DATASCI 2G03 Project Report

Elastic Collisions between Contained Particles

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Contents

1 Introduction

Visualizing the effects of colliding elastic objects enables a clearer understanding of extremely small or extremely large natural phenomena, especially in the fields

of astrophysics (eg. rotation of stars in a galaxy) and chemistry (eg. ideal gas, electron/proton interactions). Tools of this nature can provide intuition and a sense of familiarity to those studying these areas. Even in everyday life, this type of simulation often appears in video games like pong, brick breaker, and 8 ball pool. Therefore, this project attempts to simulate interactions between a large number of objects through the motion and collision of moving particles.

The simplest of these interactions are those that do not involve a change in acceleration, such as an ideal gas in a finite box. Wikipedia has an excellent example of one such simulation [1]. Further, a reasonable simulation should expect to converge to the Maxwell-Boltzmann distribution, a chi-distribution with 3 degrees of freedom [2], characterized by the large density of particles around the mean and the slow taper for higher particle speeds.

The first part of this project will consist of modelling the interaction between many particles in a containing box the hopes of achieving a 2D Maxwell-Boltzmann distribution of velocities. We also ensure correctness of our simulation by monitoring kinetic energy conservation for the system. Then, we will extend these interactions with the addition of charged particles to simulate the effects of non-constant acceleration. We do not expect the charged particles to follow the Maxwell-Boltzmann distribution, but will explore other effects of remote particle-particle interactions, like orbits.

2 Method

2.1 ODE Solver

Since this simulation is based primarily around dynamic motion, we will use the kick-drift-kick form of Leap Frog integration [3]:

$$v_{i+\frac{1}{2}} = v_i + a_i \frac{\Delta t}{2} \tag{1}$$

$$x_{i+1} = x_i + v_{i+\frac{1}{2}} \Delta t \tag{2}$$

$$v_{i+1} = v_{i+\frac{1}{2}} + a_{i+1} \frac{\Delta t}{2} \tag{3}$$

2.2 Initial Equations

The physics-based ODEs and other equations used to simulate this problem are listed below. The goal of this simulation is to track the position of objects (represented by x) over some length of time t. Each particle will have some mass m and starting velocity v.

[1] https://en.wikipedia.org/wiki/Maxwell%E2%80%93Boltzmann_distribution
[2] https://en.wikipedia.org/wiki/Chi_distribution
[3] https://en.wikipedia.org/wiki/Leapfrog_integration

Velocity (v) of one particle [4]:

$$v = \frac{dx}{dt} \tag{4}$$

Acceleration (a) of one particle:

$$a = \frac{dv}{dt} = \frac{d^2x}{dt^2} \tag{5}$$

Kinetic energy of one particle:

$$E_k = \frac{1}{2}mv^2 \tag{6}$$

The below equation is used to calculate the vectors of velocity resulting from an elastic collision [5]. Let v_1 represent the first particle's velocity and v_2 for the second particle's velocity. Additionally, let v' represent the velocity after the collision and v for the velocities prior to the collision. Swapping $*_1$ and $*_2$ will provide the velocity for particle 2.

$$v_1' = v_1 - \frac{2m_2}{m_1 + m_2} \frac{\langle v_1 - v_2, x_1 - x_2 \rangle}{\|x_1 - x_2\|^2} (x_1 - x_2) \tag{7}$$

2.3 Extended Equations

Newton's second law:

$$F = ma \tag{8}$$

Coulomb's law: Force of charged particles against one another:

$$F_{charge} = \frac{kq_1q_2}{r^2} \tag{9}$$

Electric potential energy of a system [6]:

$$U = \frac{k}{2} \sum_{i}^{N} \sum_{j}^{N} \frac{q_i q_j}{r_{ij}} \text{for} i \neq j \tag{10}$$

2.4 Configuration Parameters

- Starting position s of each particle
- Initial velocity v of each particle

[4] https://en.wikipedia.org/wiki/Equations_of_motion

[5] https://en.wikipedia.org/wiki/Elastic_collision

[6] https://phys.libretexts.org/Bookshelves/University_Physics/University_Physics_(OpenStax)/University_Physics_II_-_Thermodynamics_Electricity_and_Magnetism_(OpenStax)/07%3A_Electric_Potential/7.02%3A_Electric_Potential_Energy

- Mass m of each particle (kept at a constant 1 kg except for configuration 9)
- Radius of each particle r (kept at a constant 0.25 m)
- Charge of different particles q (kept at a constant ± 1 except for configuration 9)
- Coulomb's constant k (kept at $5Nm^2/C$ instead of $9 \times 10^9 Nm^2/C$ since we are massively downscaling real-world values)

2.5 Interesting Properties

- Speed of particles over time (momentum of all particles should remain constant) position of particles on a graph
- Distribution of particle speeds (Maxwell-Boltzmann distribution)
- Unique path of each particle (random movement of one particle) [7]

3 Testing

To ensure the correctness of our program, we compare the results of a few preset configurations against the expected behaviour of the simulation. Additionally, we examine a collection of randomly positioned particles.

3.1 Uncharged Particles

The tests for this section cover the initial model of this project, without any extensions. All particles are set to a charge of 0, so they only interact though collisions with other particles and walls. This setup mimics that of an ideal gas, so we are expecting to find that energy is conserved and the distribution of speed eventually forms the Maxwell-Boltzmann curve.

3.1.1 2 Particles in a 1D Collision

This test examines the effects of one collision between two particles moving towards one another on the x-axis, as shown below. Both particles have the same initial speed and are pointed towards the origin:

[7] `https://en.wikipedia.org/wiki/Brownian_motion`

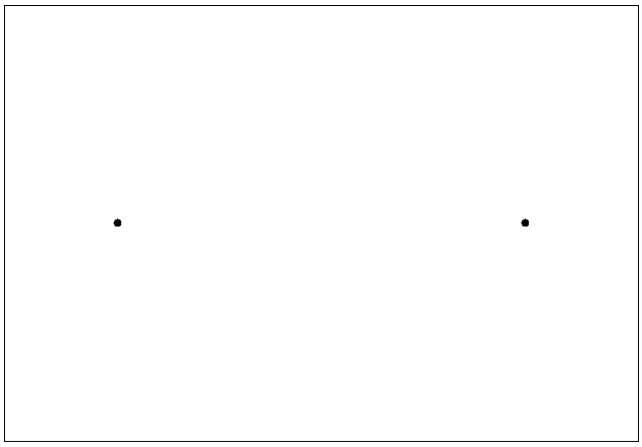

Figure 1: Two uncharged particles aligned on the x-axis. Initial velocities are equal and towards the origin.

