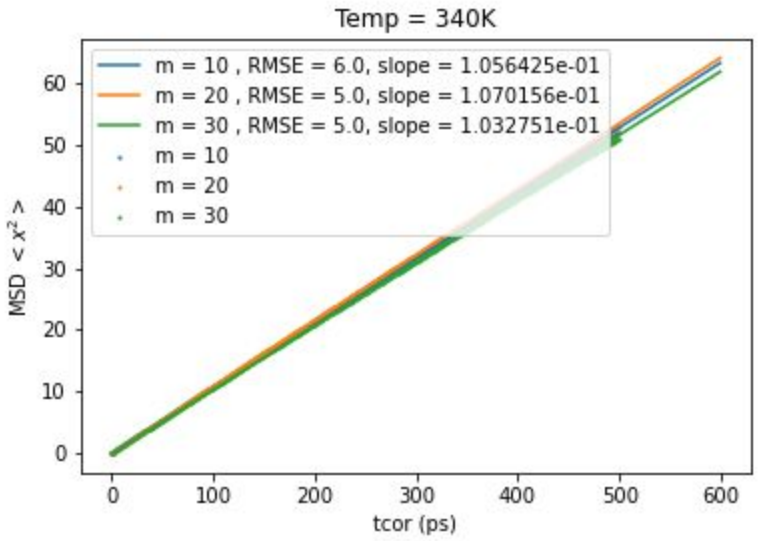


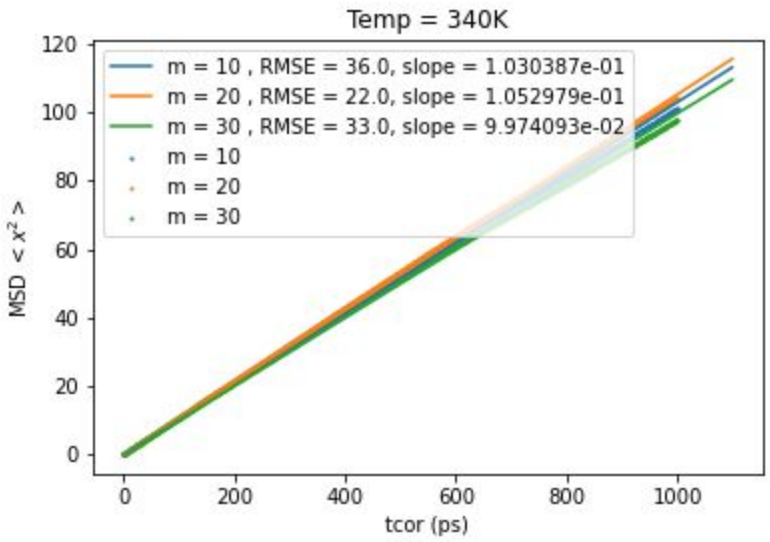
For the temperature 310K :





For the temperature 340K :





B . Tabulate your data

Now we know that

$$< x^2 > \; = \; 6 \, D \, t$$

This transforms to

$$slope \; = \; 6 \, D$$

Thus

$$D \; = \; slope \, / \, 6$$

We will divide the values of D" by 1000 to convert it to $cm^2 \, s^{-1}$

For temperature 276 K :

Molecules	**Corr Time**	**Slope**	**RMSE**	**D($cm^2 \, s^{-1}$)**
10	500	0.04880191	5.825958655	8.13E-06
20	500	0.05041397	3.410315109	8.40E-06
30	500	0.04931729	4.347296013	8.22E-06
10	1000	0.04641699	14.93685059	7.74E-06
20	1000	0.04907206	10.27582121	8.18E-06
30	1000	0.04792704	12.01314195	7.99E-06

The mean D for each time correlation can be calculated as follows

Mean 500	8.25E-06
Mean 1000	7.97E-06

For temperature 310 K :

Molecules	Corr Time	Slope	RMSE	D($cm^2\ s^{-1}$)
10	500	0.08010645	8.726245658	1.34E-05
20	500	0.07789401	5.982508724	1.30E-05
30	500	0.07845191	6.436347711	1.31E-05
10	1000	0.07935738	23.10088632	1.32E-05
20	1000	0.07646998	13.46020707	1.27E-05
30	1000	0.07593512	18.14884305	1.27E-05

The mean D for each time correlation can be calculated as follows

Mean 500	1.31E-05
Mean 1000	1.29E-05

For temperature 340 K :

