TABLE of CONTENTS

1-) INTRODUCTION 2

2-) METHODS-DISCUSSION 3

3-) RESULTS 9

4-) CONCLUSION 11

5-) CODE REVIEW 12

1) INTRODUCTION

There are ways to mathematically model dynamical systems. One of the most common ones is the designing a mass-spring system. In the smaller types of systems such as in the dynamics of the molecular systems, The Langevin dynamics approach is the most common and successful one. Basically, in physics, Langevin dynamics is an approach to the mathematical modeling of the dynamics of molecular systems. The French physicist Paul Langevin developed this type of modeling originally and name was given after his works. The approach is characterized by the use of simplified models while accounting for omitted degrees of freedom by the use of stochastic differential equations. The Langevin equation is a stochastic differential equation that describes the time-dependent variation of the degrees of freedom subset. The degrees of freedom mentioned are macroscopic variables that only slowly change with respect to other microscopic variables. The microscopic variables that are fast are responsible for the stochastic nature of the Langevin equation.

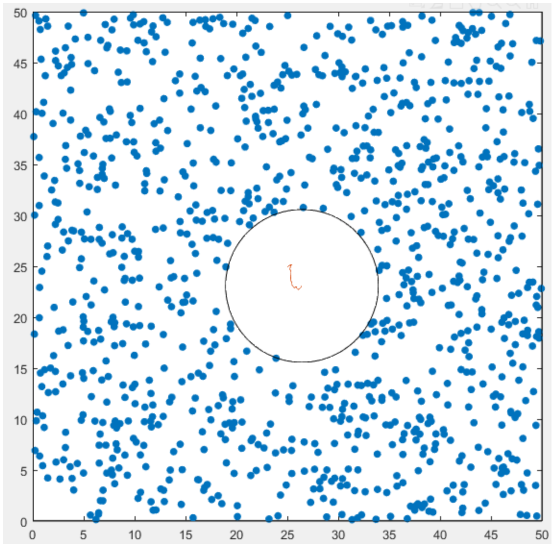


Figure.1: A schematic of small and big particles in Langevin dynamics: the blue ones are moving faster compared to white one.

The Langevin dynamics approach in modeling can be used to model thermal noise in an electrical resistor, harmonic oscillator in a fluid, trajectories of free Brownian particles and recovering Boltzmann statistics. Brownian motion can be given as an example of this. Brownian motion, also called Brownian movement, any of various physical phenomena in which some quantity is constantly undergoing small, random fluctuations while some big particles with small numbers move respectively slower.

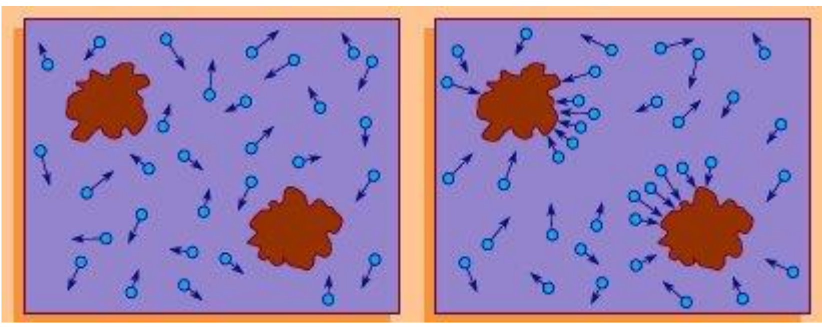


Figure.2: A schematic of Brownian motion: the big brown ones move slower than the blue small ones.

2) METHODS-DISCUSSION

In fig.1, there are 1000 blue particles and 1 big white particle and they are crashing to each other. If the system is a conversational system, that is, the mechanical energy before the impact and after the impact must be equal to each other. Therefore, both the total momentum and the total kinetic energy must be conserved.

