Derek Brown
19466599
CS 115 Final Project Report

Background:

The original goal of this simulation was to calculate the ideal gas constant, R.

Hypothesis:

My original hypothesis was that my R would be equivalent to the standard published value, approximately 8.3144621 J/(K*mol). However, as I began programing the simulation, it became apparent that my original design was would not give me timely data(see implementation for details). Therefore, recalling the conclusion of Rutherford experiment, that atoms are mostly empty space, I removed the inter-particle collisions in order to speed the simulation.

In light of this change, I altered my hypothesis such that the removal of the inter-particle collisions from the simulation would not cause a statistically significant alteration in the calculated R from the published R value. For this purpose, I defined “statistically significant” to be a deviation of >= 5% from the published value.

Implementation:

Due to my past difficulties with with event-driven simulations, I avoided the event-driven model for a time driven model to my detriment.

My initial simulation design simulated both elastic collisions with the walls, and inelastic collisions between the particles should they come to occupy the same location at the same time, changing both the direction and magnitude of the particles, while preserving the total momentum(i.e. a particle would only be sped up if the other ). However, my second design removed the inelastic collisions in an attempt to speed the simulation.

The simulation takes five parameters from the command line: radius of the container, in picometers; the number of particles (as an integer); the mass of a single particle, in kg; the temperature, in K; and the molar mass of the particles, in kg.

Observations:

The initial value was quite higher than expected, being initally over a hundred orders of magnitude larger than. Moreover, even after two days(~30 hours) of continuous running, even without the intermolecular collisions, the calculated value has still yet to fall below that threshold, although it is decreasing.

However, this may be due to the fact that the calculated pressure, a component in the calculation of R's value and should be relatively constant, is also steadily dropping.

Conclusion:

Unfortunately, the only conclusion that I can draw is that my decision to avoid an event-driven simulation was a poor one.

Data:

The following data was collected using the following inputs:

- 2*10^7//radius of sphere, in picometers
- 10//number of particles
- 1.6605402*10^(-27))//mass of each particle, in kg
- 370//temperature, in K
- 2.02*(10^(-3))//molar mass for the particles, in kg

The format is as follows: Time: (in simulated seconds), followed by calculated R value, followed by calculated pressure.

Time:1323000001:: 1.2585526951048527E157 :: 4.102239994106747E128
Time:1324000001:: 1.2576021266047363E157 :: 4.099141625533478E128
Time:1325000001:: 1.256652992924996E157 :: 4.0960479337429575E128
Time:1326000001:: 1.2557052908194328E157 :: 4.092958908154229E128
Time:1327000001:: 1.2547590170516306E157 :: 4.0898745382182305E128
Time:1328000001:: 1.2538141683949236E157 :: 4.086794813417674E128
Time:1329000001:: 1.2528707416323567E157 :: 4.0837197232669275E128
Time:1330000001:: 1.2519287335566499E157 :: 4.080649257311893E128
Time:1331000001:: 1.2509881409701616E157 :: 4.07758340512989E128
Time:1332000001:: 1.2500489606848532E157 :: 4.074522156329539E128
Time:1333000001:: 1.2491111895222518E157 :: 4.071465500550639E128
Time:1334000001:: 1.2481748243134168E157 :: 4.068413427464058E128
Time:1335000001:: 1.247239861898901E157 :: 4.065365926771611E128

Time:2140000001:: 7.780678579926194E156 :: 2.5361044456866183E128
Time:2141000001:: 7.777044447008727E156 :: 2.534919903676108E128
Time:2142000001:: 7.773413707305935E156 :: 2.533736467680546E128
Time:2143000001:: 7.769786356067635E156 :: 2.5325541361516157E128
Time:2144000001:: 7.766162388552503E156 :: 2.5313729075438872E128
Time:2145000001:: 7.762541800028059E156 :: 2.530192780314813E128
Time:2146000001:: 7.758924585770646E156 :: 2.529013752924722E128
Time:2147000001:: 7.755310741065403E156 :: 2.5278358238368102E128