Dynamic Temperature Simulations in Argon Fluid

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***Index Terms*—Simulation, C++, Argon Fluid, NVT,**

I. Introduction

This project's initial purpose is to test the effects of dynamically changing temperature an NVT environment of Argon fluid (provided by professor Vikram Jadhao) and its effects on the system. The way I tested the effects on the system was plotting the distribution of the magnitude of velocities and checking if they fall under a Gaussian Distribution.

II. Implementation

A. Identifying Temperature Effecting Variables

First I had to identify all variables that affected temperature that way I can control it. The variables that affect temperature are: "reduced-temperature". After that, I had to create another variable "temperature-change" which will be received from the user in reduced units. These variables are utilized in dynamic temperature change.

B. Temperature Ramping Algorithm

There are a total of five degrees of temperature ramping implemented in the current code. Each degree of ramp takes an equal amount of time-steps to ramp temperature up to the new temperature. Every time the temperature is incremented throughout the simulation they are done equally e.g.

$10K->20K->30K$, increments of 10K

The simulation was ran on a consistent 40,000 total time-steps, the ramp levels incremented temperature at a rate of every: 20,000, 8000, 4000, 400, and 20 time-steps which equates to changing temperature one time, four times, nine times, ninety-nine times, and 1999 times.

The way you choose your desired ramp level is through the "temp-ramp-level" variable. Changing what it is equal to (either 1,4,9,99, or 1999) will tell you how many total temperature increments there will be until your desired temperature is reached.

C. Magnitude of velocities

To measure the effects dynamic temperature has on the system we decided to track the magnitude of each particles velocity and see if it falls under a Maxwell-Boltzmann distribution.

First the sum of each particles velocity in the system was calculated and confirmed that it added to zero. Then, the magnitude of each particles velocity was calculated and stored in a file (collected every 100 time-steps).

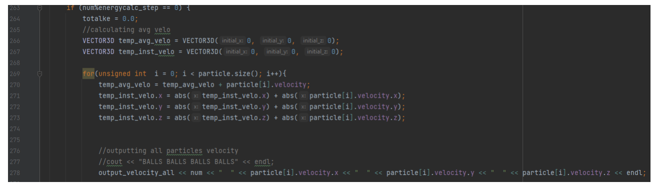

Fig. 1. C++ Code implemented to receive particle velocities.

From there figure 1. shows how the code was implemented to receive each particles velocity.

D. MATLAB: Gaussian Distribution

MATLAB was used to interpret the results after pushing all the velocity data to a file in C++. It was used to make histograms that easily visualize whether the velocities fall under a Gaussian Distribution. Unless specified, all data was taken from time-steps 5000, 25,000 and 35,000 respectively (40,000 total time-steps).

III. Results

A. Baseline results

First a sample test was taken and used to compare to. This sample had no temperature change, and the simulation ran as normal. The temperature vs. time graph and magnitude of velocity graphs can be seen in figure 2.

B. Round 1 - Constant Densities

The first round of results were conducted at each ramp level where temperature-change and density were held constant. An example of the temperature and magnitude of velocity graph of the 4 step ramping simulation can be seen in figure 3.

C. Round 2 - Differing Densities

The second round conducted similar simulations, at three different densities: 0.65, 0.8447, and 0.95 and compared against each other. An example conducted with 1 step temperature ramping can be seen in figure 4.

IV. Interpretation

A. Plateauing

Under certain conditions there seems to be a certain plateauing effect in the distribution of velocities seen in figure 5. I would normally count this plateauing effect as an abnormal distribution, although it seems to be more prominent under the following conditions: high step temperature ramping, and