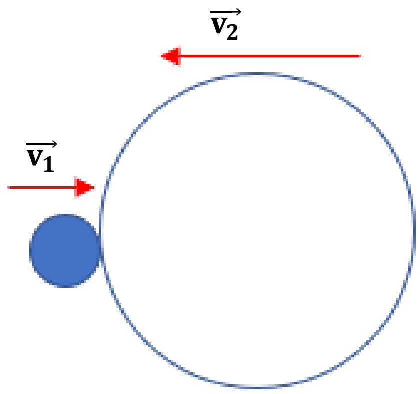


Figure.3: Representation of collision of smaller and bigger particles in Langevin dynamics

$$\vec{v_1}' = \vec{v_1} - \frac{2m_2}{m_1 + m_2} \frac{(\vec{v_1} - \vec{v_2}) * (\vec{x_1} - \vec{x_2})}{(x_1 - x_2)^2} (\vec{x_1} - \vec{x_2})$$

Where $\vec{v_1}$ is the velocity of the small particle before the collision and $\vec{v_2}$ is the velocity of big particle before the impact, $\vec{v_1}'$ is the velocity of the small particle after the collision, m_1 is the mass of the small particles, m_2 is the mass of the bigger particle, $\vec{x_1}$ is the position vector of the smaller particles and $\vec{x_2}$ is the position vector of the bigger particle.

Collisions between objects are governed by laws of momentum and energy. When a collision occurs in an isolated system, the total momentum of the system of objects is conserved. Provided that there are no net external forces acting upon the objects, the momentum of all objects before the collision equals the momentum of all objects after the collision. If there are only two objects involved in the collision, then the momentum lost by one object equals the momentum gained by the other object.

As a result, if the masses of the particles are close to each other in terms of magnitude, then the velocities of them would be affected much by each other. If the big one's mass is competerively larger than the small particles' masses, then after the collision, there wouldn't be large difference of the bigger particle's before and after velocities. If the bigger particle was not initially moving, then after the collision, the velocity direction of it would be the initial direction of the small particle's velocity.

Before going deep in Langevin dynamics, it is beneficial to mention about some phenomenon.

Drag / Dissipation

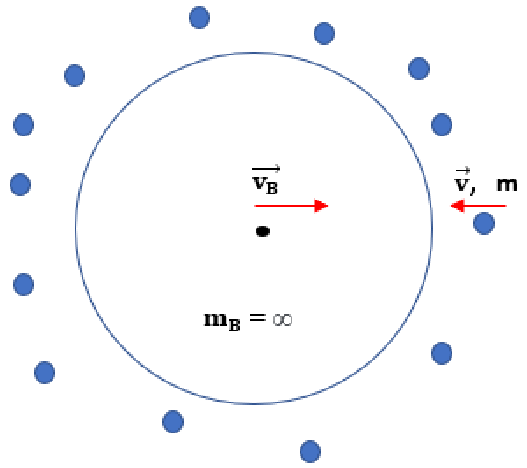


Figure.4: Collision of a huge(infinite) mass and a very small mass in opposite directions

If the velocity of the small particle is v to the left, the velocity of the bigger ball is v_B and the mass of the ball is infinity, then the new velocity of the smaller particle will be $\mathbf{v + 2v_B}$ in terms of magnitude. If the the ball with infinite mass was stationary(not moving), then the small particle would just go back with the same velocity magnitude. Since the ball is moving too, then the affect of this movement on the small particle will be in reverse direction and twice its velocity. The momentum that the small particle imparted on the ball will be $\mathbf{m(2v + 2v_B)}$ since its velocity has changed with the amount of $2v + 2v_B$.

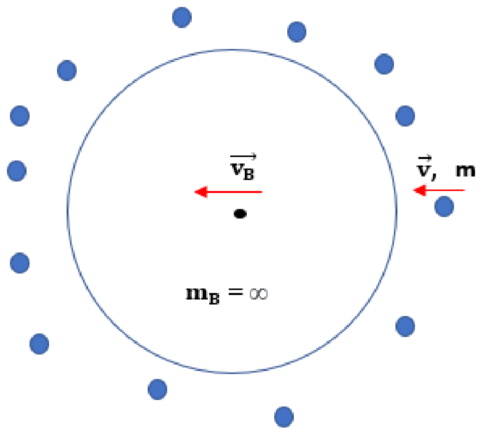


Figure.5: Collision of a huge(infinite) mass and a very small mass in the same directions

If the velocities of both the small particle and the ball are to the left. then the new velocity of the smaller particle will be $\mathbf{v - 2v_B}$ in terms of magnitude after the collision. Since the ball is moving to the left too, then the affect of this movement on the small particle will be in reverse direction and twice its velocity. The momentum that the small particle imparted on the ball will be $\mathbf{m(2v - 2v_B)}$ since its velocity has changed with the amount of $2v - 2v_B$.

Since the small particles are expected to move faster than the heavier ones, if one thinks that $v > v_B$, the direction of the ball with respect to small particle is important. The ball is getting more effect when its direction is opposite to the particle's direction than they are moving in the same direction ($\mathbf{m(2v + 2v_B)}$ > $\mathbf{m(2v - 2v_B)}$).

