Homework 8: Molecular dynamics

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1 Introduction

In this assignment, we return to N-body simulation to model a semi-ideal gas system of particles in a box, a field of computation known as molecular dynamics.

2 Results

Question 1

For the system with $E/N = -1.2$, the particles are all relatively clustered after thermalization, with only a few off on their own (Fig. 1). In the system with $E/N = 4$, however, we see the particles much more independently distributed, because they are able to break free of each others' potential wells (Fig. 2). The first is what we might see for liquid water, with a few molecules having evaporated, but most stuck together. The second is more reminiscent of water vapor, where the molecules are mostly free-standing.

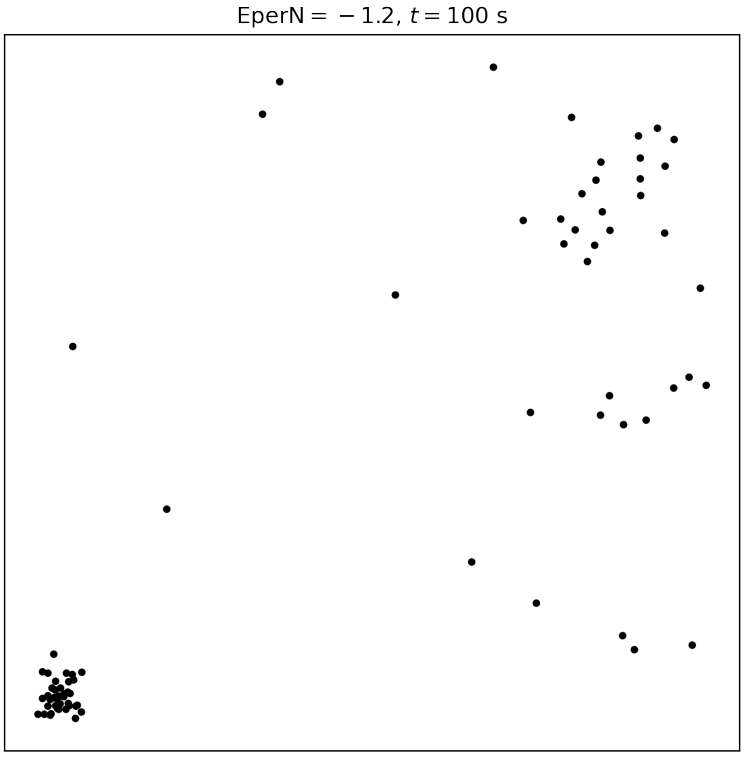

Figure 1: $N = 80$, $L = 40$, $E/N = -1.2$, and $t = 100$ s.

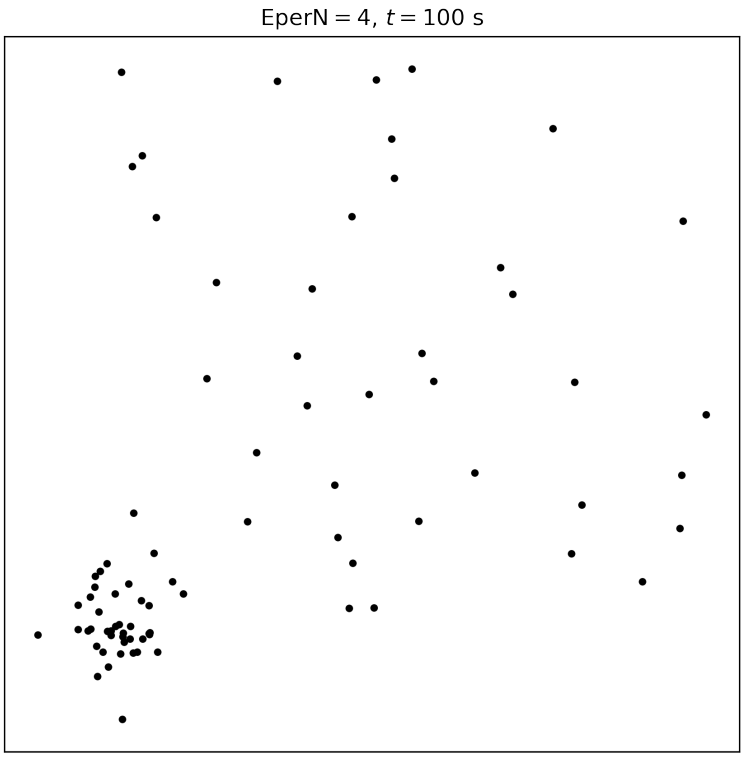

Figure 2: $N = 80$, $L = 40$, $E/N = 4$, and $t = 100$ s.