Molecules	Corr Time	Slope	RMSE	D($cm^2\ s^{-1}$)
10	500	0.10564253	5.905473397	1.76E-05
20	500	0.10701561	5.183326308	1.78E-05
30	500	0.10327508	5.257260819	1.72E-05
10	1000	0.10303866	36.39200703	1.72E-05
20	1000	0.10529788	21.97280664	1.75E-05
30	1000	0.09974093	33.05706925	1.66E-05

The mean D for each time correlation can be calculated as follows

Mean 500	1.76E-05
Mean 1000	1.71E-05

C . Estimate the the values of the slopes and the corresponding D

Solved in B

D . Comment on which one you consider the most appropriate estimate, providing your reasons.

Answer :

The most appropriate estimate for each temperature is given below

Temperature (K)	**Estimate of D($cm^2\ s^{-1}$)**
276	7.97E-06
310	1.29E-05
340	1.71E-05

We take approximately ⅛ th of 8000 ps thus the time corresponding to this value is 1000. The graph is also comparatively linear thus. Another reason for choosing this value is that the error is considerably within the acceptable range. We can also see that the value of D increases with temperature.

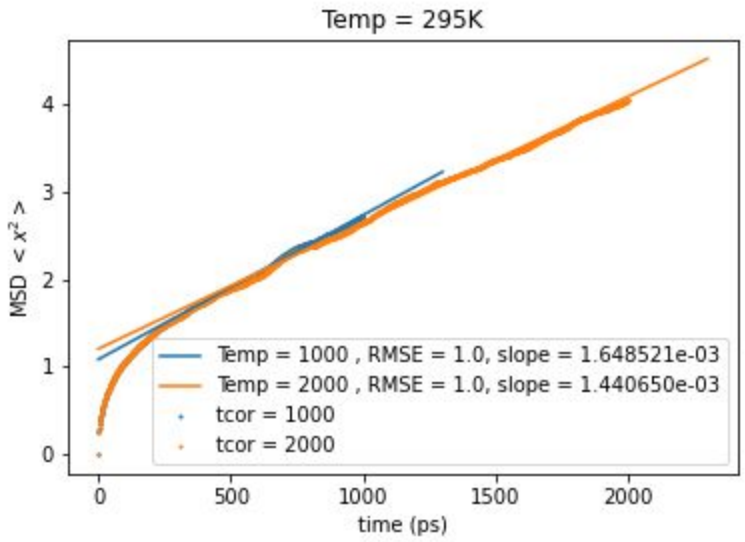
MSD_Assignment_Q3

Name : Abhay Kshirsagar **ROll.No** : 19MS172

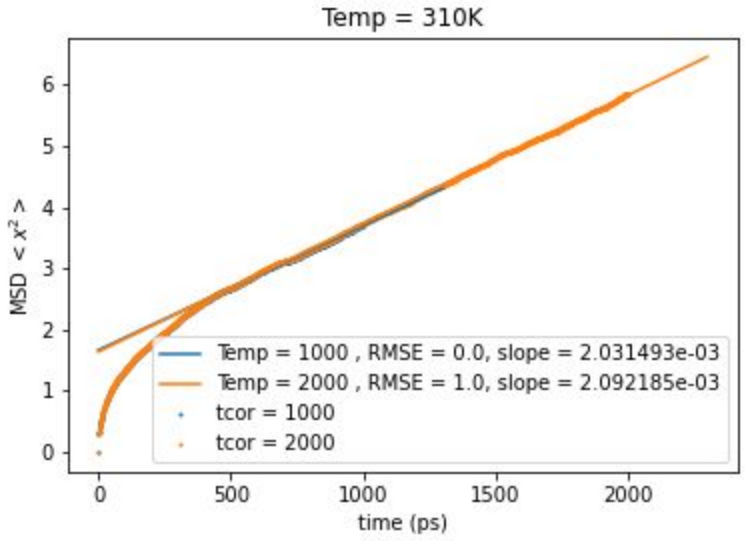
A . Calculate and plot the Mean Squared Displacement with two different values of the correlation time for each temperature

I have used the SciPy library of python for fitting the data. Below are the three plot's each for different temperatures. For each plot two correlation times are chosen 1000 ps and 2000 ps and fitted from the origin.