Plotting the total energy and speed over time (blue and green respectively), we find that kinetic energy is entirely conserved. The purple line indicates electric potential energy and can be ignored for now. Note that there is no scale for the Time axis since this graph updates by appending new data every dt seconds. This means that initial iterations take up the entire plot and then compress as time goes on and the plot holds more data.

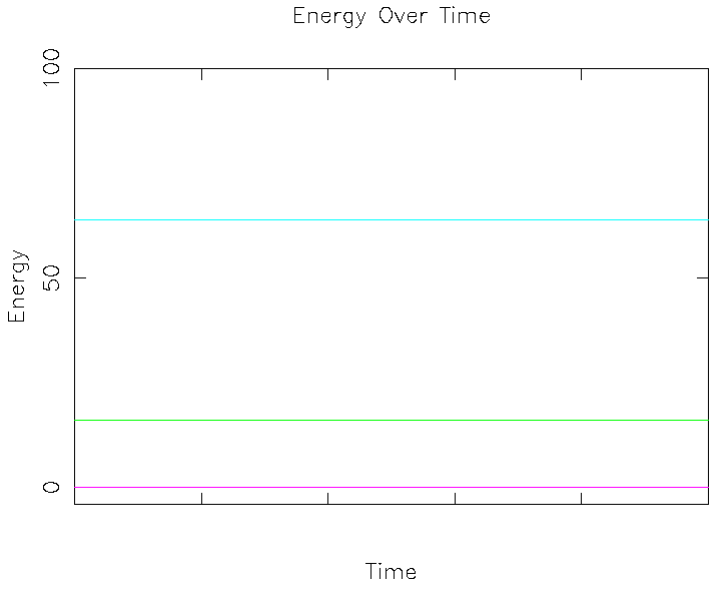

Figure 2: Energy over time for the collision of two particles. Kinetic energy (blue), speed (green), electric potential energy (pink), and total energy (black, obscured by and equal to kinetic energy) are constant.

3.1.2 2 Particles in an Angled Collision

Similar to the previous test, but we now check that the angle of deflection for both particles are correct. A simple case for examining angles is to move the point previously located at $(-1, 0)$ to $(0, 1)$ and point it towards the origin. Thus, the two particles will meet at a 90-degree angle and bounce in perpendicular directions. The initial layout of this test has particles located at the top and right with velocities toward the origin:

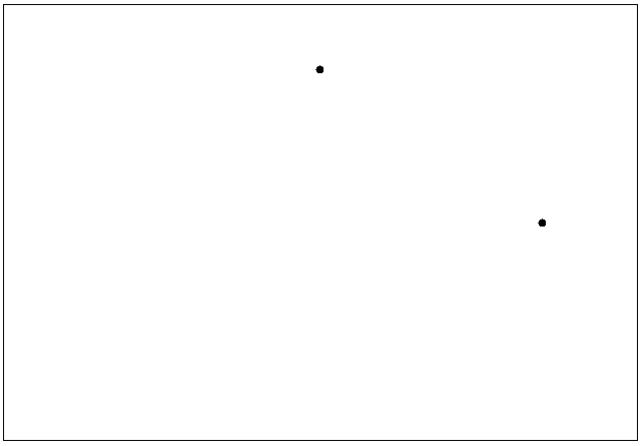

Figure 3: Particles at the top and right, facing towards the origin.

After collision, the initially top particle will be sent to the left and the right particle to the bottom. Since the particles met at a 90-degree angle, they must depart at 90-degrees in order to conserve momentum towards the bottom left.

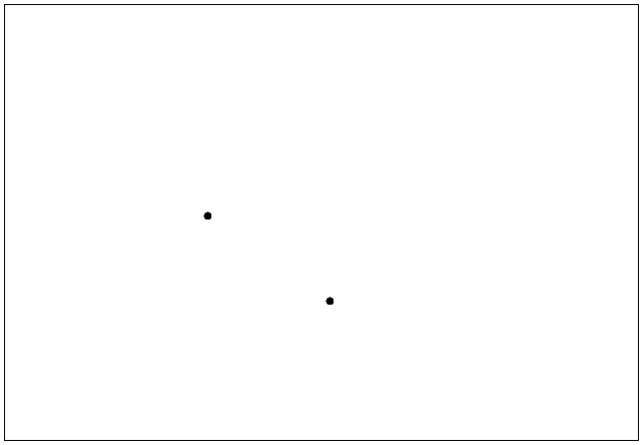

Figure 4: Particles at the bottom and left, after a 90-degree collision at the origin.

The particles will then bounce against the walls, reversing direction and colliding at the origin again. Particle locations will swap between the two quadrants until the simulation is stopped. Energy is conserved during this as both particles bounce with the same net speed (although we do not include the energy vs time graph here since it looks the same as section 3.1.1).

3.1.3 200 Random Particles

With a large amount of particles, we can now examine the distribution of speed compared to the Maxwell-Boltzmann distribution. The speed distribution of particles is separated into 30 "buckets", where each particle is sorted into a bucket based on its speed. Each bucket holds a range of $1m/s$, where he maximum speed bucket is $30m/s$ Note that the specific x-axis speeds are not especially important since it is more important to visualize the groupings of particles rather than the exact speed of the particles themselves. For example, we could scale down the interpreted particle speeds based on the maximum speed and receive a similar graph.

An image of the simulated particles is below:

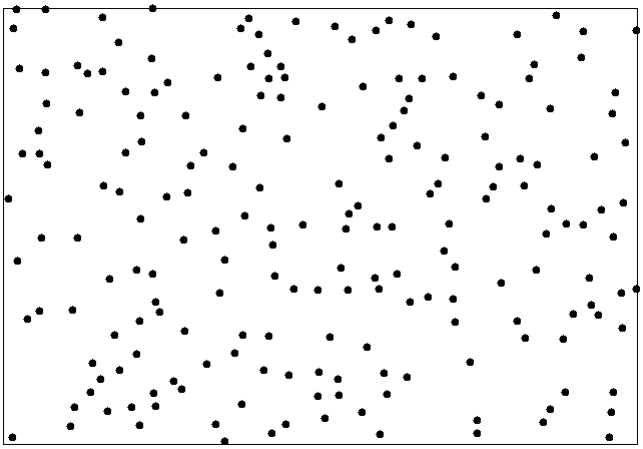

Figure 5: 200 particles with initially random positions and velocities.

