Introducing randomness to physical systems

Computational Physics Project

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Abstract

We look at the behaviour of two physical systems, the harmonic oscillator and free falling particles, when a random Gaussian force is added to every step. We use numerical forward integration (RK4 method) to simulate the systems. Our objective is to obtain few of the statistical properties for our system by following Langevin's approach and to also demonstrate that the equipartition theorem holds for the Brownian oscillator system.. In order to do that we trace Langevin's, and Chandrasekhar's equations with our numerical solution for the Brownian oscillator. The section on free-falling particles would have further application when modelled with boundary condition and realistic values of the system.

Contents

Introduction

The properties of Brownian motion and random walk have been extensively studied as a part of understanding the behaviour of fluid molecules and particles in the air. Brownian motion is the random motion of particles, caused by collisions with surrounding molecules. Robert Brown was credited with its discovery in 1827 when he observed pollen grains suspended in water executing random, jittery movements. Einstein calculated the probability distribution of the displacement of particles subject to Brownian motion and found that the solution was the normal or Gaussian distribution (a bell-curve). From this, the equation of the mean squared displacement is given by

$$x^2 = 2Dt \tag{1}$$

where D represents the diffusion constant, which is a stochastic property of the gas. Thus, Einstein showed that the mean squared displacement was directly proportional to time, rather than the mean displacement.

Using this overview of Brownian motion, our project aimed to model deterministic dynamical systems with the addition of a Gaussian random force, and examine the statistical properties over a large number of trials. We chose two physical systems- the damped driven harmonic oscillator and a collection of free-falling particles in the atmosphere.

Model 1: Harmonic Oscillator

Harmonic Oscillators

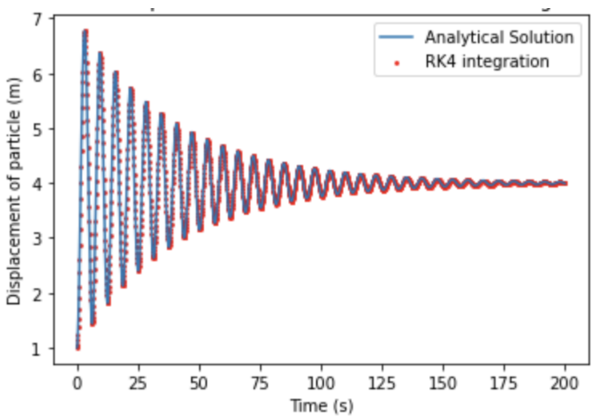
Harmonic oscillators are very common dynamical systems that are well understood and have many practical examples, such as springs and waves. A particle exhibits simple harmonic motion if its acceleration is negatively proportional to its displacement from the origin.

Driven damped harmonic oscillator

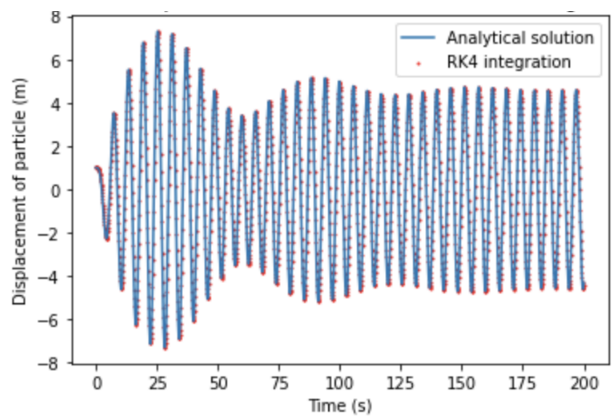
The motion of a harmonic oscillator can be damped due to friction or fluid viscosity that is proportional to the velocity of the particle and opposes the harmonic or restoring force. This gives the equation -. In some systems, there is an additional force exerted onto the particle, that may be constant or periodic. Periodic force on a damped oscillator gives rise to the transient and steady state regimes.

$$\begin{aligned} m\frac{d^2x}{dt^2} &= -m\gamma\frac{dx}{dt} - kx + \mathrm{F} \\ \frac{d^2x}{dt^2} &= -\gamma\frac{dx}{dt} - \omega^2 x + \mathrm{F} \end{aligned} \tag{2}$$

We simulated three variations of this equation- constant driving force, sinusoidal driving force and random driving force. For the first two variations, the numerical integration is plotted with the analytical solution on the same graph.



