Brownian motion and the diffusion equation, a computational simulation for simple diffusion.

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Summary — **This paper presents The Theory Developed by A. Einstein and P. Langevin required for description of the movimientor of a Brownian particle suspended in a continuous medium. First show Three results Fundamental, that the Brownian motion satisfies the diffusion equation, then the solution of the diffusion equation is obtained, and that the mean square displacement depends linearly on the timeor, then using the programming language Python This last relationship is demonstrated and two simulations are made, one in three spatial dimensions, and the second in a dimension graphing position against time of a Brownian motion.**

Keywords – **Brownian movement**, **diffusion, numerical physics.**

Abstract — **In this work presents** the **theory developed by A. Einstein and P. Langevin necessary for the description of the motion of a Brownian particle suspended in a continuous medium. First show three fundamental results, that the Brownian motion fulfills the diffusion equation, then the solution of the diffusion equation is obtained, and that the mean square displacement depends in a linear way with time, then using the python programming language it is demonstrated this last relation and two simulations are made, one in three spatial dimensions, and the second in one dimension, plotting position against time of a Brownian motion.**

Keywords — **Brownian motion, diffusion equation, numerical physics**

I. Introduction

When talking about Brownian motion they can refer to the random movement of particles that are suspended in a medium, due to the collision of the molecules of the medium that are in thermal movement with said particles, or it can refer to the mathematical model that describes this phenomenon, in mathematics it is more commonly called "a Brownian", because it is a behavior that can be applied to a wide variety of stochastic processes of continuous time, such as finance, tidal movement or paths of certain species when migrating.

The problem of Brownian motion was first solved by A. Einstein in one of his four papers of 1905, where he shows that Brownian motion complies with the diffusion equation and obtains that the mean square displacement of particles behaves linearly with time, three years later P. Langevin obtains the same result, but following a simpler path starting from Newton's second law.

In this work is structured as follows in section II, it is shown that Brownian motion complies with the diffusion equation in the way that A. Einstein does in his original paper of 1905, then the diffusion equation is solved obtaining the fundamental solution using the m Lie group theoretical methods and finally Langevin's method is used to arrive at the same result as A. Einstein which is that the value of the mean square displacement depends linearly with time, in section III the results of the simulations and a computational verification of Langevin's result are shown and finally in part IV, A list of references is presented.

II. Methodology

This section yields three important results, from Brownian motion, developed by Einstein and Langevin.

A. Einstein's proof.

First let's show that Brownian motion satisfies the diffusion equation [2]. For a number of particles experiencing a displacement that lies between and , for the time interval , is expressed as.$dn\delta\delta + d\delta\tau$

$$dn = n\phi(\delta)d\delta \qquad ...(1)$$

where is an even function and satisfies with. $\phi(\delta)$

$$\int_{-\infty}^{+\infty}\phi(\delta)d\delta = 1 \qquad ...(2)$$

We will now focus on describing the concentration of particles per unit volume for the instant between two planes perpendicular to the axis with abscissae, this concentration is given by.$f(x,t)t + \tau x\ x$ y $x + dx$

$$f(x,t+\tau)dx = \int_{-\infty}^{+\infty} f(x+\delta,t)\phi(\delta)d\delta \qquad ...(3)$$

As we have considered very small we can write.τ

$$f(x,t+\tau) = f(x,t) + \tau\frac{\partial f}{\partial t} \qquad ...(4)$$

If we expand in powers of :$f(x+\delta,t)\delta$

$$f(x+\delta,t) = f(x,t) + \delta\frac{\partial f(x,t)}{\partial x} + \delta^2\frac{\partial^2 f(x,t)}{\partial x^2} + \cdots \qquad ...(5)$$

Carrying the expansion under the sign of the integral.

$$f+\frac{\partial f}{\partial t}\tau=f\int_{-\infty}^{+\infty}\phi(\delta)d\delta\ +\int_{-\infty}^{+\infty}\delta\phi(\delta)d\delta + \frac{\partial^2 f}{\partial x^2}\int_{-\infty}^{+\infty}\frac{\delta^2}{2}\phi(\delta)d\delta\ \ldots \qquad \ldots(6)$$