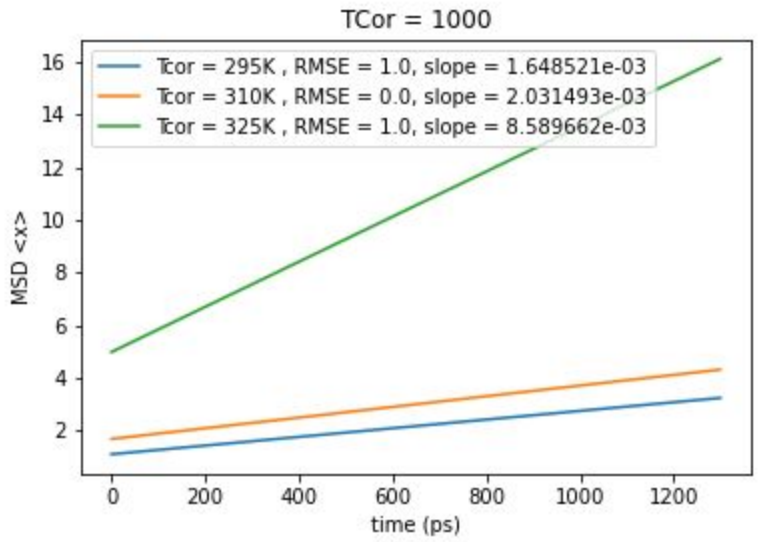
For temperature 295 K :



For temperature 310 K :



For temperature 340 K :



B . Compare the values of the slopes and the D. Comment on which one you consider the most appropriate estimate, providing your reasons

We will divide the values of "D" by 10000 to convert it to $cm^2\ s^{-1}$
For temperature 295 K:

Corr Time	**Slope**	**RMSE**	**D($cm^2\ s^{-1}$)**
1000	0.01683314	1.577428136	2.81E-07
2000	0.01690834	1.579947772	2.82E-07

For temperature 310K:

Corr Time	**Slope**	**RMSE**	**D($cm^2\ s^{-1}$)**
1000	0.0209854	1.844785199	3.50E-07
2000	0.02109161	1.848014577	3.52E-07

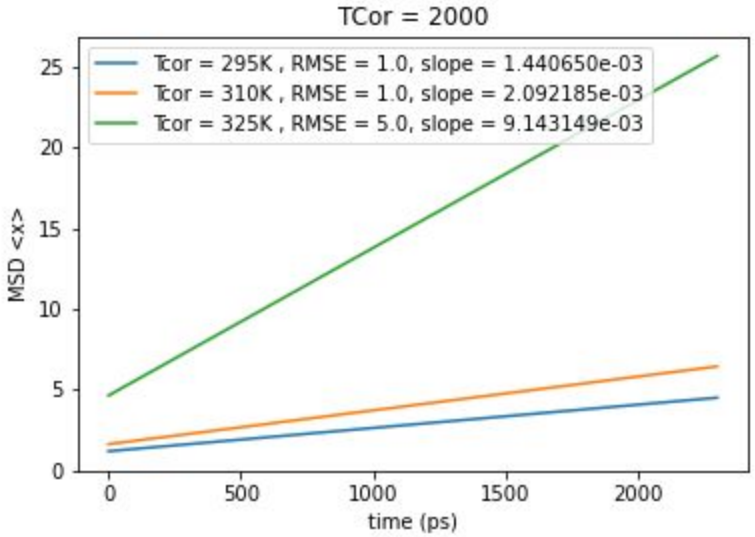
For temperature 340 K:

Corr Time	**Slope**	**RMSE**	**D($cm^2\ s^{-1}$)**
1000	0.05446275	3.125355253	9.08E-07
2000	0.05456998	3.126253311	9.09E-07

From the "D" we can see that there isn't much difference in Diffusion coefficient the error is in an acceptable range. Although the value obtained for 2000 frames is still a better approximation to the original value. This is a type of subdiffusion where the msd is lower than the msd of a normal diffusion thus we have fitted the curve for initial linear data points to get a tangent from the origin to the curve.

C . Report if D scales with temperature in this case. Provide a short discussion

Yes as the temperature scales up the msd also increases. As msd is directly proportional to D the DIffusion coefficient will also increase this can be seen in the following plots for 2000 ps correlation time.



The more temperature we add to the system we increase its energy as well this leads to more and more molecules gaining more energy and thus the rate of diffusion increases as the velocity of the particles increases.