(a) Driven Damped Oscillator with constant driving force.



(b) Driven Damped Oscillator with Sinusoidal driving force

Figure 1

Analytical solution for the damped harmonic oscillator with constant driving force A and damping constant γ:

$$x(t) = Ae^{-\frac{1}{2}\gamma t}\cos(\omega_d t) \text{ where } \omega_d = \sqrt{\frac{k}{m} - \frac{\gamma^2}{4}} \tag{3}$$

Analytical solution for the damped harmonic oscillator with sinusoidal driving force F and damping constant γ:

$$\begin{aligned} F &= F_0\cos(\omega_f t) \\ \omega_d &= \sqrt{\frac{k}{m} - \frac{\gamma^2}{4}} \\ B &= \frac{F_0}{\sqrt{(\omega_0^2 - \omega_f^2)^2 + \gamma^2\omega_f^2}} \\ \phi &= \tan^{-1}\left(\frac{-\gamma\omega_f}{\omega_0^2 - \omega_f^2}\right) \\ x(t) &= Ae^{-\frac{1}{2}\gamma t}\cos(\omega_d t + \theta) + B\cos(\omega_f t + \phi) \end{aligned} \tag{4}$$

Brownian Oscillator

In the simulation of a Brownian oscillator, the force applied to the damped, harmonic motion is randomly generator according to the Gaussian distribution.

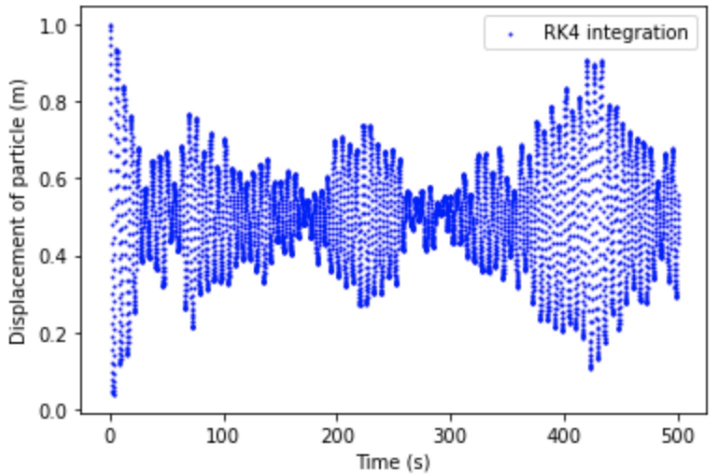


Figure 2: Driven damped oscillator with random driving force generated by the Gaussian distribution.

Equipartition Theorem

The equipartition theorem is a concept arising from classical statistical mechanics, which states that the energy of the system is equally divided amongst the energies in different degrees of freedom. It also gives a relation between the temperature of the system to its average kinetic and potential energies. Our model has potential energy arising from the harmonic force, and one degree of freedom for kinetic energy.

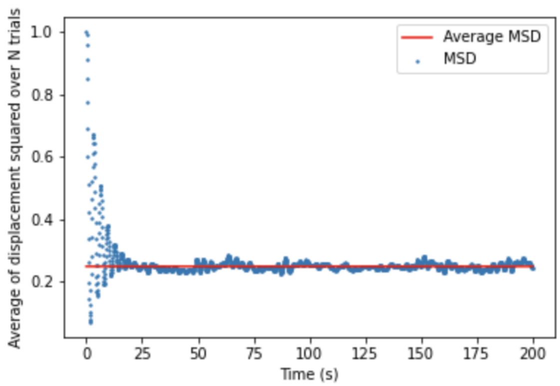
$$\begin{aligned} \text{Kinetic energy} &= \frac{1}{2}mv^2 \\ \text{Potential energy} &= \frac{1}{2}kx^2 \end{aligned} \tag{5}$$

Each component of energy contributes $\frac{1}{2}k_bT$ joules of energy, where k_b represents the Boltzmann constant and T represents temperature. Thus the total energy of the system is given by:

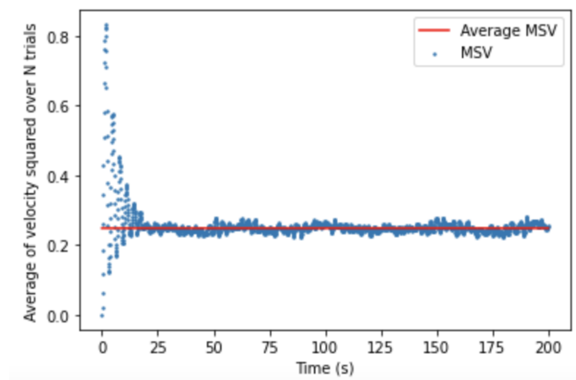
$$\frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}k_bT + \frac{1}{2}k_bT = k_bT \tag{6}$$

In the below graphs, the system had $k = 1$ and $m = 1$. Therefore,

$$\frac{1}{2}k\langle x^2\rangle + \frac{1}{2}m\langle v^2\rangle = \frac{1}{2} \times 1 \times 0.249 + \frac{1}{2} \times 1 \times 0.249 = \frac{1}{2}k_BT$$



(a) The Mean squared displacement over time, along with the calculated average. The average over time was calculated to be 0.249 m^2.



(b) The Mean squared velocity over time, along with the calculated average. The average over time was calculated to be 0.249 $m^2\ s^{-2}$.

Figure 3: Graphs of MSD and MSV used to demonstrate the equipartition theorem. The initial few values were not included in the calculation of the overall average.

By using the values for the brownian oscillator calculated by the numerical integrator, we can calculate the squares of the velocities and displacements over time and check that the simulated oscillator satisfies the equipartition theorem. To obtain the aforementioned results we use the Langevin's approach to compare the energy values of kinetic energy and potential energy. Following Langevin's approach will also get us the temperature of our system. Considering the energy equipartition theorem which states that

$$\frac{1}{2}m\langle v^2\rangle = \frac{1}{2}k_B T$$

and mean value of $\langle v \rangle = 0$, this gives us an equation for the temperature of our system, in terms of derivatives of the standard deviation of x.

$$\frac{d^2\sigma_x^2}{dt^2} + \beta\frac{d\sigma_x^2}{dt} + 2\omega^2\sigma_x^2 = 2\frac{k_b T}{m} \tag{7}$$

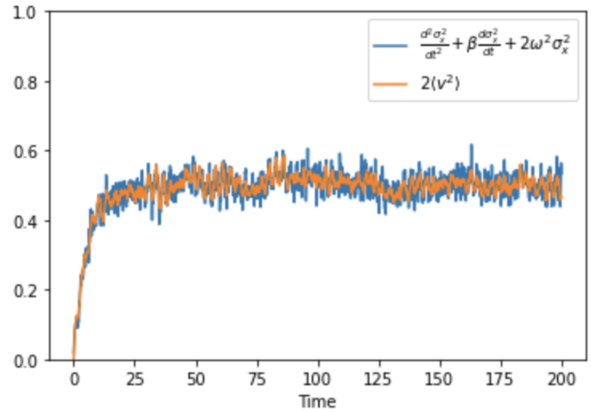


Figure 4: Comparing the left hand side and right hand side of the equation giving us the value of $\frac{k_b T}{2}$. This confirms that the simulated system does follow this equation and can give us a good approximation of the temperature.

The above graph gives us the value of $k_B T/m = 0.251\ m^2\ s^{-2}$ so, the temperature of our system where $m = 1$, T is the temperature and k_B is the Boltzmann constant is

$$T = 1.824 \times 10^{22}$$

Langevin's approach

Langevin's equation is a stochastic differential equation that describes the state of a system subjected to random forces. We attempted to replicate the results of a paper by O. Contreras-Vergara et al. in which the authors compared the approach by Langevin to the approach by Chandrasekhar to finding a deterministic equation for the mean squared displacement and mean squared velocity of the Brownian oscillator. Chandrasekhar's equations were calculated to be exact, taking into consideration the random force, whereas Langevin's approach was to eliminate the fluctuating force. He based his theory on the independence of the fluctuating force and the mean trajectory of the particle. His solutions did not mach with Chandrasekhar's or the numerically calculated ones in the short term, but over time it converged and in the long time limit, does match the other two. The principle of the difference between the two solutions is similar to that of the transient and steady state regimes. The factor that differs between the two solutions is multiplied by a decaying exponential, so that the amount they differ by decreases over time, leaving only predominant forces and conditions.
The system was modelled by the equation:

$$\frac{d^2x}{dt^2} + \beta\frac{dx}{dt} + \omega^2 x = \frac{1}{m}\zeta(t) \tag{8}$$