After a few seconds of simulation, the distribution graph for 200 particles visibly relaxes from a random distribution into the Maxwell-Boltzmann distribution.

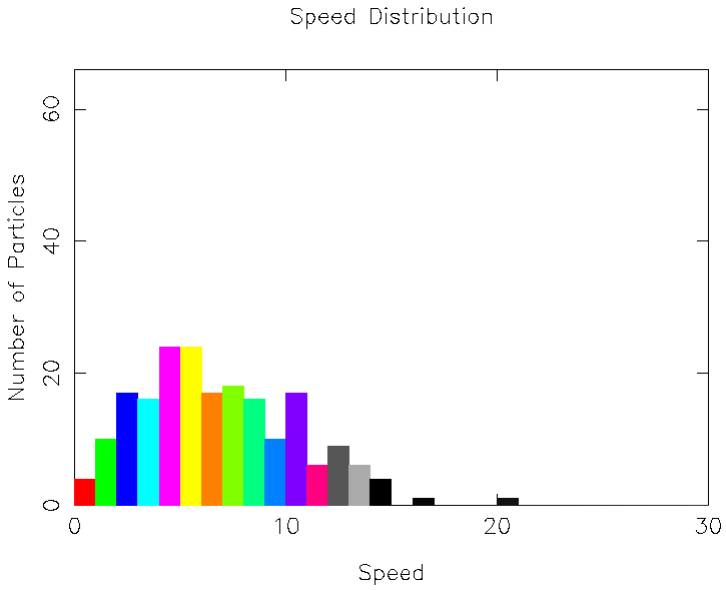

Figure 6: Speed distribution of 200 random particles. Most particles stay within the 2 to 12m/s range

Calculating the exact curve of the distribution is slightly out of the scope of this project since we do not collect any information on gas-specific statistics

(ie., temperature, pressure, heat), but the characteristic bulge and slow taper can be visually estimated and compared with Wikipedia's simulation:

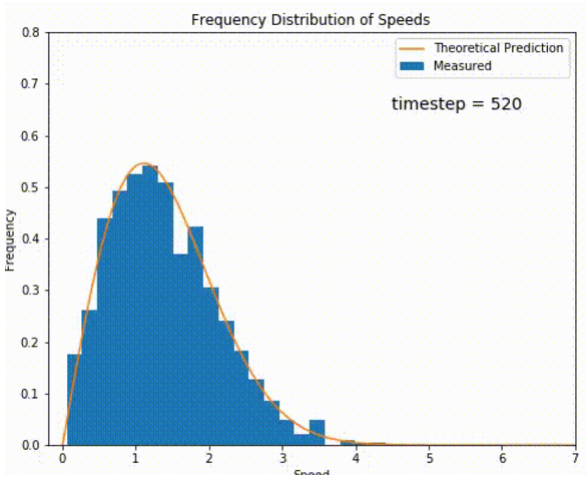

Figure 7: Wikipedia image of the Maxwell-Boltzman distribution against the actual speed distribution of particles.

Finally, we see that kinetic energy is indeed conserved, although total speed fluctuates within a margin of error.

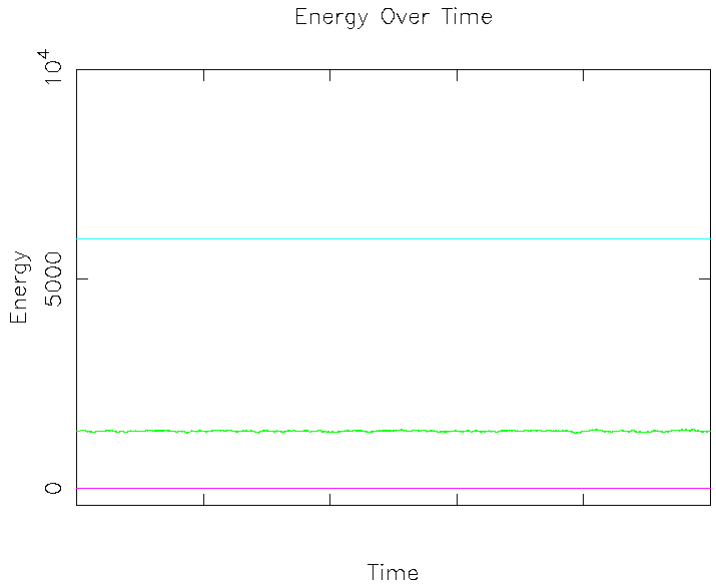

Figure 8: Energy over time for the collision of 200 particles. Kinetic energy (blue), speed (green), electric potential energy (pink), and total energy (black, obscured by and equal to kinetic energy) are constant.

3.2 Charged Particles

The inclusion of charged particles within the simulation adds an additional ODE for our consideration, namely, a non-constant acceleration due to Coulomb's Law. The focus of this extension is to demonstrate how equations for dynamic particle movement can be manipulated and reused to provide an idea of orbital movement. Similar to gravity, the acceleration of charged particles is remotely influenced through other nearby particles.

3.2.1 2 Particles Interacting in 1D

The same experiment for uncharged particles can be performed on charged particles.

For particles with the same charge, the setup is as follows (initial velocity towards the origin):

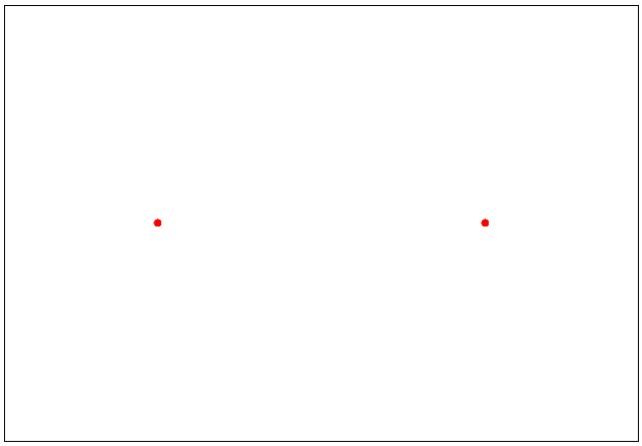

Figure 9: Two positively charged particles with initial velocities towards the origin.