Question 2

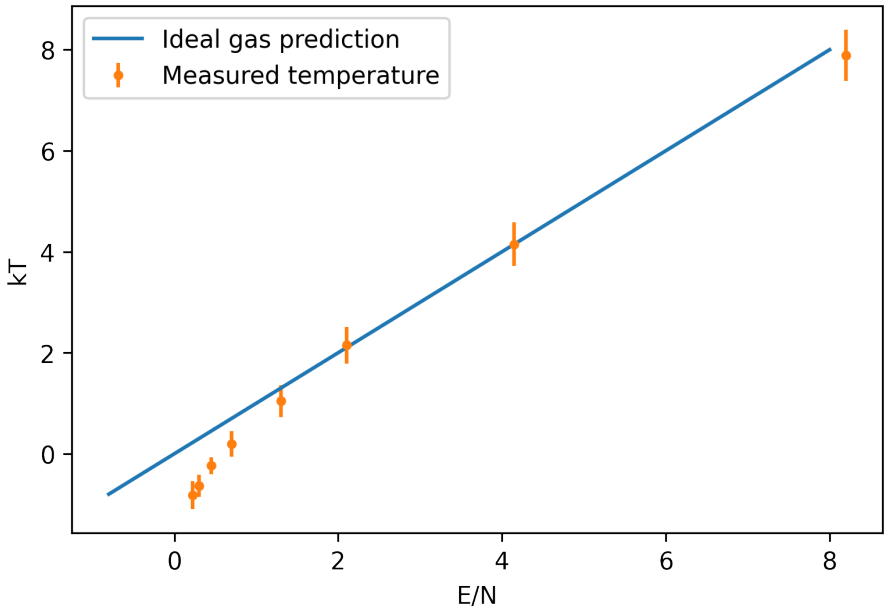

Figure 3: Comparison of simulation ($N = 20$, $L = 40$, and $dt = 10^{-3}$) temperature and ideal gas prediction as a function of $\frac{E}{N}$. We see that the simulation is only really good for $\frac{E}{N} > 0$.

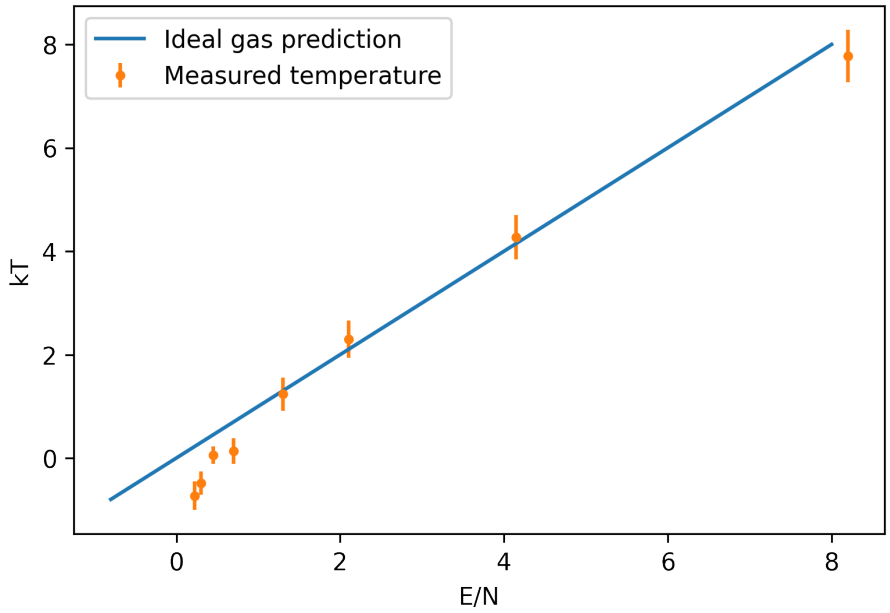

Figure 4: Comparison of simulation ($N = 20$, $L = 16$, and $dt = 10^{-3}$) temperature and ideal gas prediction as a function of $\frac{E}{N}$. This plot is not qualitatively substantially different from Fig. 3, so changing the dimensions (and therefore density) does not seem to significantly change the restriction of the simulation to $\frac{E}{N} > 0$.

Question 3

The velocity distributions for each scenario are shown in Fig.5 and Fig. 6, respectively.

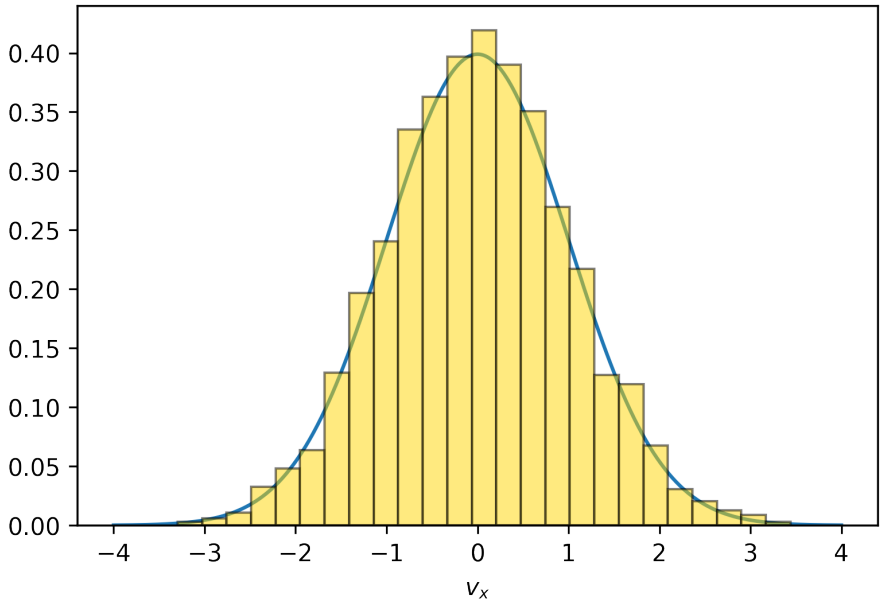

Figure 5: Distribution of x-velocities when $N = 40$, $L = 40$, and $E/N = 1.2$. We observe a close agreement between the simulation histogram (in gold) and the theoretical Maxwell-Boltzmann distribution (in blue).