ζ, represents the fluctuating gaussian force applied to the harmonic system. The system behaves differently depending on the damping factor β, which can be divided into two distinct cases- overdamped oscillator, where $\beta > 2\omega$, and the underdamped case, where $\beta < 2\omega$. In the underdamped case, the system will oscillate to the equilibrium position, while in the overdamped case, the moves slowly towards the equilibrium without (much) oscillation.
Langevin's equations for the mean squared displacement of the Brownian oscillator are calculated with the assumption that $\langle\zeta(t)\rangle = 0$ and $\langle x\zeta(t)\rangle = 0$. Two equations are formed from Eqn. 8, one by multiplying by x and then taking the ensemble average, and the other by first taking the ensemble average and then multiplying by $\langle x\rangle$. From this process, we get the equations for the overdamped and overdamped cases.
For each case, we have plotted the numerically calculated (using RK4) values of the mean square displacement, and mean square velocity along with Langevin's approximations and Chandrashekhar's exact equations.

Underdamped Case

Underdamped case for a brownian harmonic oscillator includes the condition where ($\beta < 2\omega$). The equations below are provided by Langevin are an approximation to the exact solution by Chandresekhar. We have compared the results with our numerical solutions.

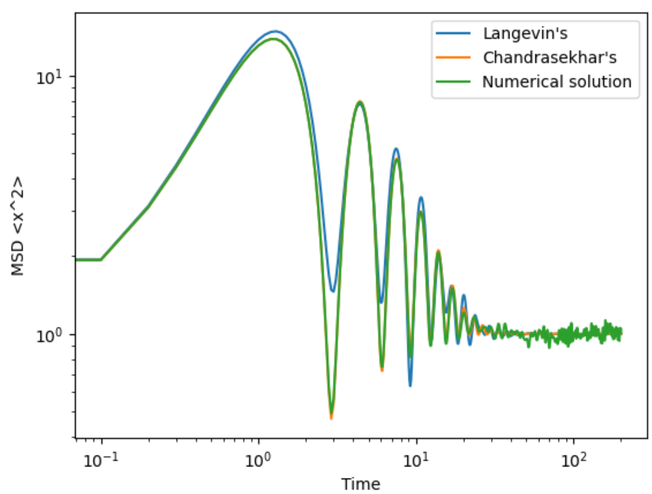


Figure 5: Harmonic Brownian Oscillator Underdamped Case ($\beta < 2\omega$)

The equations below are for the mean square displacement:
Langevin's eqn.

$$\bar{\omega}_1 = \sqrt{\omega^2 - (\beta^2/8)}$$
$$\langle x^2(t)\rangle_o = \langle x(t)\rangle^2 + \frac{k_B T}{m\omega^2} \times \left\{1 - e^{-\frac{1}{2}\beta t}\left(-2\sin^2\frac{\sqrt{2}}{2}\bar{\omega}_1 t + \frac{\beta}{\sqrt{8}\bar{\omega}_1}\sin\sqrt{2}\bar{\omega}_1 t + 1\right)\right\} \tag{9}$$

Chandrashekhar's eqn.

$$\omega_1 = \sqrt{\omega^2 - (\beta^2/4)}$$
$$\langle x^2(t)\rangle_c = \langle x(t)\rangle^2 + \frac{k_B T}{m\omega^2}\left\{1 - e^{-\beta t} \times \left(\frac{\beta^2}{2\omega_1^2}\sin^2\omega_1 t + \frac{\beta}{2\omega_1}\sin 2\omega_1 t + 1\right)\right\} \tag{10}$$

Mean Squared velocity Equations

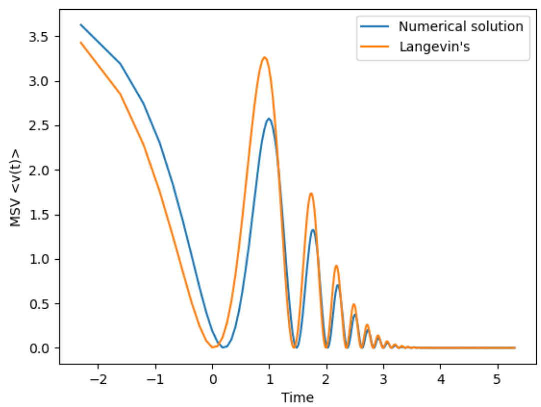


Figure 6: Harmonic Brownian Oscillator underdamped case ($\beta < 2\omega$).