As the particles approach one another, their speed and kinetic energy transform into electric potential energy. Eventually, the particles stop a small distance before collisions and begin moving in the opposite direction. Then, when moving apart, the potential energy is converted back into kinetic and the particles speed into the wall. An oscillation pattern between the kinetic energy (blue) and electric potential (pink) can be seen below. Note that the total energy of the system (black) is conserved throughout and total speed (green) follows the

kinetic energy.

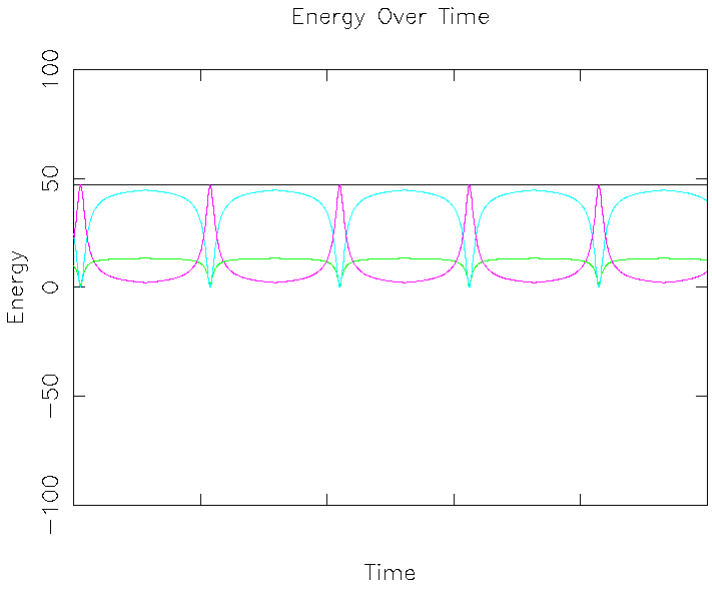

Figure 10: Energy over time for two positively charged particles. Note that electric (pink) and kinetic (blue) energy oscillate but always add up to the total energy (black).

Similar behaviour can be seen for opposite charges, with the energy curves flipped. There is a slight, repeated fluctuation in total energy at the moment of collision, but the overall energy of the system does not change.

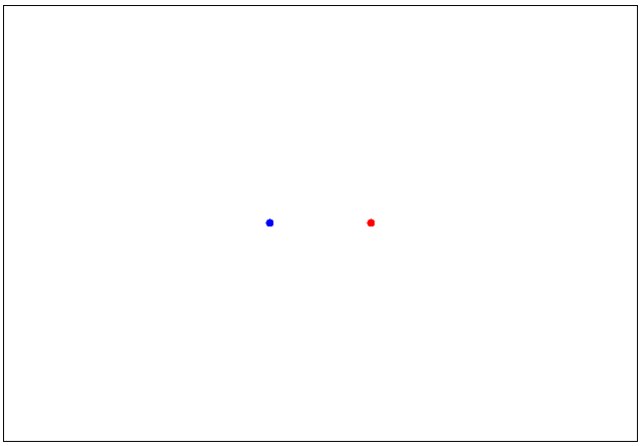

Figure 11: Two oppositely charged particles with initial velocities towards the origin.

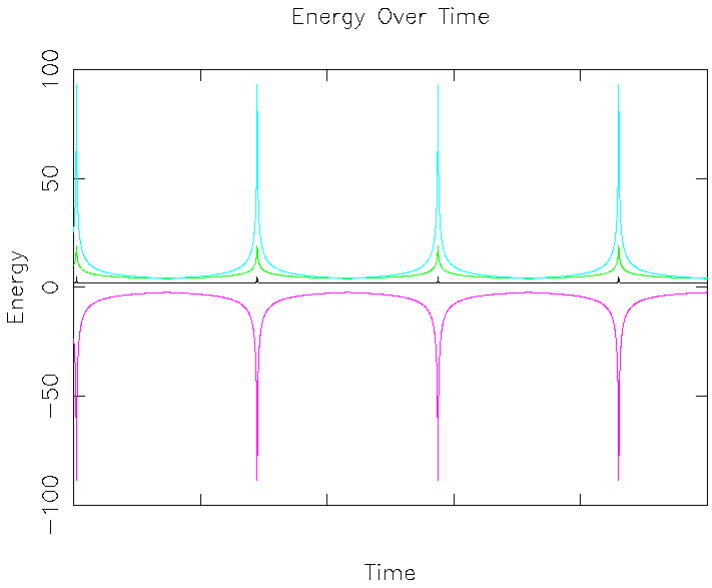

Figure 12: Energy over time for two oppositely charged particles. Once again, electric (pink) and kinetic (blue) energy oscillate but always add up to the total energy (black).

3.2.2 Orbiting Particles

The below setup places two oppositely charged particles at equal and opposite distances from the origin, with initial velocity parallel to the y-axis. This led to a stable elliptical orbit about the origin.

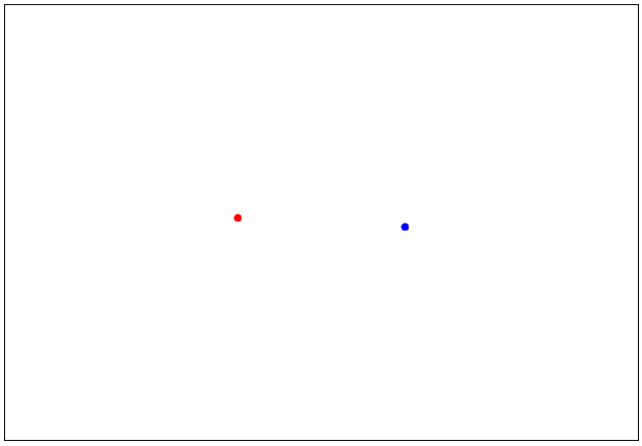

Figure 13: Two particles orbiting about the origin. The blue particle has velocity downward, while the red particle has velocity upward.

In the below graph, fluctuations in kinetic energy (blue) and electric potential energy (pink) oscillate opposite to one another, as the two particles get closer/faster and further/slower to one another. We still note that the total energy (black) remains constant throughout.