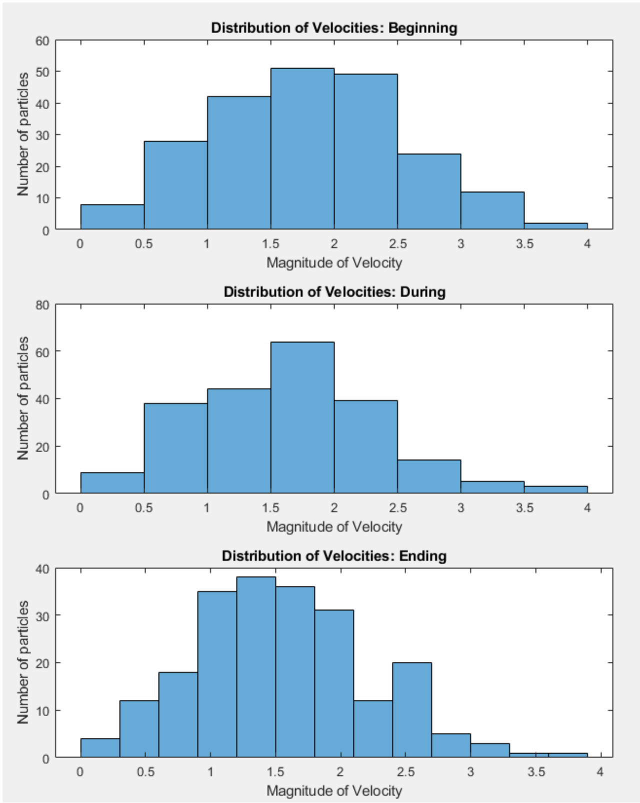

Fig. 2. Baseline velocity Distribution (No temperature ramping)

usually in the middle (15,000-25,000 time-steps) of the simulation. With current data the reason for an effect to occur at all is unknown, the most likely explanation is that the data seems this way due to the low resolution graphs of the histograms provided in MATLAB.

B. Big Jumps - nothing noticeable

I was interested to see whether the distribution faltered when the temperature jump was drastic like in temperature ramp level 1. After plotting many different distributions near the massive jump, there seemed to be no noticeable differences.

C. General interpretation

When Density was held to a constant temperature, temperature ramp seems to have little to no effect on the distribution of particles, although there is a clear Gaussian trend. As one might expect, there was a clear increase in max temperature when increasing the temperature.

V. Conclusion

In conclusion there seemed to be predictable behavior of the system when ramping the temperature up in varying levels of intensity in the argon fluid system. The velocities always seemed to follow a Gaussian distribution even under unusual conditions, and the only peculiarities that occurred where most likely due to low resolution plots in MATLAB.