Langevin's eqn.

$$\langle v^2(t)\rangle_o = \langle v(t)\rangle^2 + \left(\sigma_0^2 - \frac{k_B T\omega^2}{m(\omega^2+\beta^2)}\right)e^{-2\beta t} + \frac{k_B T\omega^2}{m(\omega^2+\beta^2)}e^{-\frac{1}{2}\beta t} \times \left[\cos\sqrt{2}\bar{\omega}_1 t - \frac{3\beta}{\sqrt{8}\bar{\omega}_1}\sin\sqrt{2}\bar{\omega}_1 t\right] + \frac{C_1}{\beta m}\Big(1 - e^{-2} \tag{11}$$

Chandrashekhar's eqn

$$\langle v^2(t)\rangle_c = \langle v(t)\rangle^2 + \frac{k_B T}{m}\left\{1 - e^{-\beta t} \times \left(\frac{\beta^2}{2\omega_1^2}\sin^2\omega_1 t - \frac{\beta}{2\omega_1}\sin 2\omega_1 t + 1\right)\right\} \tag{12}$$

Overdamped case

Overdamped case for a brownian harmonic oscillator includes the condition where ($\beta > 2\omega$). The equations below are provided by Langevin are an approximation to the exact solution by Chandresekhar. We have compared the results with our numerical solutions.

The equations below are for the mean square displacement:

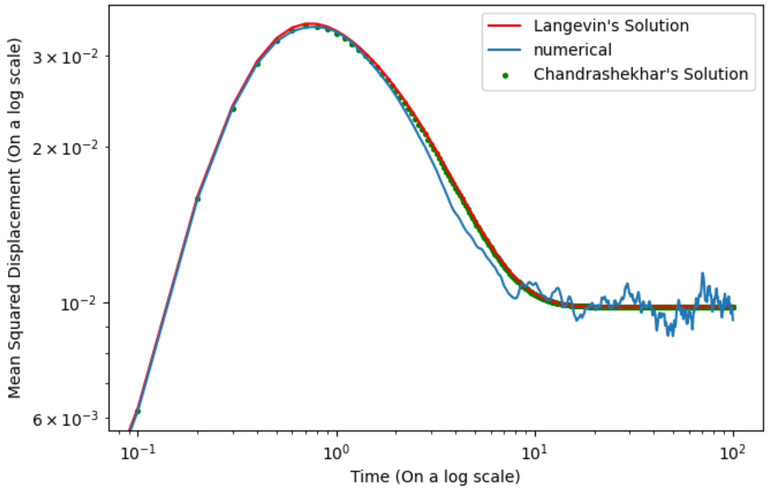


Figure 7: Mean squared displacement in the overdamped case.

Langevin's approach.

$$\begin{aligned}\bar{\beta}_1 &= \sqrt{\beta^2 - 8\omega^2} \\ \langle x^2(t)\rangle_o &= \langle x(t)\rangle^2 + \frac{k_B T}{m\omega^2}\Big\{1 - e^{-\frac{1}{2}\beta t}\Big(2\sinh^2\frac{1}{4}\bar{\beta}_1 t + \frac{\beta}{\bar{\beta}_1}\sinh\frac{1}{2}\bar{\beta}_1 t + 1\Big)\Big\}\end{aligned} \tag{13}$$

Chandrashekhar's exact solution.

$$\begin{aligned}\beta_1 &= \sqrt{\beta^2 - 4\omega^2} \\ \langle x^2(t)\rangle_c &= \langle x(t)\rangle^2 + \frac{k_B T}{m\omega^2}\Big\{1 - e^{-\beta t}\Big(2\frac{\beta^2}{\beta_1^2}\sinh^2\frac{1}{2}\beta_1 t + \frac{\beta}{\beta_1}\sinh\beta_1 t + 1\Big)\Big\}\end{aligned} \tag{14}$$

Next we move on the Mean Squared velocity Equations.