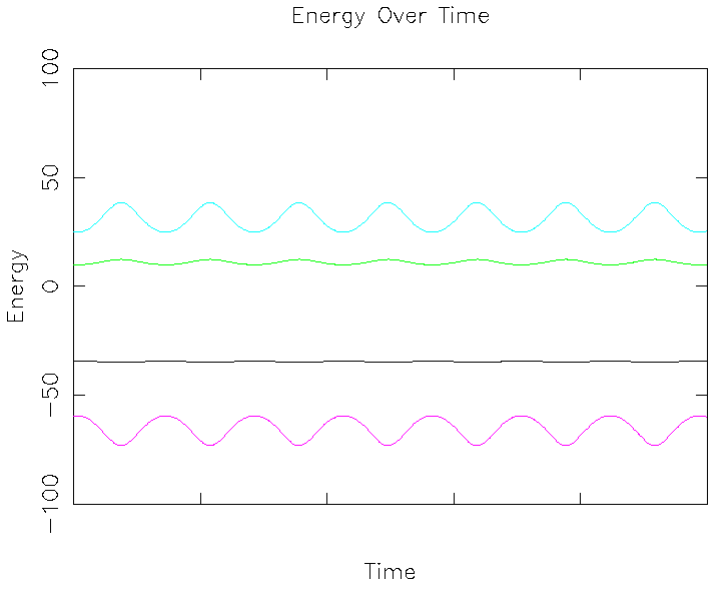

Figure 14: Energy over time between orbiting particles. Electric (pink) and kinetic (blue) energy oscillate and sum to total (black).

Orbits akin to Bohr-Rutherford models of the atom, where small charges orbit a large central charge, can be seen by configuring several negatively charged masses initially travelling perpendicular to the electric force from a large red mass. The energy over time is shown below, following the same oscillation as above.

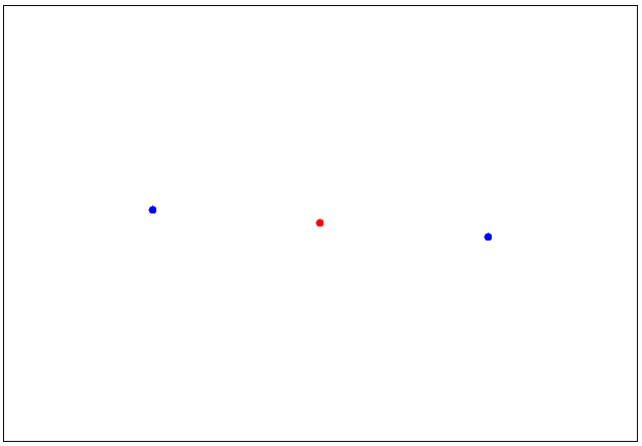

Figure 15: Two negatively charged low-mass particles orbiting a highly positively charged central particle, akin to electrons and protons in an atom.

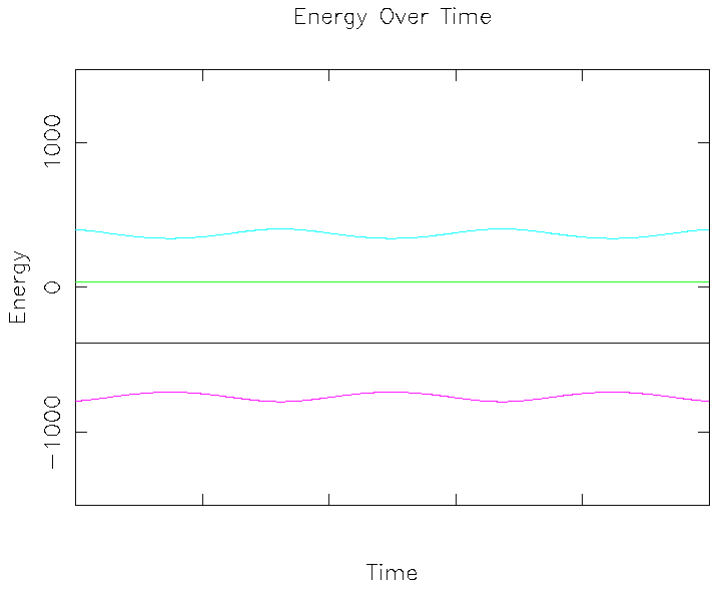

Figure 16: Energy over time for particles orbiting around another particle. Electric (pink) and kinetic (blue) energy oscillate and sum to total (black).

3.2.3 200 Random Particles

This test is similar to that of the uncharged particles, but all particles have been either assigned a positive (red) or negative (blue) charge. The setup and energy graphs are listed below:

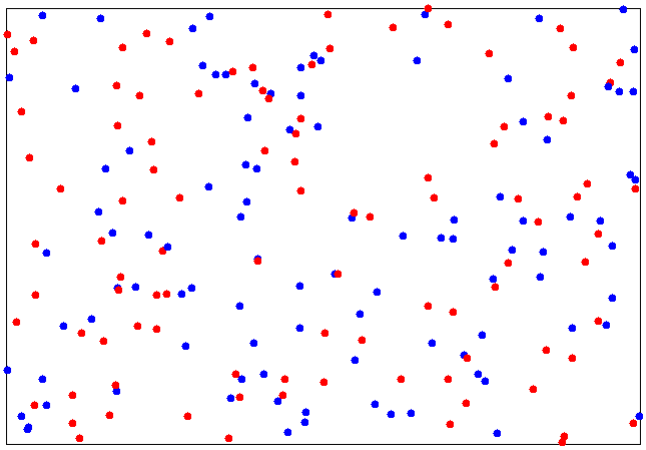

Figure 17: 200 randomly charged particles.

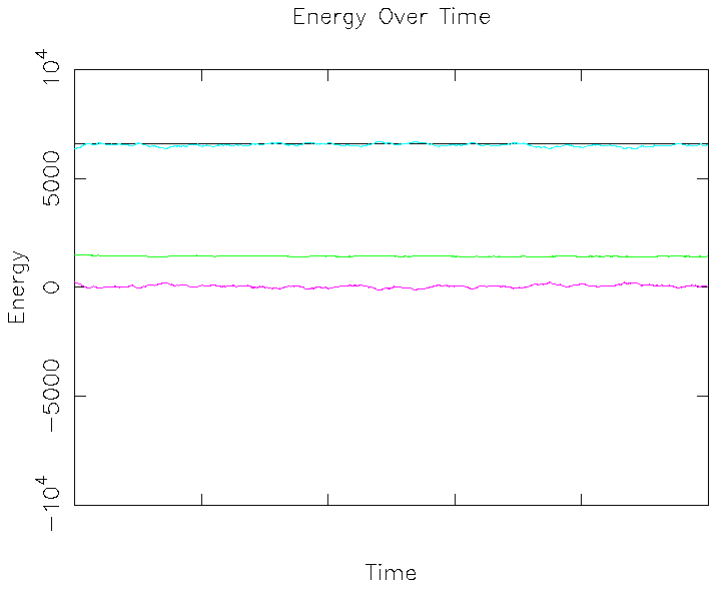

Figure 18: Energy over time for 200 randomly charged particles. The total energy (black) remains constant.

