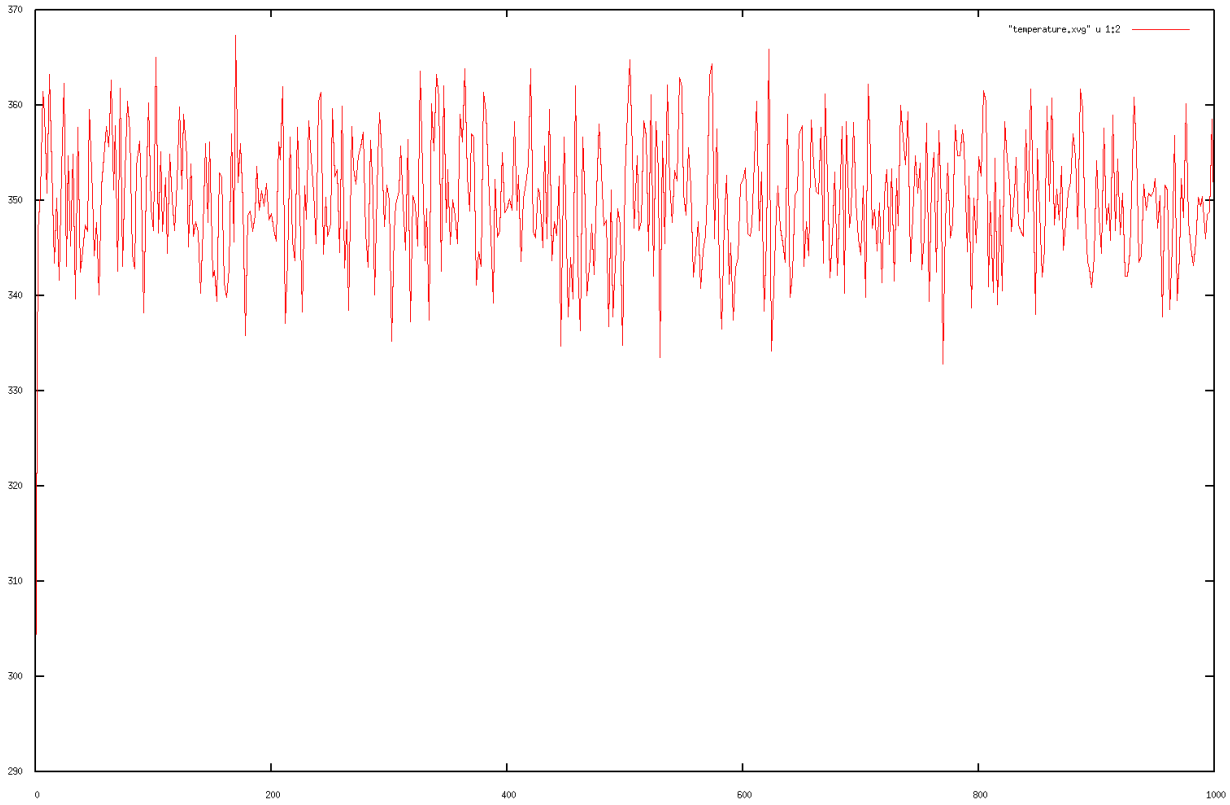
MOLSIM-HW3

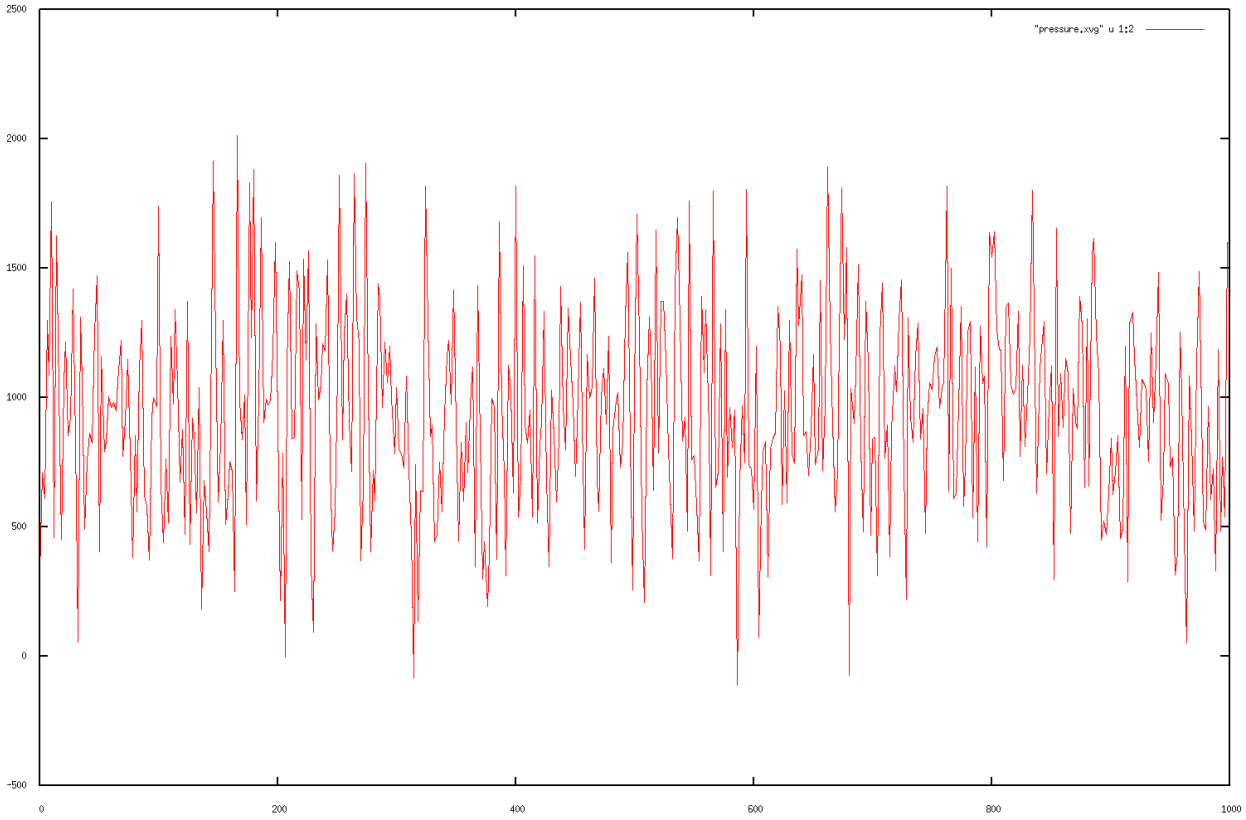
1) a) The NVT simulation was run and the average and RMSD temperature was recorded. The plot is shown below as well.

Energy	Average	Err.Est.	RMSD	Tot-Drift
Temperature	349.868	0.24	7.08983	-0.832525 (K)



b) The NVT simulation was run and the average and RMSD pressure was recorded. The plot is shown below as well.

Energy	Average	Err.Est.	RMSD	Tot-Drift
Pressure	939.752	10	393.862	34.6238 (bar)

