Simulation of Brownian Motion Driven Internally by White Noise and an External Electric Oscillator

NORODIN A. RANGAIG*,1, NORHAMIDA D. MINOR*,2, GREMA FE I. PEÑONAL*,3, VERNIE C. CONVICTO*,4 , and JAE LORD DEXTER C. FILIPINAS*,5

ABSTRACT

Understanding the Brownian motion of a random particle caused by the contribution of randomness can lead to a great physical interpretation into the behavior of any stochastic phenomena. In this study, we used a mathematical and analytical modeling of realistic stochastic processes with a numerical treatment on the random force addressed as white noise term. The transition of motion from the classical Langevin equation was treated; and the ballistic to diffusive regime due to the inertial term on the Langevin equation for a short time was then considered. Furthermore, we examined the diffusive regime without the inertial term and subjected it to a varying electric oscillator with fixed fluctuation of frequency for a short time. Lastly, plots for the displacements, and mean squared displacements, when with or without inertial term and when it is subjected to an electric oscillator were obtained.

Keywords: Brownian motion, White noise, Electric oscillator, Langevin equation, Diffusion.

I. INTRODUCTION

Brownian motion is a great example of a stochastic phenomenon that has a very wide application, and some of its applications are in modeling stock market, molecular biology, nanodevices etc. Although the process of understanding directly the behavior of the stochastic phenomena requires the use advanced and expensive tools; starting with a simple stochastic process may give an insight on the dynamics of stochastic processes. Understanding can be achieved by doing numerical experiments which are cheap and affordable and are done with the use of a computer[1].

Consider a microscopic Brownian particle that is suspended in a fluid [2] and that due to the thermal agitation from collisions with the molecules of the fluid, it provides a dependency on the temperature and the fluid's viscosity. This becomes a good example in studying a stochastic phenomenon. It is possible that studying the Brownian particle when the fluid is electrically charged, to reveal whether it produces an external electric field and induces a deterministic force. With this, we propose a Langevin equation that can describe such Brownian particle in the form:

$$M\ddot{x}(t) = -\gamma \dot{x}(t) - k \sin(2\pi f t)\, x(t) + \sqrt{2k_B T\gamma}\,\xi(t) \quad (1)$$

where x is the particle's position, M as its mass, γ is the friction factor, k is the induced stiffness due to the electric field defined as $k = E_o \times 10^{-6}\,C/m$ $\sqrt{2k_B T\gamma}\,\xi(t)$ is the random force due to the random impulses from the neighboring molecules of the fluid, k_B is the Boltzmann's constant, and T is the absolute temperature. Equation (1) is an example of a stochastic differential equation [3] and a common tool in studying stochastic phenomena by adding the white noise term. We did not use any advance mathematical tools, instead, numerical calculation on the Langevin equation (1) can be done directly using a finite difference algorithm [1].

II. METHODS AND MATERIALS

In the following sections, we show how to solve the Langevin equation by means of finite difference algorithm. Before that, we discuss the simulation of the random walk and the white noise term as well as the simulation of the diffusion of Brownian particle and its transitions due to the inertial effects. Subsequently, we investigate the effect of the electric oscillator on the motion of the Brownian particle. The

*Department of Physics, College of Natural Science and Mathematics, Mindanao State University, Marawi City 9700, Philippines
1Corresponding Author
 E-mail Address: azis.norodinp6@gmail.com
2E-mail Address: vanderwaalsmida@yahoo.com
3E-mail Address: grempens@gmail.com
4E-mail Address: vernieconvicto@gmail.com
5E-mail Address: jaelordcf@gmail.com

simulation of this work was mainly done by using the associated MATLAB program which is freely available.

Random Walk and White Noise

The continuous-time solution x(t) of equation 1 is approximated by a discrete-time sequence x_n which is a solution for the finite difference approximation equation evaluated at time steps $t_n = n\Delta t$. For small Δt, $x_n \sim x(t_n)$. In which we can write the differential equation in terms of its solution x(t) and replace it with x_n. Then we have :

$$\dot{x} = \frac{x_n - x_{n-1}}{\Delta t} \qquad (2)$$

and

$$\ddot{x} = \frac{x_n - 2x_{n-1} + x_{n-2}}{(\Delta t)^2} \qquad (3)$$

Hence, for any ordinary differential equation, we can obtain its solution by solving for x_n and using the iterated values for x_{n-1} and x_{n-2}

