Computational Physics HW7

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1 Introduction

In this assignment we simulate a small system of particles in an pseudo-ideal gas scenario.

2 Results

2.1 Question 1

Seen below are snapshots of 2 different systems with similar starting configurations, but different instal energies. The lower energy system would correspond to something akin to a droplet of water. Some molecules have enough energy to escape the system i.e. evaporate, while the high energy system is like that of a gas where every molecule is energetic enough to turn to steam.

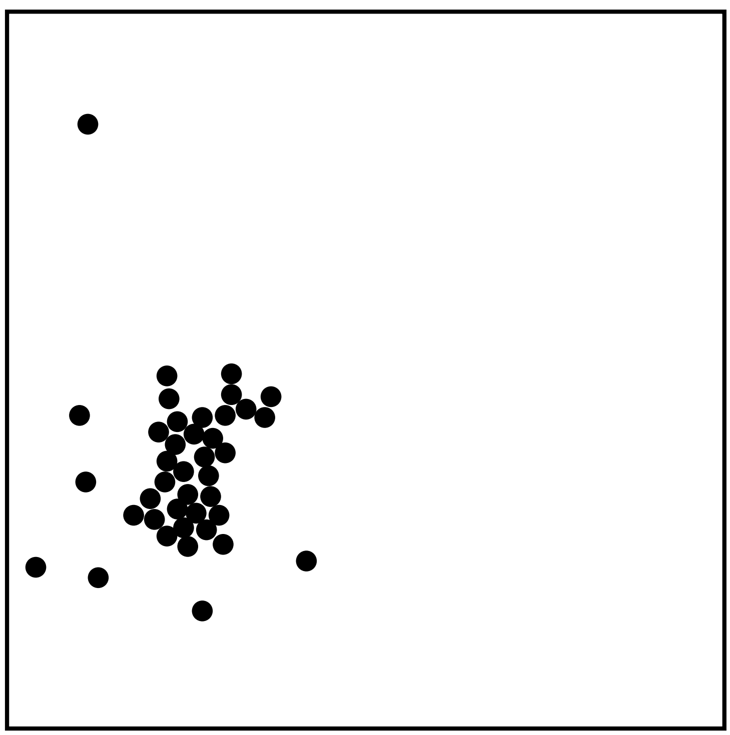

Figure 1: A system of 80 molecules where initially $\frac{E}{N} = -1.2$: Most remain clustered together after thermalization.

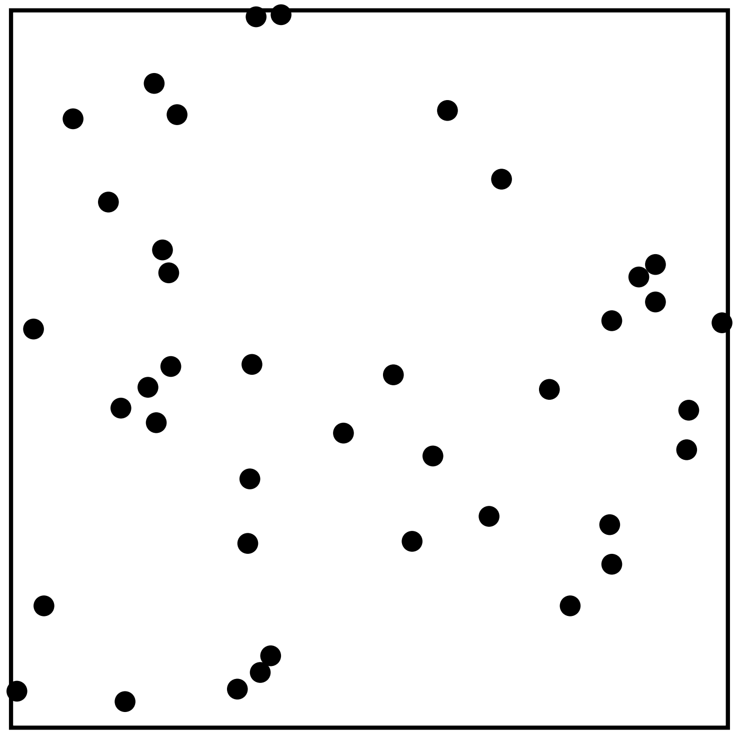

Figure 2: A system of 80 molecules where initially $\frac{E}{N} = 4$: The molecules rapidly escape the potential wells of the other molecules.