These random particles have a similar shape to the Maxwell-Boltzmann distribution, likely due to the high ratio of kinetic to electric potential energy.

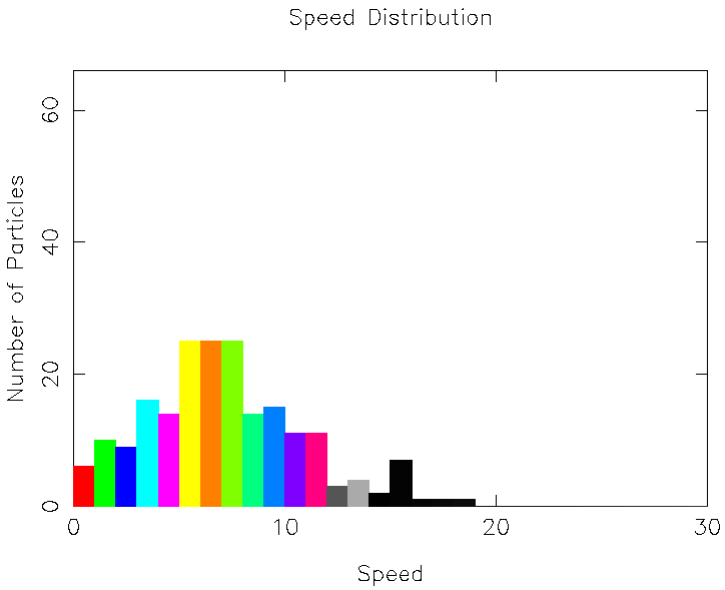

Figure 19: Speed distribution 200 randomly charged particles, appearing similar to the Maxwell-Boltzman distribution.

4 Results

Overall, both models of uncharged and charged particles behaved as expected with respect to energy conservation and speed distribution. Selected tests also demonstrated the conservation of momentum and distance-based forces. Outside of exceptional circumstances, Leap Frog integration had a high degree of precision throughout all iterations of the simulation, demonstrating its effectiveness for dynamic systems.

4.1 Initial Model - Uncharged Particles

Initially, I faced difficulties with conservation of kinetic energy for uncharged particles since some collisions would last for longer than one dt instant. To counter this, I implemented a directional check to ensure that particles only collide when they are facing towards one another [8].

Along with the above bug in collision calculations, I had also mistakenly tried calculating new velocities based on the contributions of each particle at one point in time. However, doing so led to very unpredictable behaviour when 3 or more particles collided at once, where involved particles would either explode with speed or slow down immensely. Eventually, this was resolved by calculating the pairwise collisions of every particle in some arbitrarily chosen order.

Although the energy-time graphs are not very interesting in section 3.1, they serve as a constant, visual examination of the total energy of the system. For a simulation with no explicit acceleration changes, all lines on the graph should and do appear as flat line.

4.1.1 Extended Testing: 8-Ball Pool with 225 Particles

From the experiment in section 3.1.3, we can hypothesize that given a high enough density of particles in an enclosed space, the initial distribution does not matter. To test this claim, we select an experiment grounded with the real world: what would happen if we removed the friction and pockets from a pool table when making a "break" shot? For better visualization of the Maxwell-Boltzman distribution, we increase the number of balls on the pool table to 200. The initial layout of the test is shown in the following figure along with the initial speed distribution. Note that only one particle is moving to the right at $100m/s$ while all others are at rest.

[8] Dr. Wadsley initially told me about the equation, but the linked forum post also states the same method: `https://math.stackexchange.com/questions/1438002/determine-if-objects-are-moving-towards-each-other`

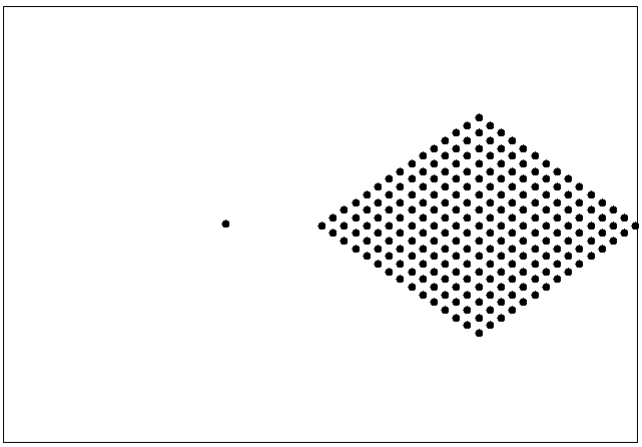

Figure 20: Initial setup similar to the game of 8-ball pool. One high-speed particle from the left strikes a diamond of still particles.

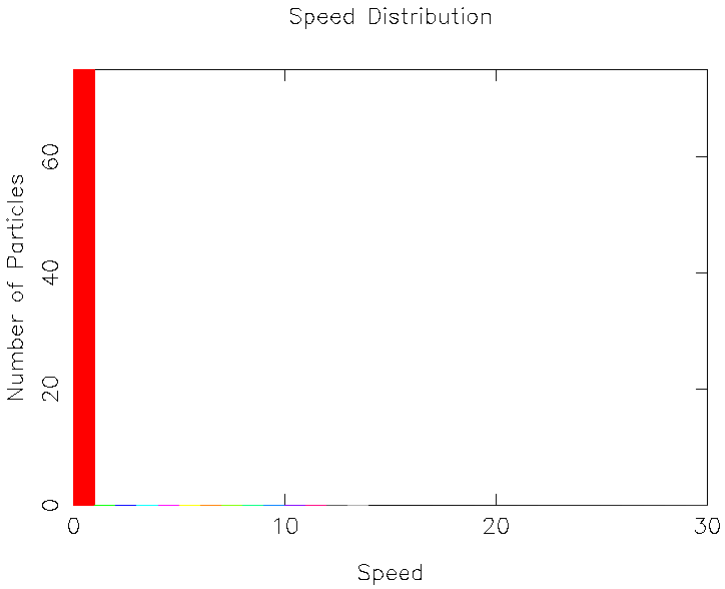

Figure 21: Initial speed distribution for the above setup. All particles are at rest, except for the "cue" ball, which has a speed $> 30m/s$.