This situation can be inverted to the situations with different cases with opposite directions of the particle and the ball:

First case:
If the ball is moving with 1m/s velocity opposite to the small particle with velocity of 5m/s and with mass of m, then the ball will be affected with momentum of **m(2*5m/s + 2*1m/s).**
Second case:
If the ball is moving with 2m/s velocity opposite to the small particle with velocity of 5m/s and with mass of m, then the ball will be affected with momentum of **m(2*5m/s + 2*2m/s).**

m(2*5m/s + 2*2m/s) > m(2*5m/s + 2*1m/s)

As it can be seen, the ball is more affected by the small particle when the ball is moving faster opposite to the small particle. This situation is called drag and can be represented with:

$\overrightarrow{\mathbf{Drag}} = -\boldsymbol{\gamma} * \overrightarrow{\mathbf{v_B}}$ where γ is a proportionality constant and $\overrightarrow{v_B}$ is the velocity of ball.

When the larger materials try to move in a cloud of respectively small particles, their movement is affected negatively.

If the vehicles going through the air are taken into account to make more sense:

Drag is the aerodynamic force that opposes a materials motion through the air. Drag is generated by the parts of the material that interact with the air. Drag is a type of mechanical force. The interaction of a rigid body with a fluid(can be gas or liquid) produces drag. It isn't caused by a force field in the form of a gravitational or electromagnetic field, in which one object will influence another without physical contact. For drag to be generated, the solid body must be in contact with the fluid. If there is no fluid, there is no drag. The solid body must be in contact with the fluid to produce drag. There is no drag if there is no fluid. The difference in velocity between the solid object and the fluid causes drag. Between the object and the fluid, there must be movement. There is no drag if there is no movement. If the object moves through a static fluid or the fluid moves past a static solid object makes no difference. It is enough for the drag to be generated that the object and fluid move oppositely.

Figure.6: Drag affecting on a plane moving through air

Fluctuation

Fluctuation basically describes the exposure of an object to forces of different magnitude at multiple points at different times.

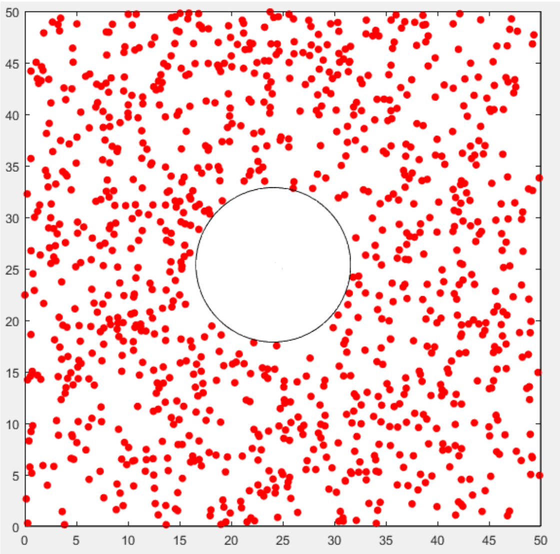
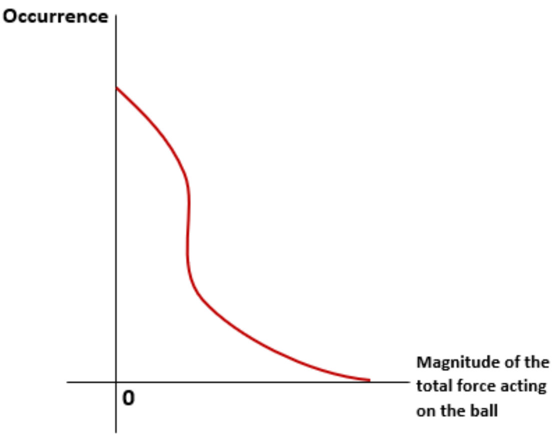


Figure.7: A ball inside the cloud of small particles with small masses.

According to Figure.7, red small particles hit the ball with more mass in the center at intervals and apply different amounts of force on it. The distribution of the forces and their occurence probability is represented by Gaussian normal distribution:



Graph.1: Distribution of the magnitude of the total forces acting on the ball

According to graph above, 0 force acting on the ball is the most common probability to occur. In addition, with increasing total force on the ball, the occurence gets smaller.