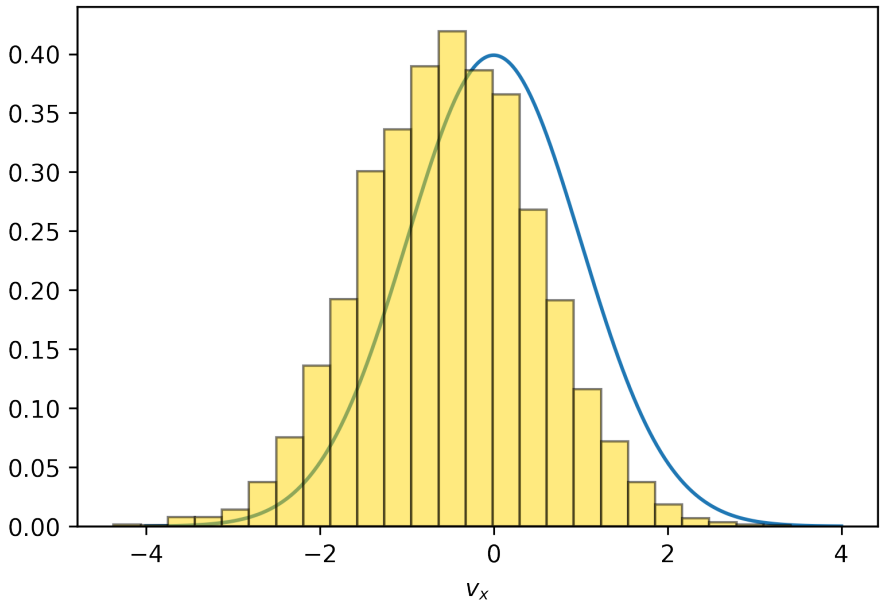

Figure 6: Distribution of x-velocities when $N = 40$, $L = 40$, and $E/N = -0.8$. We observe a slight skew between the simulation histogram (in gold) and the theoretical Maxwell-Boltzmann distribution (in blue), which could be attributed to some kind of overall motion of the group of particles.

Question 4

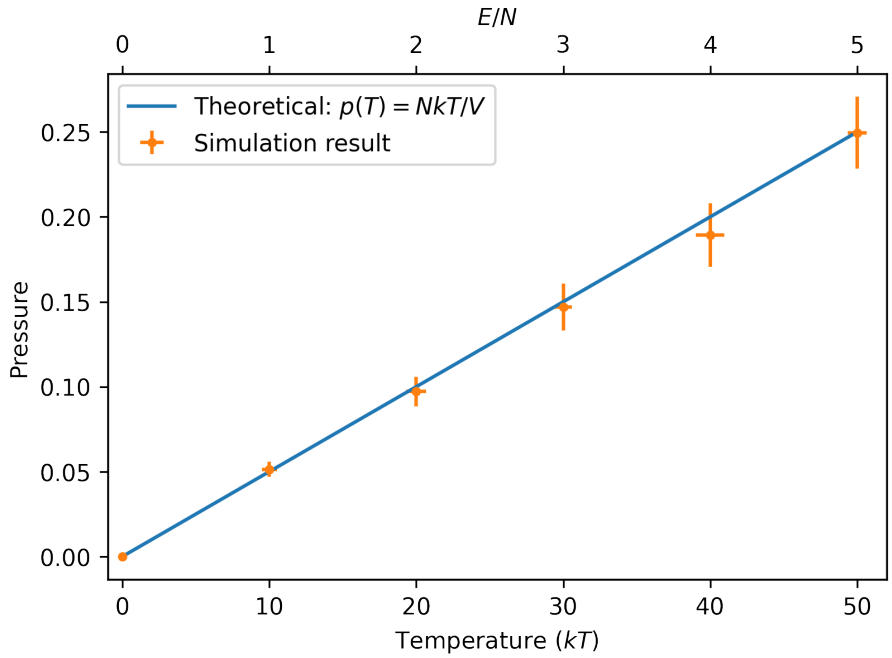

Figure 7: Comparison of simulation results (blue) and theoretical ideal gas formula for pressure (orange). In general we observe a reasonable degree of agreement between the two.

3 Conclusions

This assignment was a bit challenging, and the fact that my computer took quite a while to run each simulation with $dt = 10^{-3}$ was a bit of an obstacle, but in the end I learned quite a lot about the principles of molecular dynamics. I was especially interested in this topic because it is closely related to the material I am studying concurrently in another class, Thermal & Statistical Physics.