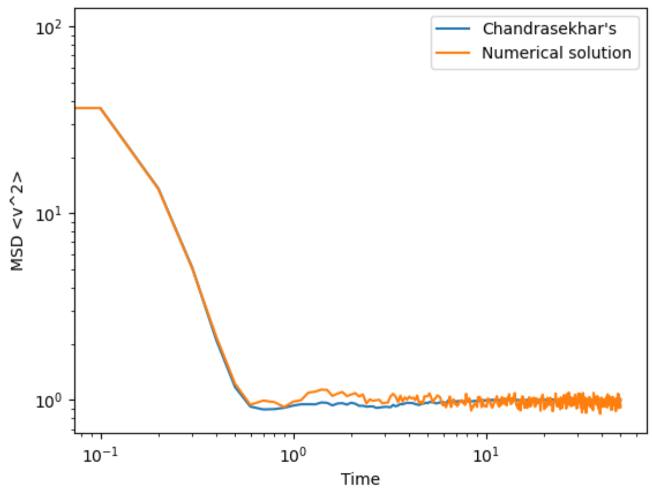


Figure 8: Mean squared velocity in the overdamped case.

Langevin's eqn.

$$\langle v^2(t)\rangle_o = \langle v(t)\rangle^2 + \Big(\sigma_0^2 - \frac{k_B T\omega^2}{m(\omega^2+\beta^2)}\Big)e^{-2\beta t} + \frac{k_B T\omega^2}{m(\omega^2+\beta^2)}e^{-\frac{1}{2}\beta t}\times\Big[2\sinh^2\frac{1}{4}\bar{\beta}_1 t - \frac{3\beta}{\bar{\beta}_1}\sinh\frac{1}{2}\bar{\beta}_1 t\Big] + \frac{C_1}{\beta m}\Big(1 - e^{-\frac{1}{2}\beta \tag{15}$$

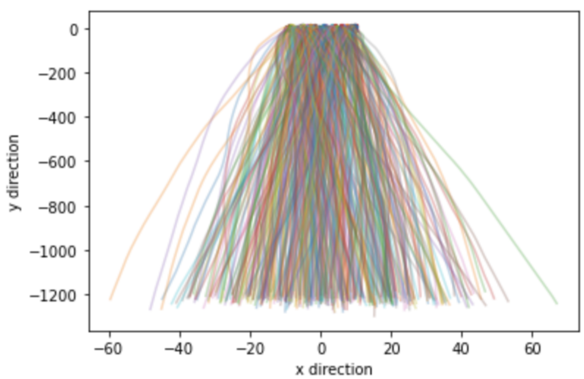
Chandrashekhar's eqn

$$\langle v^2(t)\rangle_c = \langle v(t)\rangle^2 + \frac{k_B T}{m}\Big\{1 - e^{-\beta t}\Big(2\frac{\beta^2}{\beta_1^2}\sinh^2\frac{1}{2}\beta_1 t - \frac{\beta}{\beta_1}\sinh\beta_1 t + 1\Big)\Big\} \tag{16}$$

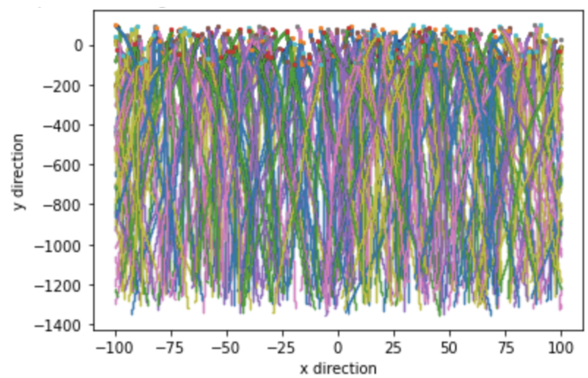
The derivation and implementation of the Langevin's MSV overdamped equation is more complex, and requires further work at this time.