Langevine Dynamics

Langevine dynamics is a stochastic differential equation as mentioned before.

Langevine dynamics can be shown as:

$$\mathbf{m}\left(\frac{\mathbf{d^2x}}{\mathbf{dt^2}}\right) = -\boldsymbol{\gamma}\frac{\mathbf{dx}}{\mathbf{dt}} + \sqrt{\mathbf{2\,\gamma k_B T}}\;\vec{\mathbf{R}}(\mathbf{t})$$

where;

m is the mass of the particle

γ is the microscopic friction

k_B is the Boltzmann constant

T is the temperature

$\vec{R}(t)$ is a vector pointing at random direction at each time step having a magnitude that is picked out of normal distribution with standard deviation equals to one.

In the equation above;

$-\boldsymbol{\gamma}\frac{\mathbf{dx}}{\mathbf{dt}}$ is the drag part. This part tends to stop the ball from moving by acting against it.

$\sqrt{\mathbf{2\,\gamma k_B T}}\;\vec{\mathbf{R}}(\mathbf{t})$ is the fluctuation part. This can be thought as the driving force that tends to moove the ball since the small particles hit the ball and start fluctuation.

This two parts in the equation describe the motion of the big ball, to very high precision indeed. Fluctuation and drag/dissipation parts are entengled to each other since they have the common microscopic friction(γ).

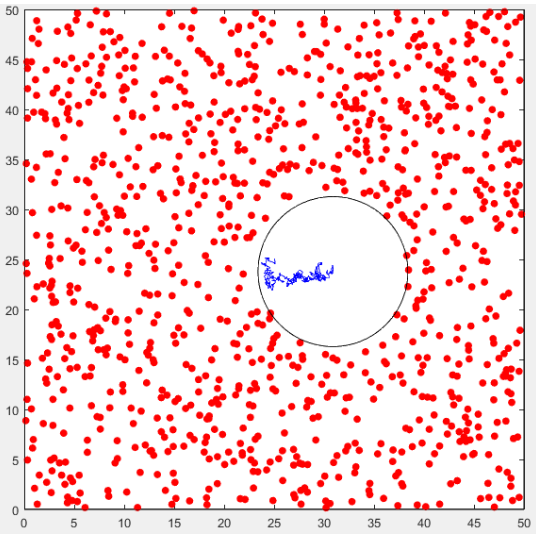


Figure.8: Representation of the Langevin dynamics:The drag and the fluctuation parts affect the way the ball took after a while.

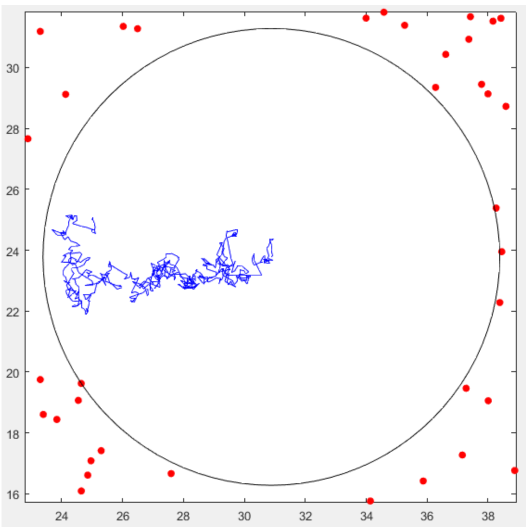


Figure.9: The path the ball took after a while, blue path shows the way the center of the ball passes.

Diffusion

After a while, the ball will diffuse from one place to another(from one end of the blue path to another end)