2.2 Question 2

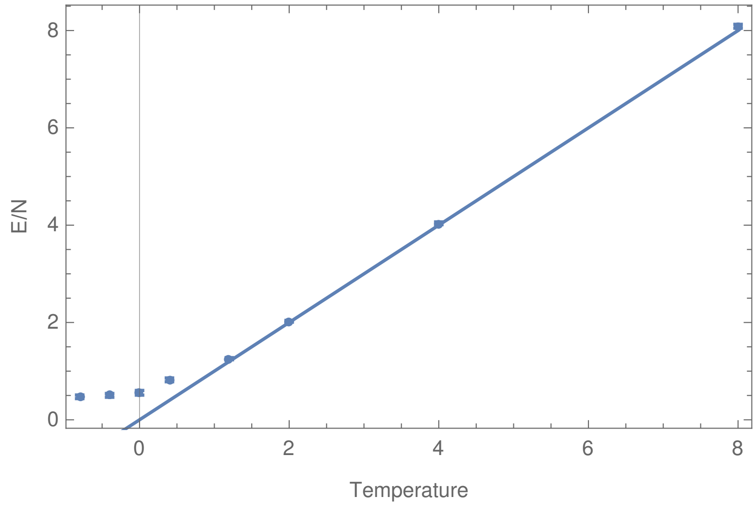

Figure 3: The E/N vs Temperature of the simulation (points) and the Ideal Gas Law (L = 20)

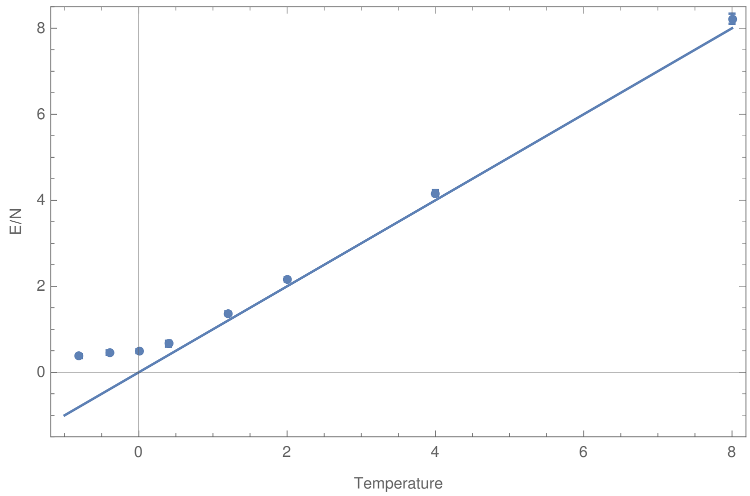

Figure 4: The E/N vs Temperature of the simulation (points) and the Ideal Gas Law L=16

The size of the box had little effect on the accuracy of the Ideal Gas Law, with major deviation occurring only after the temp drops below 1.7 for both L = 20 and L = 16

2.3 Question 3

We see close agreement between the predicted and the observed in the following graphs, though the -0.8 system has a negative skew. I believe that to be an artifact from the system rebounding off of the wall, causing a bulk movement of condensed particles.