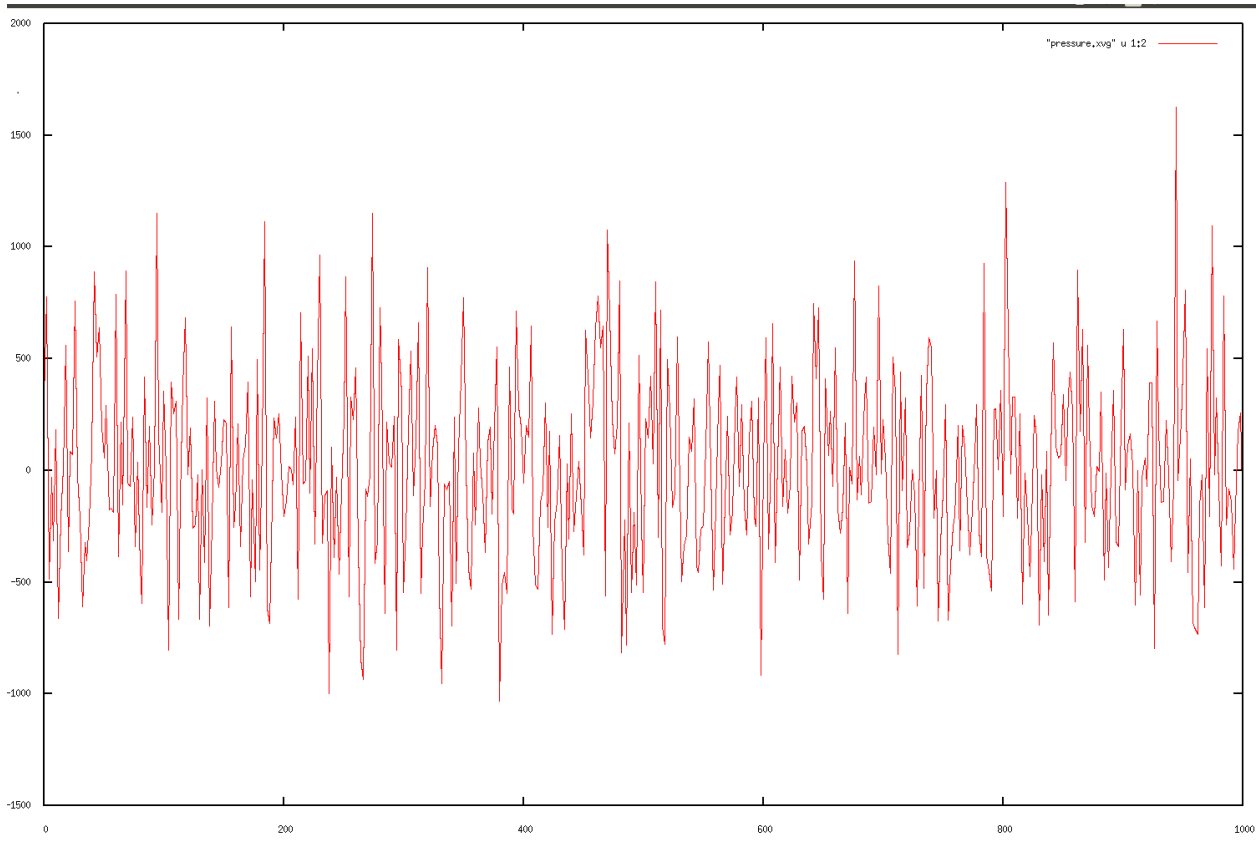


The NPT simulation was run and the average and RMSD temperature and pressure was recorded for:

a) 0.1 tau, also the graph for this particular pressure simulation is shown below

Energy	Average	Err.Est.	RMSD	Tot-Drift
Temperature	349.868	0.24	7.08983	-0.832525 (K)

Energy	Average	Err.Est.	RMSD	Tot-Drift
Pressure	7.60542	8.7	424.804	13.959 (bar)



b) 1 tau

Energy	Average	Err.Est.	RMSD	Tot-Drift
Temperature	349.435	0.41	6.98059	-1.60213 (K)

Energy	Average	Err.Est.	RMSD	Tot-Drift
Pressure	-4.4555	11	395.082	34.9963 (bar)

c) 10 tau

Energy	Average	Err.Est.	RMSD	Tot-Drift
Temperature	351.753	1.2	9.12858	3.13464 (K)