Model 2: Settling dust in the atmosphere

In this model, we simulated a number of freely falling particles, subjected to the forces of gravity, damping, and Brownian random forces from the air particles surrounding them. This model used the same RK4 numerical integration as the brownian oscillator. The particles experience a downwards acceleration due to gravity and damping in both vertical and horizontal directions. At every time step, each particle also experiences a random force in either vertical or horizontal direction, generated by a gaussian random function. To begin the simulation, we randomly distribute 400 particles across a 20 unit by 20 unit area using a uniform random number generator. This determines their initial X- and Y- positions, and their initial veolcities are all set to be zero. We also impose an additional boundary condition on the particles to ensure that they do not disperse indefinitely, so that when a particle is about to move out of the defined space, it re-enters the boundary from the other side. Then we allow the RK4 integrator to calculate subsequent velocities and positions for each particle.



(a) Particles subject to brownian motion without the boundary condition. The particles slowly drift apart, and the distribution of particles across the horizontal axis comes to resemble a bell curve.



(b) Particles subject to brownian motion with the boundary condition. The particles stay within the specified range which ensures a constant and uniform density of particles.

Figure 9: Two simulations of particles with brownian motion- one with (b) boundary conditions enforced, and one without (a).

We also varied the magnitude of the mean Brownian force driving the particles and measured how the standard deviation of the particles' distributions changed. This was shown to be a linear relationship.

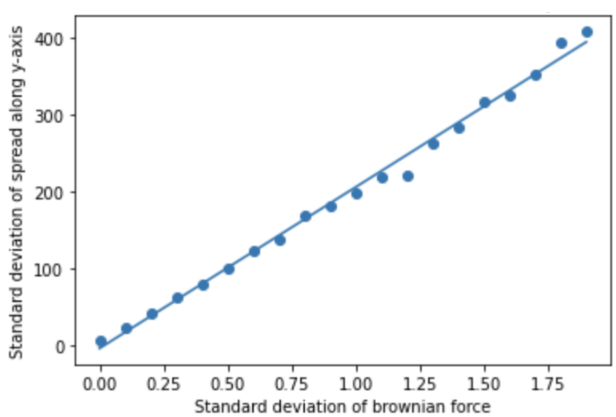


Figure 10: Distribution of standard deviation with varying mean Brownian force, along with the line of best fit for the data.

Methods

Runge-Kutta Method

Runge-Kutta is collection of methods used in numerical analysis to calculate solutions to differential equations. The most widely known method among the collection is the RK4 method, it is a fourth-order runge kutta method which uses four approximations to the slope. RK4 calculates the solution to an initial value problem (IVP) such as,

$$\frac{dy}{dt} = f(t,y), \quad y(t_o) = y_0$$

For the above equation there is a general formula to calculate the solution,

$$k1 = f(t_n, y_n),$$

$$k2 = f(t_n + \frac{dt}{2}, y_n + dt\frac{k1}{2}$$
$$k3 = f(t_n + \frac{dt}{2}, y_n + dt\frac{k2}{2}$$
$$k4 = f(t_n + dt, y_n + dtk3)$$
$$y_{n+1} = y_n + \frac{1}{6}(k1 + 2k2 + 2k3 + k4)dt$$
$$t_{n+1} = t_n + dt$$

Here dt is the time step and $n \in [0, \infty]$.

The reason behind using RK4 method is because of its better approximation and faster computation. When compared to other methods the RK4 method shows more authentic results. To test this for our own system we first look at the energy difference for each method and then the relative error. These two test were programmed using three different numerical integrator, Euler, Leapfrog and RK4.

Testing accuracy of RK4 method using Energy Difference

To check the energy difference we program simple harmonic oscillator. A simple harmonic oscillator is a very simple system, like a spring attached to a rigid body on one end and to a small mass on the other end. This gives us two terms; spring constant k for the spring and and $F = ma$ from newton's second law.

$$m \cdot \frac{d^2x}{dt^2} + kx = 0$$

Now plotting energy as function of time for the three methods.