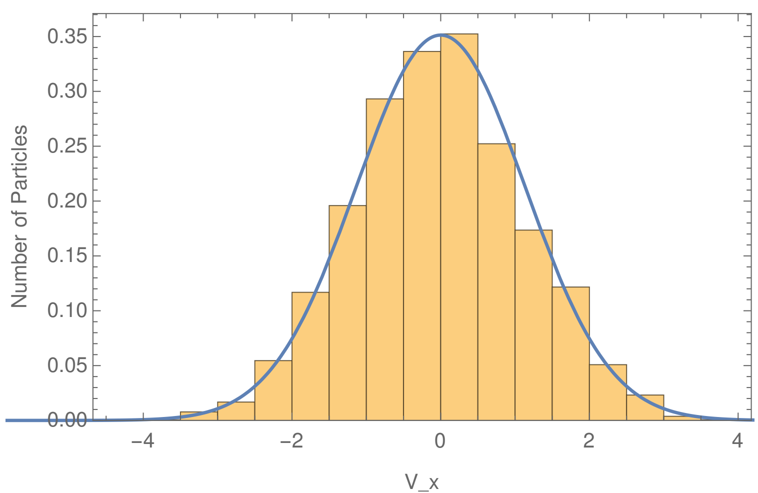

Figure 5: $\frac{E}{N=1.2}$The Histogram represents the fraction of particles found at various speeds, while the line represents the predicted value

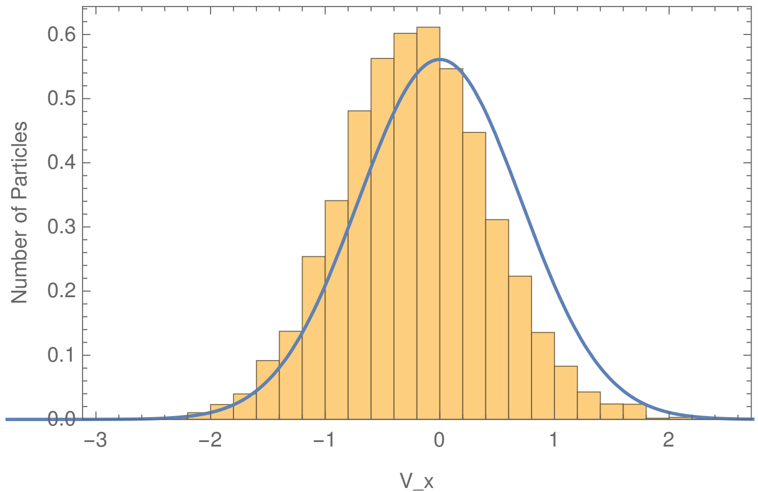

Figure 6: $\frac{E}{N} = -0.8$The Histogram represents the fraction of particles found at various speeds, while the line represents the predicted value

2.4 Question 4

Very close agreement between the Observed and Theoretical models for Pressure.

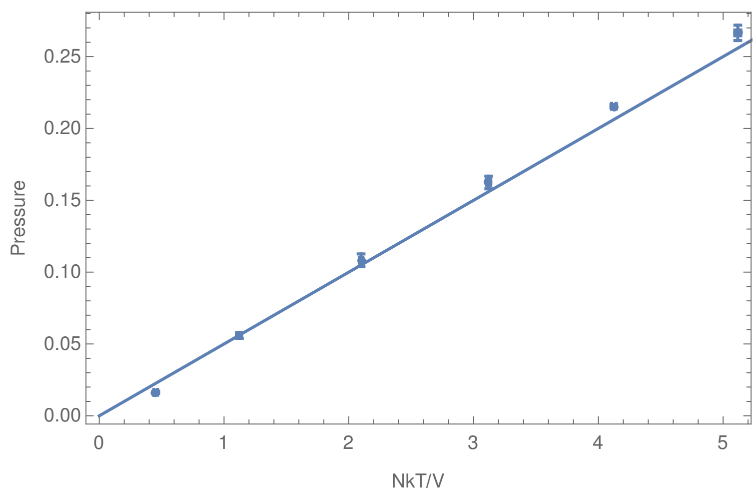

Figure 7: $\frac{E}{N} = -0.8$The Histogram represents the fraction of particles found at various speeds, while the line represents the predicted value

3 Conclusion

Monte Carlo simulations are useful windows into understanding bulk properties of fluids.