Using the algorithms (2) and (3), we approximate the solution for (1) except for the white noise term $\xi(t)$ which is on the third term. $\xi(t)$ is characterized by its basic properties such as: $\langle \xi(t) \rangle = 0$ for any t; $\langle \xi(t)^2 \rangle = 1$ for every time t. In other words, $\xi(t)$ is a Gaussian process that everywhere continuous but nowhere differentiable. To understand $\xi(t)$, we start by considering a differential equation

$$\dot{x}(t) = \xi(t) \qquad (4)$$

Where the solution is sometimes called random walk. Providing a discrete sequence of a random numbers η_n that mimics the properties of $\xi(t)$, we obtain a variance $1/\Delta t$. Upon obtaining random numbers, we then rescale it to obtain sequences $\xi(t) = \eta_n / \sqrt{\Delta t}$. $\xi(t)$
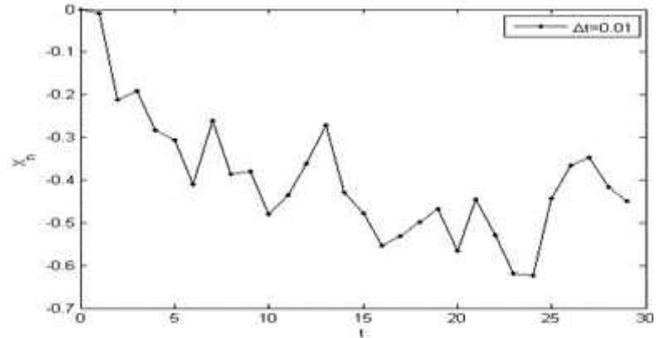
Figure 1 shows the behavior of in terms of difference equation
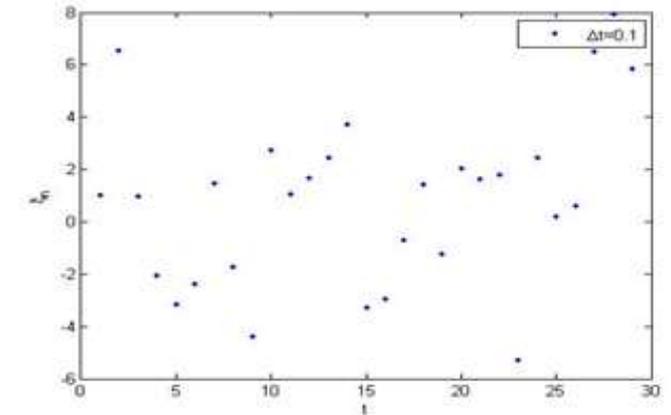
$$x_n = x_{n-1} + \sqrt{\Delta t}\eta_n \qquad (4)$$

It is evident that for $\Delta t \rightarrow 0$, values of $\xi(t)$ increase and are diverging. This suggests that Δt should be much smaller compared to the characteristic time scale of the stochastic process, otherwise, numerical solution will diverge and will show unphysical behavior.
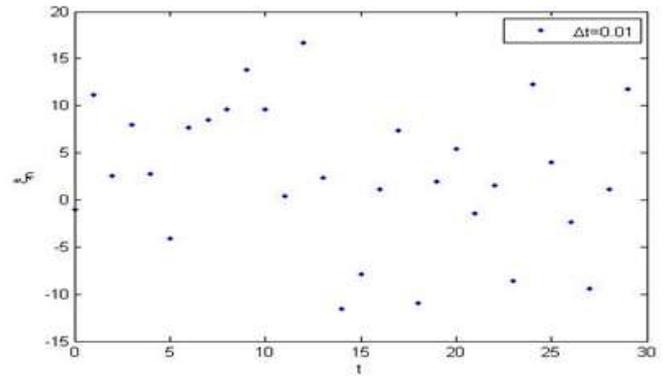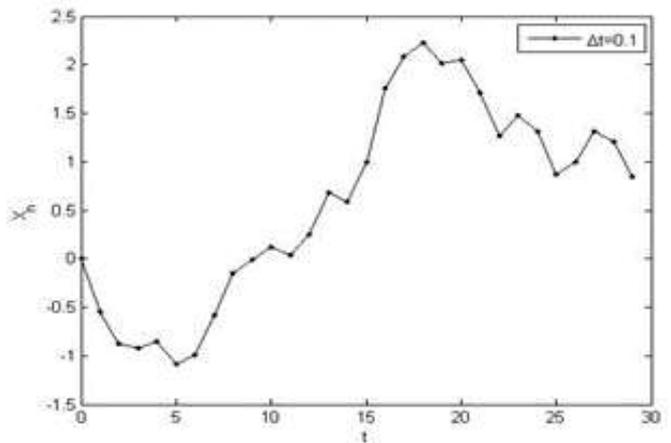
(a)

(b)

(c)