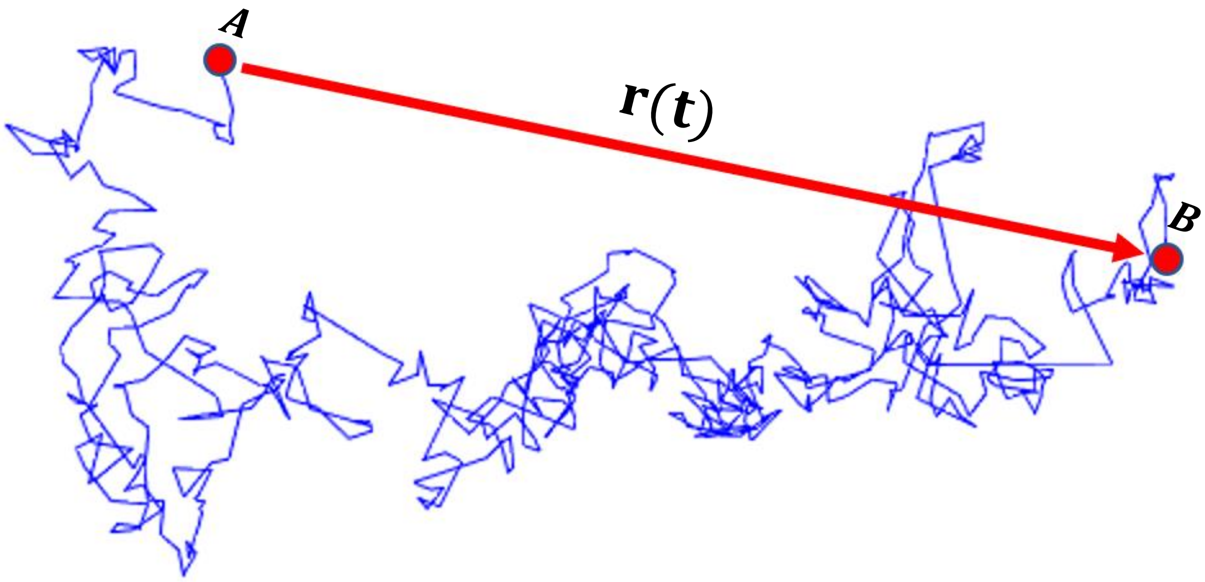


Figure.10: Showing of the diffusion from one point to another. The ball has been diffused from A to B.

$$|\mathbf{r(t)}|^2 = \mathbf{2.D.t}$$

where;
r(t) is the distance between the points,
D is the diffusion constant and $\mathbf{D} = \frac{\mathbf{k_B T}}{\boldsymbol{\gamma}}$
t is the elapsed time

For each time range, the square of r(t) should be linearly proportional to time elapsed until this moment. To make sure of it, the square root of the r(t) at this time range is taken several times(like thousands) and then the average of this several results is used. This can be shown as below:

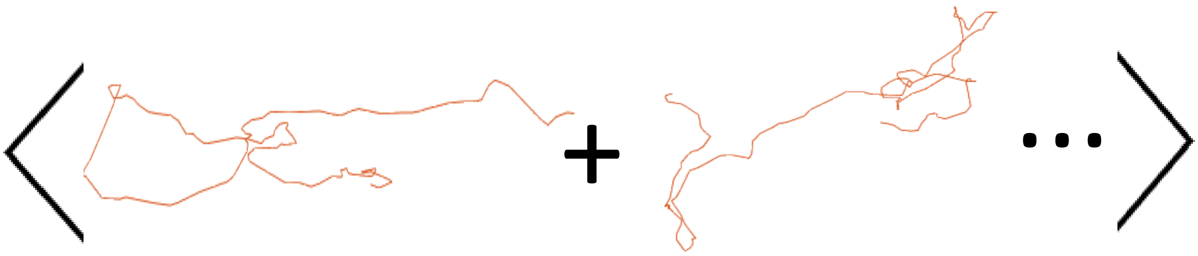


Figure.11: Summation of N different squares of the distances for a particular time range

If the repeats are made at each steps N times, N different results of square of distances between center and the final point reached are summed up and divided by N to get average of them.

$$< |\mathbf{r(t)}|^2 > = \frac{\sum_{\mathbf{i=1}}^{\mathbf{N}} (\mathbf{r(t)})^2}{\mathbf{N}}$$ where r is the distance between center and the final point reached