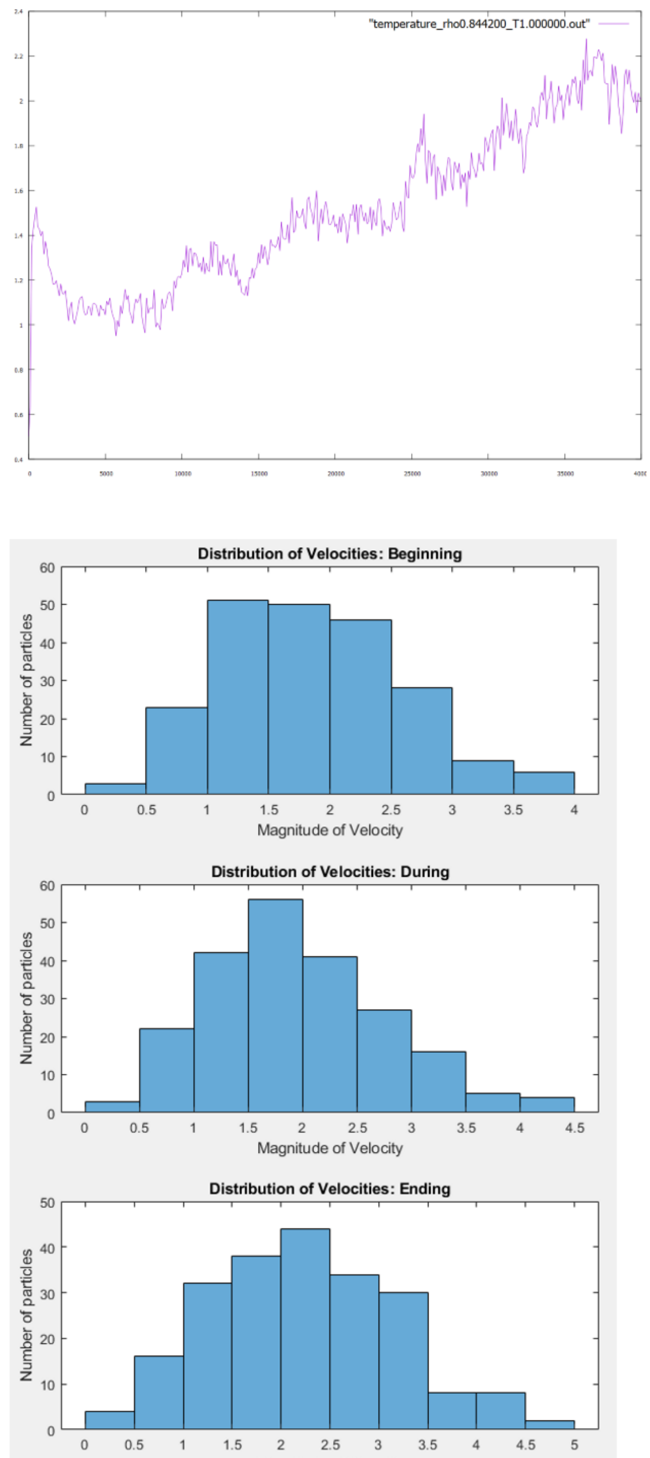

Fig. 3. 4-step ramp, Top: Temperature change throughout, Bottom: Mag. of Velocity Distributions

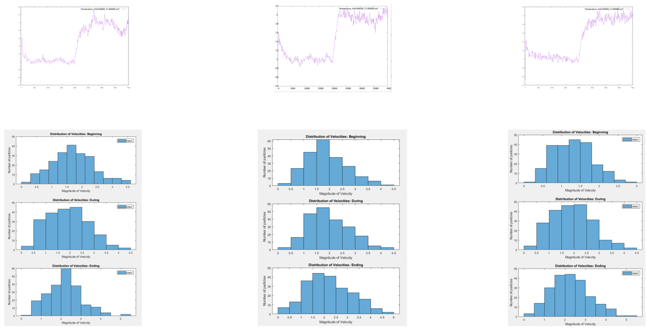

Fig. 4. 2-step ramp, densities 0.65, 0.8447, 0.95, Top: Temperature change throughout, Bottom: Mag. of Velocity Distributions

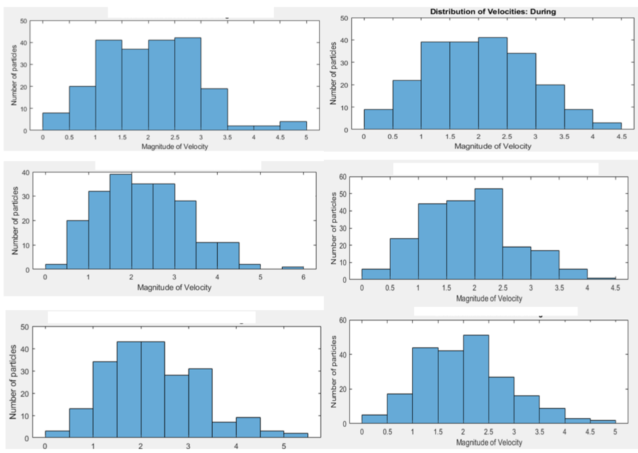

Fig. 5. Left: 9 step ramp - plateauing, Right: 99 step ramp - plateauing

A. Future Work

Future works might include looking into plateauing further, graphing the magnitude of the velocities at a higher resolution. If this plateauing still persists, more simulations should be done to characterize the phenomena.

Furthermore, Taking a look at density vs. pressure graphs and ovito movies would be interesting to see if there is any interesting crystal-forming behavior that occurs, or seeing if temperature ramping could assist in curating a specific crystal formation.