(d)

Figure 1 - Plots of $\xi(t)$ for different values of Δt

Ballistic Motion to Brownian Diffusion

At this juncture, we now consider the Brownian motion of realistic particles. A microscopic particle immersed in a fluid will undergo diffusion due to the collisions of the surrounding molecules that will alter the velocity of the particle. Here we solve the Langevin equation for when the fluid is electrically charged which excite the molecules in the fluid and will then cause rapid collision on the particle, thus, limiting the kinetic energy of the particles. Starting from equation (1), and employing the finite difference algorithm and solving for the solution yields:

$$x_n = \frac{2 + \frac{\gamma}{M}\Delta t}{1 + \frac{\gamma}{M}\Delta t + \frac{k}{M}(\Delta t)^2 \sin(2\pi f t)} x_{n-1}$$
$$- \frac{1}{1 + \frac{\gamma}{M}\Delta t + \frac{k}{M}(\Delta t)^2 \sin(2\pi f t)} x_{n-2}$$
$$+ \frac{\sqrt{2 k_B T \gamma}(\Delta t)^{3/2}}{M \left(1 + \frac{\gamma}{M}\Delta t + \frac{k}{M}(\Delta t)^2 \sin(2\pi f t)\right)} \eta_n \quad (5)$$

We consider a silica microparticle in accordance to the work of Volpe and Volpe [1] with the following parameters: radius of R=$1\mu m$, mass M=11pg, viscosity $v = 0.001$Ns/m², $\gamma = 6\pi R v$, temperature T=300K, and electric field E_0=1.5N/C at a frequency f=2.5 $\times$ 10^{-6}Hertz.

We give a sample plot for a trajectory of a particle with inertial effect for a large time to see its behavior for a continuous time rather than for a small time only. Realizations with respect to **Figure 2** include the following: that for small time, it shows that the mean motion of a particle follows a linear diffusion; and that for continuous time, vibration on molecules increases the collisions, thus affecting the particle's motion.

According to Li et. Al, (2010) to measure the particles position that is sufficiently fast is to obtain its instantaneous velocity from the ballistic to diffusive regime. It is then possible to drop the inertial term, and without the electric oscillator, we have the freely diffusive particle:

$$\dot{x}(t) = \sqrt{2D}\xi(t) \quad (6)$$

or by difference approximation

$$x_n = x_{n-1} + \sqrt{2D\Delta t}\eta_n$$

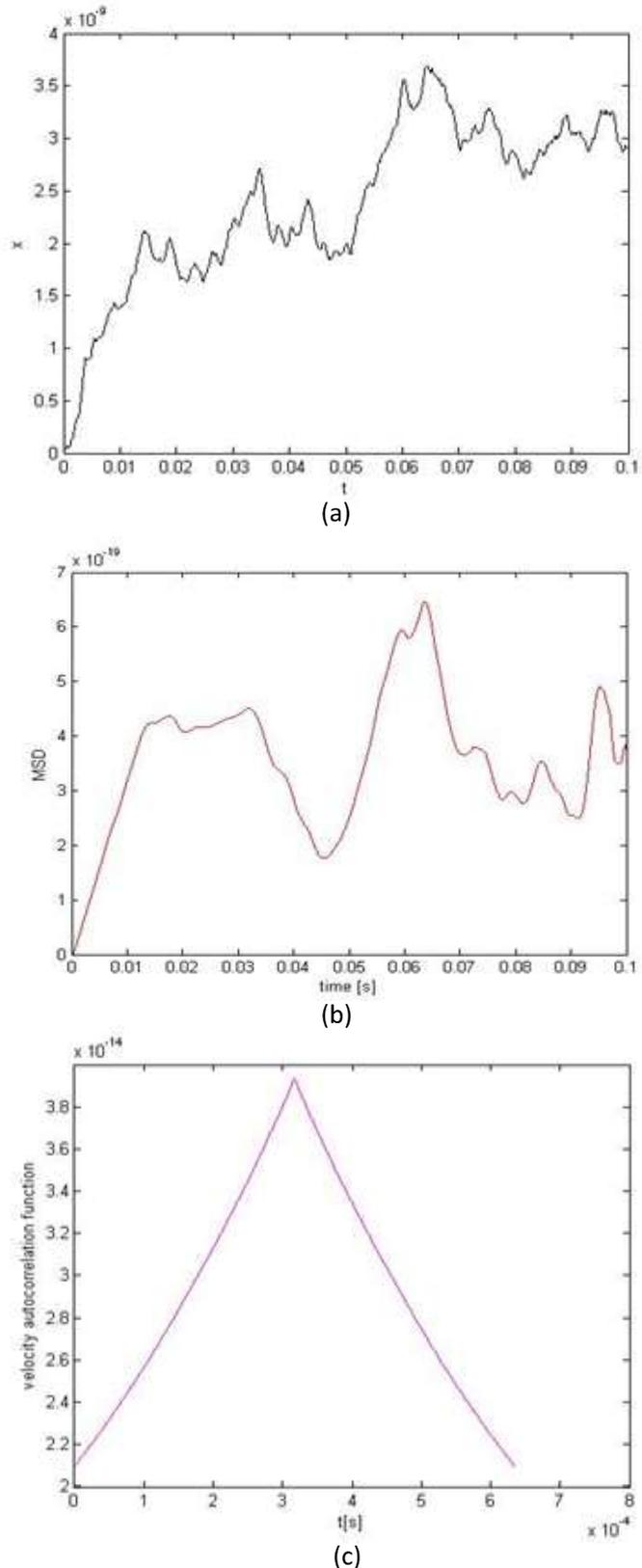Where D is the diffusion coefficient. Direct simulation of free diffusive particle yields **Figure 3**.
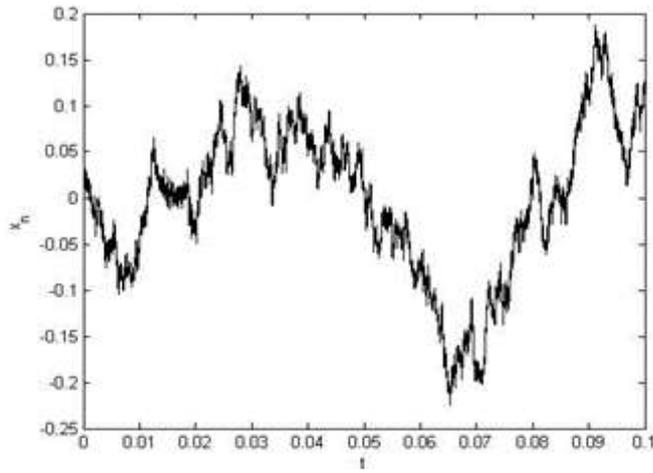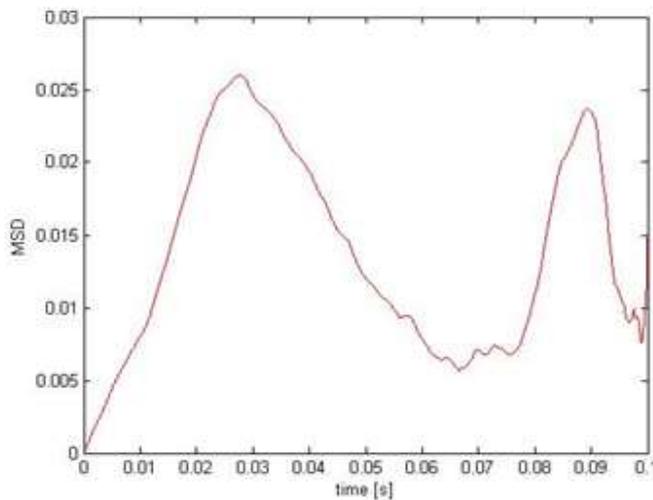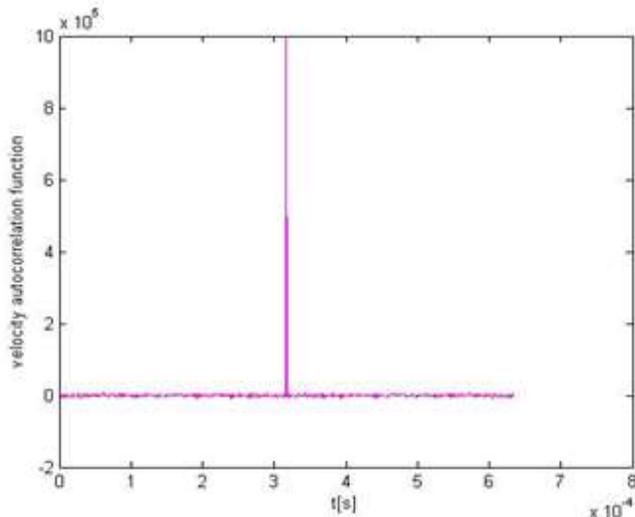

(a)

(b)

(c)

Figure 2- Plots for the Trajectory of a Silica Particle in an electrically charged environment

(a)

(b)

(c)

Figure3-Plots for the Trajectory of a Silica Particle without inertial term and oscillator

It is clear from the graphs that without the inertial mass, the particle is more random and discontinuous. The purpose of

the velocity autocorrelation function provides a measurement of the time to take the particle away from the initial velocity.