3) RESULTS

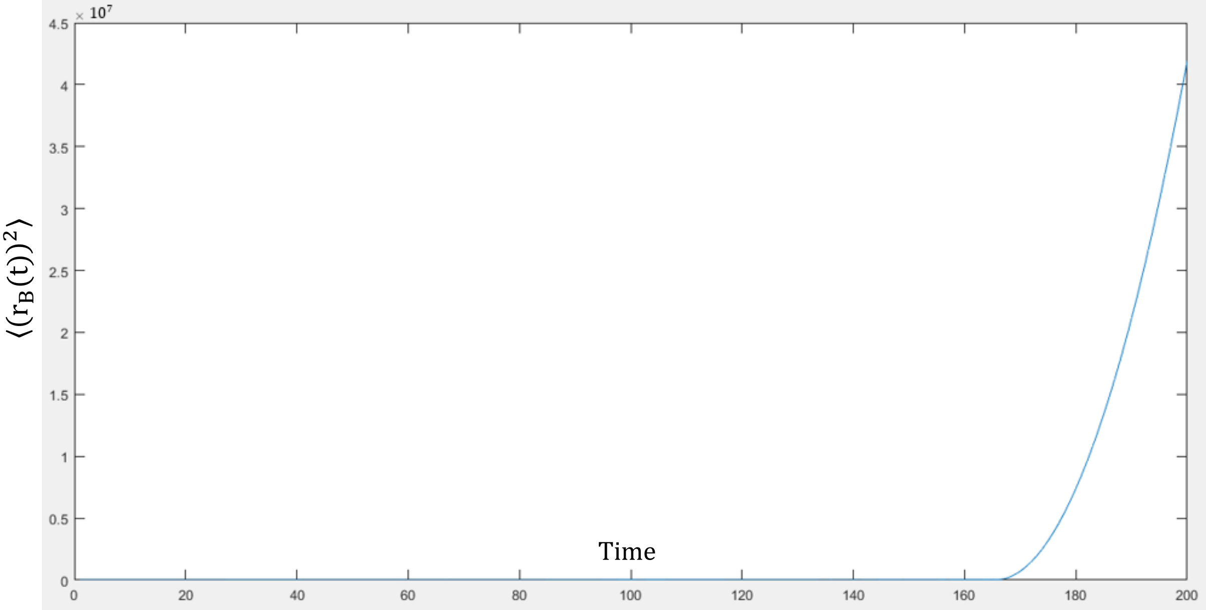


Figure.12: The representation of the average of the squares of the distances with respect to time: The time range is taken 0 to 200 and 200 repeats are made at each step.

Firstly, time step number of 200 was used with 200 repeats for each time step. Therefore, the corresponding calculation becomes:

$$\langle(r_B(t))^2\rangle = \frac{\sum_{i=1}^{200}\left(r_B(t)\right)^2}{200} \text{ with changing } r_B \text{ in each time step from 0 to 200.}$$

where $\langle(r_B(t))^2\rangle$ is the average of the square of distances in each time step until a certain time

While using time range from 0 to 200, the results were very close to 0 up to t = 166. When the time 166 is reached, the behavior of the ball motion overlaps with the expected results of linearity with Einstein's equation. The slope of this linear dependence is very much close to $\frac{\mathbf{2k_BT}}{\boldsymbol{\gamma}}$.

From the code → $\frac{4.2*10^7-0}{200-166} = 1235294$

From the Einstein's equation(ignoring the Boltzmann constant) → $\frac{2*T}{\gamma} = \frac{2*13000}{0.02} = 1300000$

where T is 13000 and γ is 0.02. We can ignore what the Boltzmann constant is because we are looking for proportionality and linearity overlapping with Einstein's equaiton.

1235294 and 1300000 are very close to each other.

$$1 - \frac{1235294}{1300000} = 4.98\%$$

There is 4.97% difference between them.