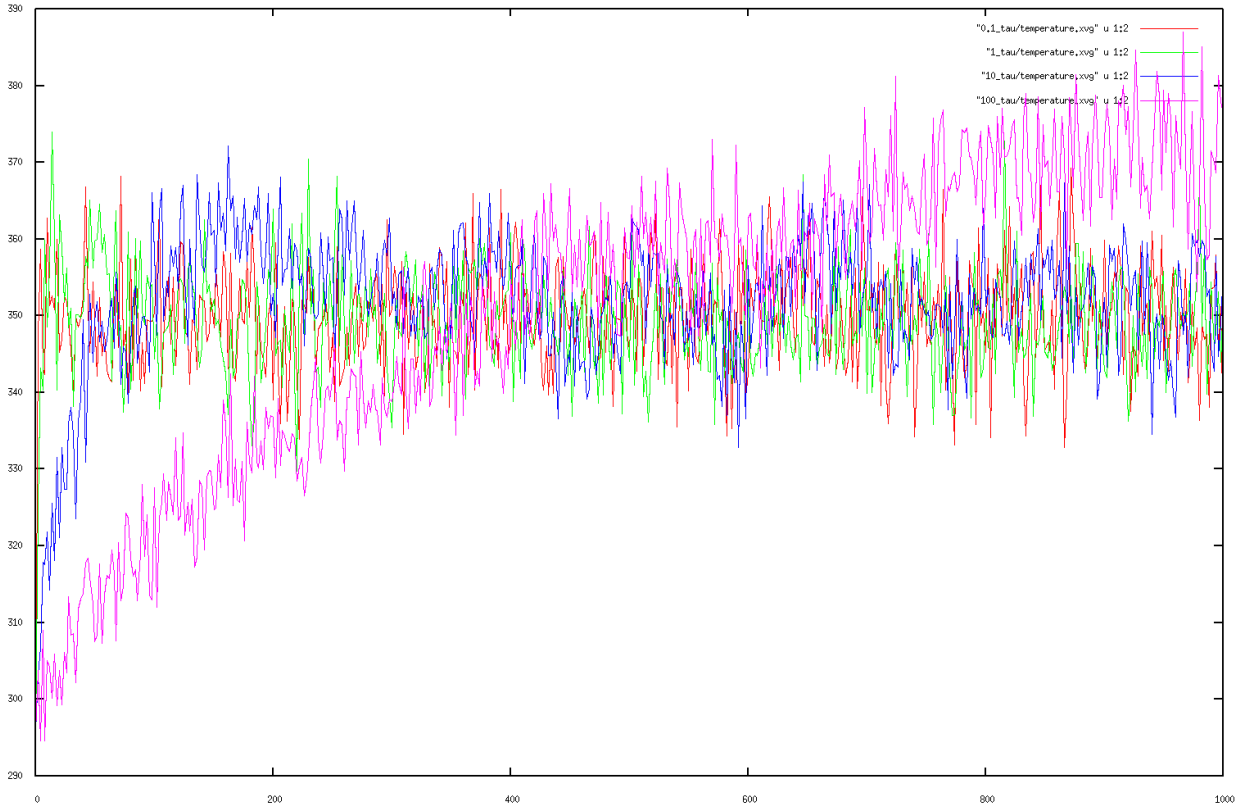
Energy	Average	Err.Est.	RMSD	Tot-Drift
Pressure	29.351	13	395.288	-21.957 (bar)

d) 100 tau

Energy	Average	Err.Est.	RMSD	Tot-Drift
Temperature	350.699	9.1	19.8475	62.4284 (K)

Energy	Average	Err.Est.	RMSD	Tot-Drift
Pressure	-7.07886	29	390.885	-155.789 (bar)

The Plot of temperature v/s time for all the 4 NPT simulations is shown below:



Inferences drawn:

- The simulation with the lowest temperate RMSD is for NPT when tau =1. The value is 6.98059.
- The plot for pressure in the NVT simulation differs from the plot for pressure in the NPT simulation for tau_0.1.The average pressure is 939.752 bar for the former and 7.60542 bar for the latter.

- The RMSD (Root mean square deviation) is the measure of the average distance between the atoms. For values of tau _0.1 and tau_1, the RMSD is almost the same. However, for tau_10 and higher, the values increase greatly. Hence for values of tau greater than 1, the simulations seem unreliable.
- For NVT, the thermostat used is v-rescale. As pressure is not regulated, no barostat is used.
- For NPT, the thermostat used is v-rescale and the barostat used is parrinello-rahman.

  Question:
  Which barostat or thermostat should be used for which applications? Is there a way to regulate that on Gromacs or is it designed for specific applications?