We demonstrate another method on holding the particle since it is more random without the inertial term in the next section.

III. RESULTS AND DISCUSSION

In the previous sections, we have shown the propagation of a Brownian particle with and without the inertial effect. Based on the observed dynamics of Brownian particle, it is useful to hold some of it and in such case, optical tweezers or optical traps [4] are one of the effective ways of holding Brownian particles. Another way is the study of the physical and chemical properties of cells and biomolecules [5] and using inert microscopic particles as force transducers [6].

A Brownian particle subjected to an electric oscillator tends to move toward the equilibrium point. With the thermal noise, it may push towards the different directions. From the previous equations, we can obtain the time-scaling for the electric oscillator that acts on the Brownian particle given by $\varphi = \frac{\gamma}{k}$. Studying the Brownian particle in electric oscillator is convenient by imposing the non-inertial approximation so that the only relevant time scale is φ.

The motion of the particle can be described using equation (1) without the inertial term thus giving us the equation:

$$\dot{r}(t) = -\frac{k}{\gamma}\sin(2\pi f t)\,r(t) + \sqrt{2D} \qquad (7)$$

where $r = [x, y, z]$ represents the particle position at time t_n and a random Gaussian number $\eta_i = [\eta_x, \eta_y, \eta_z]$ with zero means. We have the corresponding difference equation:

$$r_n = r_{n-1} - \frac{k}{\gamma}\sin(2\pi f t)r_{n-1}\Delta t + \sqrt{2D\Delta t}\,\eta_i$$

Although we may not be able to say that the electric oscillator acts as a trap, it is

efficient enough to hold the Brownian particle as shown in **Figures 4(a) and 4(b)**.

As shown in Figure 4, the particle is being held into a certain region which is caused by the electric oscillator. It is enough evidence, as part of an introductory work on electric oscillator, to show that we can use it as another factor in holding Brownian particle.
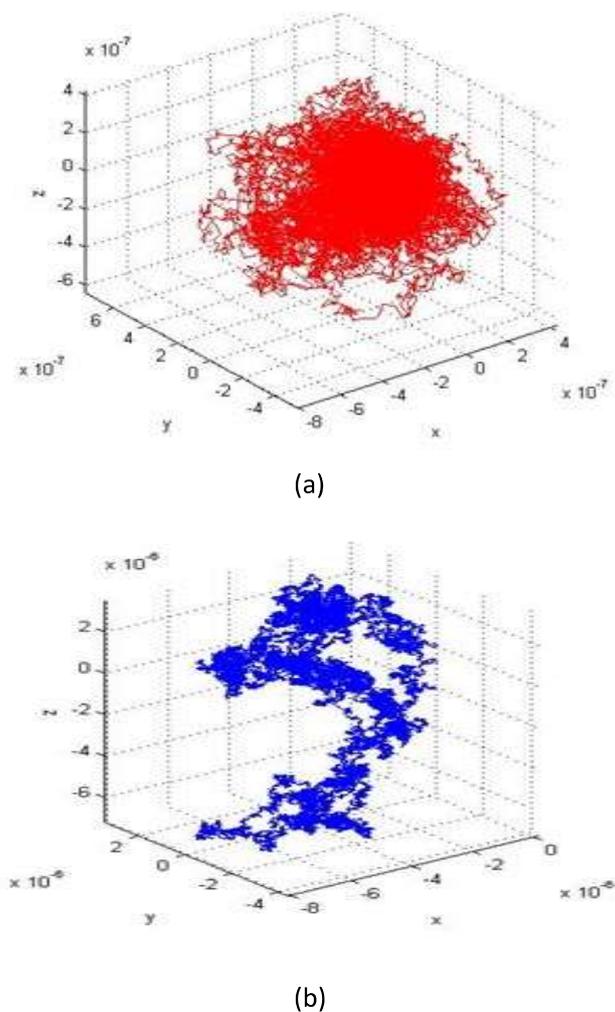

(a)

(b)

Figure 4. Trajectory of a Particle in an electric oscillator

IV. CONCLUSIONS AND RECOMMENDATIONS

The authors conclude that the electric oscillator can be treated as one method in controlling or holding the Brownian particle. In real world application, existing methods in holding Brownian particles, like optical trapping may be expensive. In contrast, this method offers an easy way and inexpensive tool.

Extension of this paper can be done by investigating the effect of the different intensities of the frequency and the electric field, and the relationship of the induced stiffness k to the propagation of a Brownian particle.

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