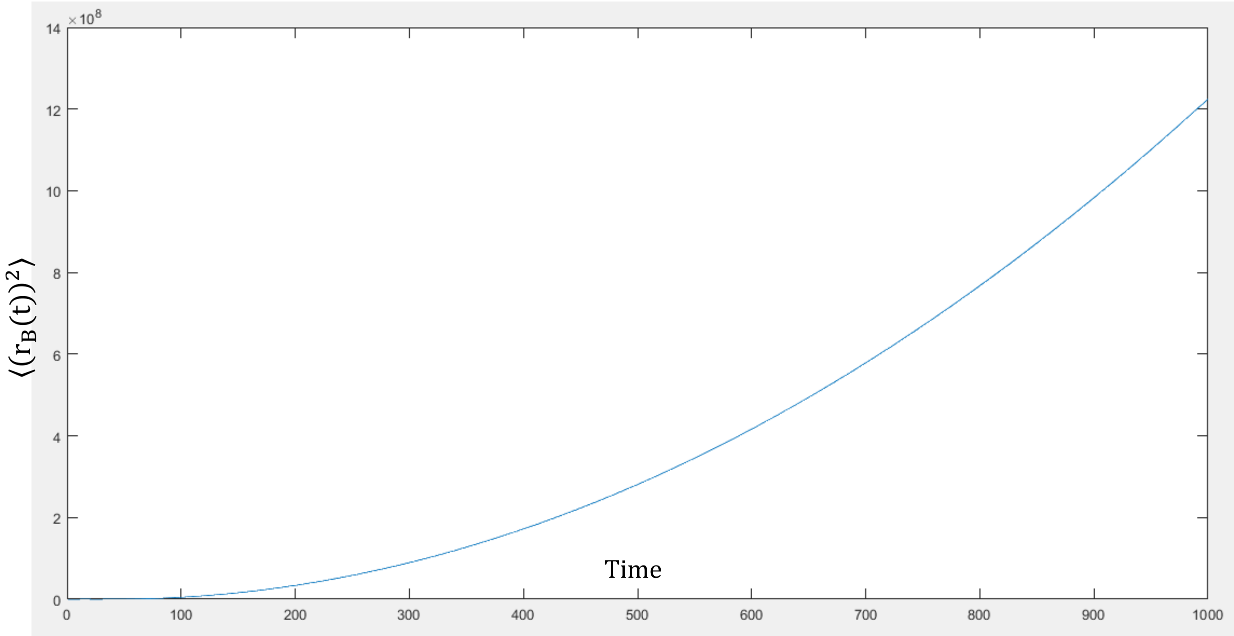


Figure.13: The representation of the average of the squares of the distances with respect to time: The time range is taken 0 to 1000 and 200 repeats are made at each step.

Secondly, time step number of 1000 was used with 200 repeats for each time step. Therefore, the corresponding calculation becomes:

$$\langle (r_B(t))^2 \rangle = \frac{\sum_{i=1}^{200} \left(r_B(t)\right)^2}{200} \text{ with changing } r_B \text{ in each time step from 0 to 1000.}$$

where $\langle (r_B(t))^2 \rangle$ is the average of the square of distances in each time step until a certain time

While using time range from 0 to 1000, the results initially started to increase rather than being very close to 0 as in the previous plot. The behavior of the ball motion overlaps with the expected results of linearity with Einstein's equation. The slope of this linear dependence is very much close to $\frac{\mathbf{2k_B T}}{\boldsymbol{\gamma}}$.

From the code → $\frac{12.5*10^8-0}{1000-0} = 1250000$

From the Einstein's equation(ignoring the Boltzmann constant) → $\frac{2*T}{\gamma} = \frac{2*13000}{0.02} = 1300000$

where T is 13000 and γ is 0.02. We can ignore what the Boltzmann constant is because we are looking for proportionality and linearity overlapping with Einstein's equaiton.

1250000 and 1300000 are very close to each other.

$$1 - \frac{1250000}{1300000} = 3.85\%$$

There is 3.85% difference between them.

4) CONCLUSION

The average of the square of the distance is linearly increasing with time. When the time interval is smaller, it moves away from linearity, and when the time interval is relatively large, linearity is approached even more. As the number of repetitions in each step increases, linearity increases and as the number of repetitions decreases in each step, getting linearty becomes harder. With increasing linearity, the result becomes closer to the Einstein's equation results which is error decreases.

When the time is elapsed later on, the ball goes beyond the boundaries of 50 x 50 and the ball continues to move on its motion.

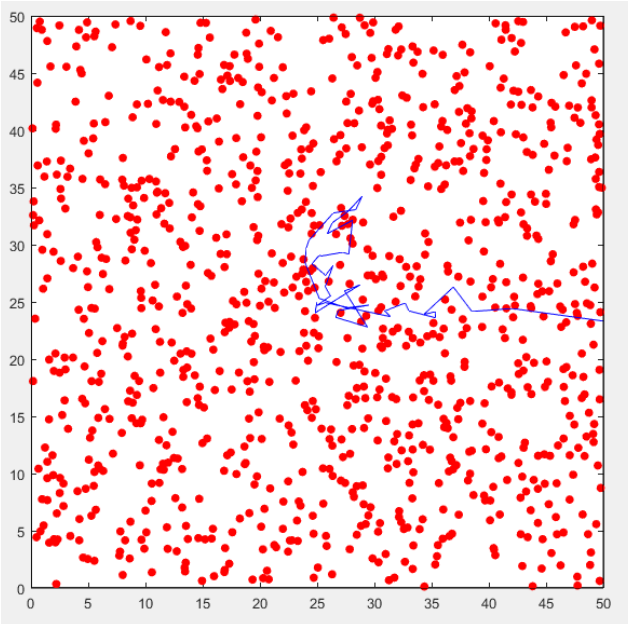


Figure.14: The ball moves outside the boundaries which is not a problem. If the boundaries were set to be 100 x 100 then it would be in the boundaries.