After about one minute, we see a very similar result as in section 3.1.3. In fact, aside from the differences in initial energy, the two plots are nearly indistinguishable.

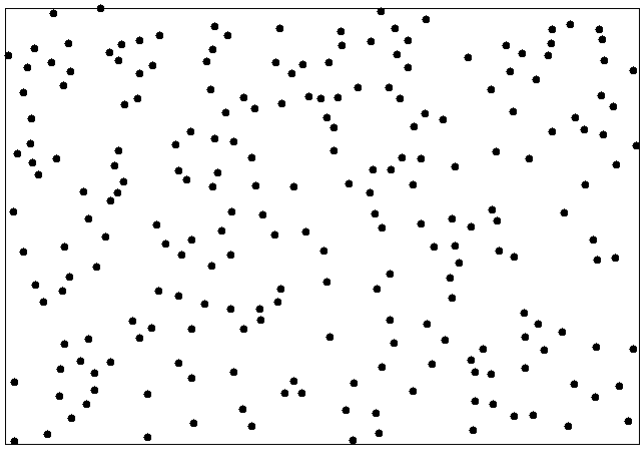

Figure 22: Particles of the pool setup after some time. The random movement is similar to that of the 200 random particles

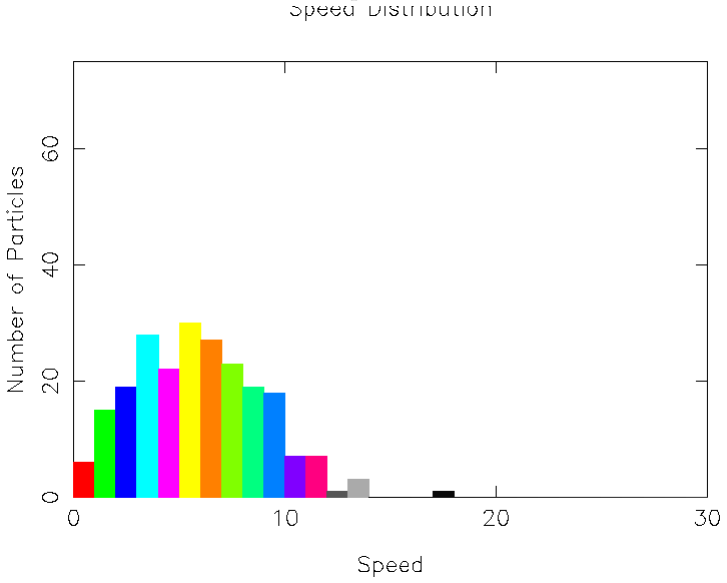

Figure 23: Speed distribution the pool setup after some time. The shape of the curve is similar to that of the 200 random particles

4.2 Extended Model - Charged Particles

Since charged particles were used with a mass of $1kg$ and charges equal to $\pm 1C$, a far lower Coulomb constant k was necessary to prevent extreme changes in acceleration. Dealing with extreme values in the case of charged particles was especially difficult, as small errors in transforming continuous phenomena into

discrete often occurred as a result of particles escaping the boundaries or coming in close contact with one another.

Enabling collisions during testing produced all results as expected with respect to the conservation of energy and distribution of speed In the case of two charged particles interacting with one another, the oscillation between kinetic and electric potential energy matched expectations and maintained conservation rules.

For tests with collisions disabled, as mentioned in section 3.2.1, monotonic changes in the total system energy could be caused by a combination of the transition to discrete steps and the soft max function limiting acceleration due to surrounding charges.

While the charged particle model massively simplifies all the complex interactions between particles in the real world, the visualization of interacting particles is more than reasonable for most common configurations. With the charged model, we can plainly see physical phenomena like orbital movement as a product of a constant central acceleration and an appropriate starting velocity.

4.2.1 Extended Testing: 2 Particles Interacting in 1D Without Collisions

This section is an extension of section 3.2.1.

For particles of opposite charge, the total energy of the system remained constant when collisions were enabled. However, when collisions were disabled (so that particles had a radius of 0 and could become arbitrarily close to one another), the energy of the system behaved erratically. Disabled collisions allowed the particles to pass through one another (and the distance between them to become infinitesimally small) rather than colliding. This drastic change in behaviour is likely due to the imprecision of integration at high acceleration and velocity values. Consider the following timeline for two particles:

- The two particles start far away and move towards one another at a moderate but increasing velocity
- At some critical point, the particles reach their closest point. They experience a high force of attraction
- The first part of Leap Frog converts that high acceleration into high velocity, enough such that the particles swap places. In other words, the particle on the right is now on the left and vice versa.
- Leap Frog then recalculates the force of acceleration, based on the new particle positions. However, the two particles are farther apart from one another than they were in step 2. Thus, the new force of acceleration is opposite but not equal to that step.
- Since there is asymmetry in the moments before and after the particles swapped places, the particles zoom into the bounding walls before meeting again and performing the reverse.

We have attempted to mitigate these errors through an additional epsilon term to prevent the distance of two particles from reaching 0, but the above situation is still applicable. All previous tests, have collisions enabled to remove errors of this kind. The second graph below is the same as the first energy-time graph with dt set to half of the original time step. The final graph is the energy over time at a tenth of the original time step.