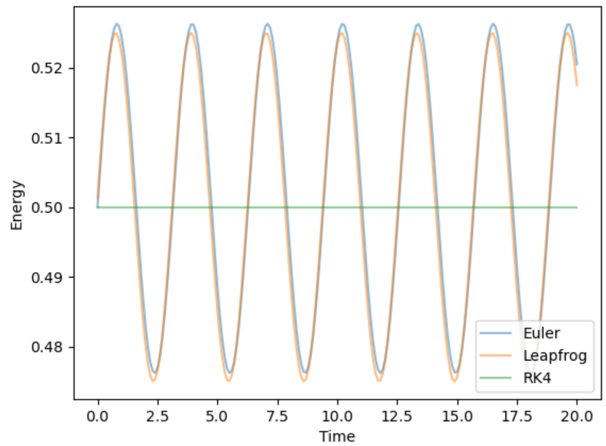


Figure 11: Plot of Energy vs Time.

Energy difference of the system for all three methods gives us,

$$\text{Energy difference for Euler method} = 0.020474379277524046$$

$$\text{Energy difference for Leapfrog method} = 0.016225000348893293$$

$$\text{Energy difference for RK4 method} = -1.3871508627860685 \times e^{-6}$$

It is evident from the Energy difference value of all three that RK4 method works better for simple harmonic oscillator.

Testing accuracy of RK4 method using Relative Error

To check for relative error we program a damped driven oscillator. It is just like a damped oscillator, but with an extra force acting on it to stop it from dying out due to frictional energy loss.
Following is the equation for damped driven oscillator:

$$F_o \cos \omega t = m \cdot \frac{d^2x}{dt^2} + b \cdot \frac{dx}{dt} + kx \tag{17}$$

Here b is the damping constant, k is the spring constant and $F_o \cos \omega t$ acts as a sinusoidal force.

In order to compare the different integrators the relative difference between the exact solution and numerical solution are plotted on the same graph.

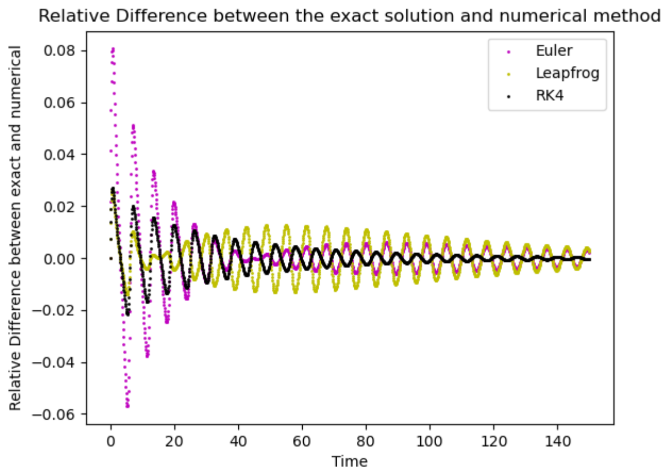


Figure 12: Relative difference between the exact solution and numerical solution.

It is evident from the graph that the RK4 method reaches the solution faster and with better approximation, hence low relative error.

Conclusion

In this work, we have successfully modeled the harmonic Brownian oscillator and also approached it using a different mathematical approximation i.e. Langevin's approach. Using this large time scale approximation we obtained various statistical properties of our system, like the temperature and energy distribution. The energy distribution further helped in proving the energy equipartition theorem for our system.

$$\frac{1}{2}m\langle v^2\rangle = \frac{1}{2}k_BT$$

The last part of our project included modelling the motion of particles in the atmosphere under the forces of gravity, viscous damping, and brownian force. We also showed how the standard deviation of the distribution varies the magnitude of brownian force. Further work on this model would be to calculate the realistic values for the damping constant, Brownian force, etc. and then re-examine the various properties and distributions of the model under those conditions.

References

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[4] Einstein, A.B. (2004). On the Motion of Small Particles Suspended in Liquids at Rest Required by the Molecular-Kinetic Theory of Heat.

[5] *Runge-Kutta method.* Runge-Kutta method - Encyclopedia of Mathematics. (n.d.). Retrieved September 18, 2022, from https://encyclopediaofmath.org/index.php?title=Runge-Kutta-method

Appendix

Attached here are the code files written in python, using Google Drive Colab.
[1] Simple oscillators and Brownian oscillators
[2] Langevin’s equations- the underdamped case
[3] Langevin’s equations- the overdamped case
[4] Modelling settling dust