5) CODE REVIEW

```
tic
clear; clc; clf;
T = 1000;
L = [50 50]; % dimensions of the box
N = 1000; % number of particles
D = 1/4; % diameter of particles
r(1:N,1) = rand(N,1)*(L(1,1)-D/2); % define initial positions
r(1:N,2) = rand(N,1)*(L(1,2)-D/2); % define initial positions
v = randn(N,2); % define initial velocities
dt = 0.1; % time step
```

Time step number, dimensions of the box, number of the particles, diameter of the particles, initial positions, initial velocities and the time step size are defined.

```

mp = 1; % particle mass
mb = 10; % ball mass

vb = [0 0]; % velocity of the ball
rb = [25 25]; % coordinate of the ball
pb(T,2) = 0; % path of the ball
Db = 15; % diameter of the ball
```

Smal particles' and the larger ball's masses are defined, initial velocity of the ball and the initial position of the ball are defined. The diameter of the ball is defined.

```

nv = find((r(:,1) - rb(1,1)).^2 + (r(:,2) - rb(1,2)).^2 < ((Db+D)/2)^2);
for n = 1 : size(nv)
    th = rand*2*pi;
    r(nv(n),:) = r(nv(n),:) + (Db+D)*[cos(th) sin(th)];
end
```

This parts find the particles inside the ball and take them out of the ball

```


for t = 1 : T
    summ = 0;
    pb(t,:) = rb;
    for a = 1:200
```

Initiating the loop to investigate all time steps

Gathering the new ball coordinates

Initiating the loop to repeat each time step

```



        plot(r(:,1),r(:,2),'.r','MarkerSize',20);
        hold on;
        plot(pb(1:t,1),pb(1:t,2),"b");
        rectangle('Position',[rb(1,1)-Db/2 rb(1,2)-Db/2 Db Db],'Curvature',[1 1]);

        rectangle('Position',[0 0 L(1,1) L(1,2)]);
        hold off;
        axis equal;
        axis([0 L(1,1) 0 L(1,2)]);
        drawnow;
```

Plotting the ball motion and small particles's motions

```
        [sx,nx] = sort(r(:,1));
        for kn = 1 : N-1
            n = nx(kn);
            for km = kn+1:N
                m = nx(km);
                if (sx(km) - sx(kn) > D)
                    break
                else
                    rp = r(n,:)-r(m,:);
                    nrp = norm(rp);
                    if (nrp < D)
                        rv = v(n,:)-v(m,:);
                        if (rv*rp'<0)
                            v(n,:) = v(n,:) - (rv*rp')*rp/nrp^2;
                            v(m,:) = v(m,:) + (rv*rp')*rp/nrp^2;
                        end
                    end
                end
            end
        end
```

Defining the collisions between balls
Scanning particles from left to right
Stops if x's differ more than D which is the diameter of the small particles.
Defining the vector between two balls(before and after)
Defining the velocity difference vector

```
        for n = 1 : 2
            nv = (v(:,n) > 0).*(r(:,n) > L(1,n)-D/2); v(nv==1,n) = -v(nv==1,n);
            nv = (v(:,n) < 0).*(r(:,n) < D/2); v(nv==1,n) = -v(nv==1,n);
        end

        nv = find((r(:,1) - rb(1,1)).^2 + (r(:,2) - rb(1,2)).^2 < ((Db+D)/2)^2);
        for n = 1:size(nv,1)
            m = nv(n,1);
            rp = (r(m,:)-rb); nrp = norm(rp); rv = v(m,:) - vb;
            if (rv*rp' < 0)
                v(m,:) = v(m,:) - 2*mb/(mp + mb)*(rv*rp')*rp/nrp^2;
                vb = vb + 2*mp/(mp + mb)*(rv*rp')*rp/nrp^2;
            end
        end
```

Defining the particles when they bounce the ball

```
        r = r + v * dt; % move particles
        rb = rb + vb * dt; % move the ball

        %plot(t,result)
        %hold on
        mp*sum(v(:,1).^2 + v(:,2).^2) + mb*(vb(1,1)^2 + vb(1,2)^2);
        summ = summ + (abs(rb(1)-25))^2 + (abs(rb(2)-25))^2;
    end
    average = summ/200;
    result(t)=average;
end
plot((1:T),result)
toc
```

Moving the particles and the ball according to new datum