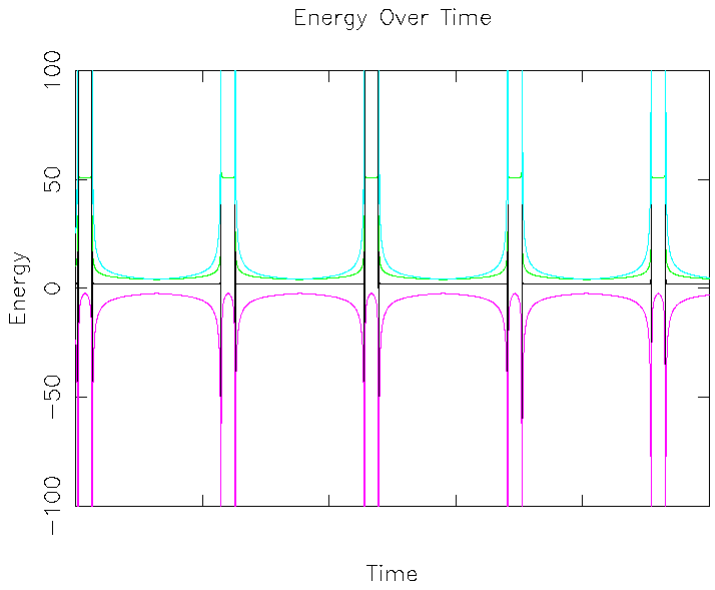

Figure 24: Energy over time for two oppositely charged particles with no radius (collisions disabled).

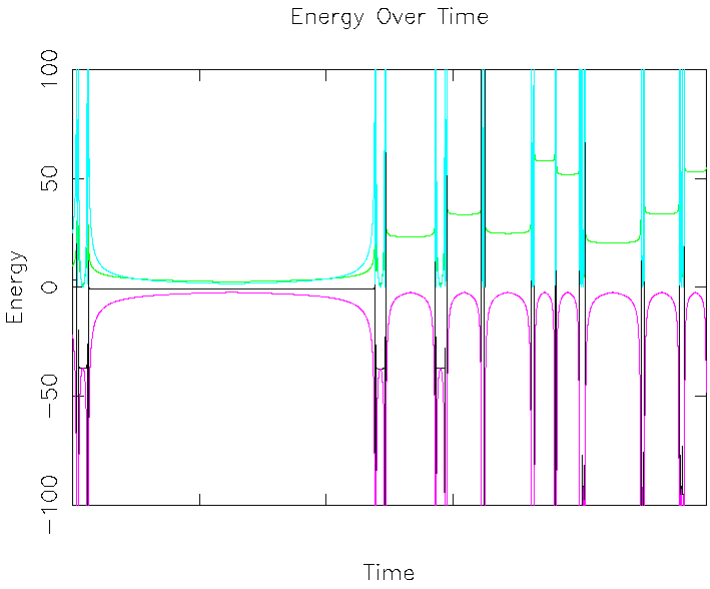

Figure 25: Same as above, but with $dt = 0.005s$ (half of above)

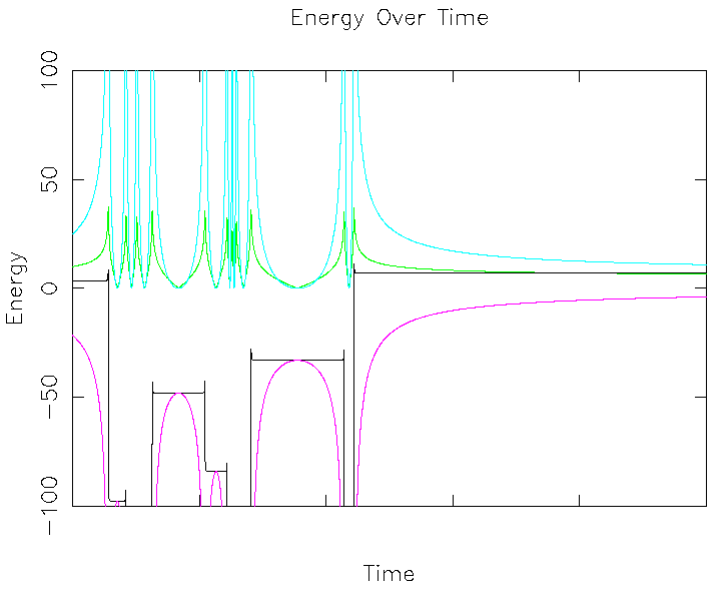

Figure 26: Same as above, but with $dt = 0.001s$ (a tenth of the first graph)

5 Conclusion

Both models performed well to simulate moving particles, but there is far more that could be done to explore this topic further:

- Incorporation of gravity as an optional force. Implementing this with the current state of my project should not be terribly difficult, since a developer would only need to add the force of gravity to the collection of acceleration contributions. The two independent variables required to calculate gravitational force (mass and distance) are readily accessible within each particle's object.
- Expanding the container to a variety of different shapes. This would necessarily involve improvements to wall collision calculations in accommodating angles or curves.
- Improve wall bounce calculations to ensure that out-of-bounds objects are pushed back in bounds. Currently, if objects have enough velocity and acceleration away from the origin, the naive velocity reversal calculations of `Container::get_collision_velocity` may not be enough to keep it in bounds.
- Improve program efficiency from $O(n^2)$ to $O(n \log n)$ by dividing the space and calculating collisions only for those objects close to one another. One of the more recent lectures have also explored an optimal method of calculating distant-dependent forces using a divide and conquer method.
- Add friction or an electric field map to provide non-constant acceleration outside of particle-particle interactions. This would enable the model to run other physics-based simulations like a mass spectrometer or even projectile motion (eg. a positively charged particle moving parallel to a negatively charged bottom plate).
- Count the number of collisions between particles against a wall. 3Blue1Brown has an excellent video exploring a special case where large masses collide with small masses with a ratio $\pi \times 10^x$ where x is based on the ratio of the object masses [9].
- Examine the overall (conservation of) momentum of the system over time. The visualization of momentum could be plotted on the moving particle graph with vectors showing the momentum of each particle.
- Calculations for pressure, temperature, etc. in the context of the ideal gas law. This would also enable a direct overlay of the Maxwell-Boltzman distribution on the energy distribution graphs seen above.

[9] `https://www.youtube.com/watch?v=jsYwFizhncE`

- Interactivity improvements, like adding energy to the system in the form of heat, controlling select particles, or tracing the path of selected particles to find random walk behaviour [10]. Adding containers that react to pressure differences may serve as a more realistic simulation of the physical world.

Exploring and researching about particle simulation in the context of C++ helped me gain a deeper understanding and appreciation of physical interactions. Among the most interesting findings was the mimicking of orbiting objects through charged particles with select initial velocities, the Maxwell-Boltzmann distribution of neutral particles, and the behaviour of charged particles given pre-selected configurations. Both models serve as an excellent tool to better visualize and interpret miniscule molecule-level movements.

[10] `https://en.wikipedia.org/wiki/Brownian_motion`