The even terms cancel out because the function is even, only the first, third, fifth, etc. survive. terms, these terms becomeϕsmaller and smaller, if we consider the following integral equal to the diffusion coefficient D.

$$\frac{1}{\tau}\int_{-\infty}^{+\infty}\frac{\delta^2}{2}\phi(\delta)d\delta=D \qquad \ldots(7)$$

Andtaking into account only the first and third term on the right side, we get the following equation.

$$\frac{\partial f}{\partial t}=D\frac{\partial^2 f}{\partial x^2} \qquad \ldots(8)$$

Which is the diffusion equation that offers an approximation of the temporal evolution of the probability density function associated with the position of the particle that goes under a Brownian motion in the physical definition remember that the approximation is valid on short time scales so we supposed. τ

B. Solution of the diffusion equation.

Making the variable change, known as the parabolic scale

$$v=\lambda x, u=\lambda^2 t \qquad \ldots(9)$$

$$f(v,u)=\tilde{f}(x,t)=f(\lambda x,\lambda^2 t) \qquad \ldots(10)$$

This new function also satisfies the diffusion equation, and we know that if this happens then so will a multiple of it because we have the function on both sides of the equation$\tilde{f}$.

$$\tilde{f}(x,t)=f(v,u)=af(\lambda x,\lambda^2 t) \qquad \ldots(11)$$

To determine the constant that any scalar can be, but if $a$you think in terms of the Brownian particles at any given time, then we know that their integral must be equal to the total number of suspended particles, so we can use the following relationship.$\tilde{f}$

$$\int_{-\infty}^{+\infty}af(\lambda x,\lambda^2 t)dx=n \qquad \ldots(12)$$

Making the corresponding variable change.

$$\frac{a}{\lambda}\int_{-\infty}^{+\infty}f(\lambda x,\lambda^2 t)dv=n \qquad \ldots(13)$$

Again we require that the integral gives us the total number of particles for what we can do . $a=\lambda$So then, we have a transformation set under which the equation is invariant, the next step is to reduce the number of variables in the equation this is obtained by making the following variable change.

$$\lambda=\frac{1}{\sqrt{t}} \qquad \ldots(14)$$

That's how we have.

$$\tilde{f}(x,t)=\lambda f(\lambda x,\lambda^2 t)=\frac{1}{\sqrt{t}}f\left(\frac{x}{\sqrt{t}},1\right) \qquad \ldots(15)$$

To convert the components of the function into dimensionless components we use the diffusion coefficient, writing , $\lambda=\frac{1}{\sqrt{Dt}}z=\frac{x}{\sqrt{Dt}}$.

$$\tilde{f}(x,t)=\frac{1}{\sqrt{Dt}}f\left(\frac{x}{\sqrt{Dt}},\frac{1}{D}\right)=\frac{1}{\sqrt{Dt}}\bar{f}(z) \qquad \ldots(16)$$

Which is already a function of a single variable .z

$$\tilde{f}(x,t)=\frac{1}{\sqrt{Dt}}\bar{f}(z) \qquad \ldots(17)$$

Calculating the corresponding derivativess and substituting them into the diffusion equation we obtain.

$$-\frac{t^{-\frac{3}{2}}}{2\sqrt{D}}\left(z\frac{\partial\bar{f}(z)}{\partial z}+\bar{f}(z)\right)=D\frac{1}{Dt}\frac{\partial^2\bar{f}(z)}{\partial z^2}\frac{1}{\sqrt{Dt}} \ldots(18)$$

Here the derivatives are total derivatives, and we can reduce it to the following expression by noting theterms that correspond to the derivative of a product.

$$\frac{d^2\bar{f}(z)}{dz^2}+\frac{1}{2}\frac{d}{dz}\left(z\bar{f}(z)\right)=0 \qquad \ldots(19)$$

$$\frac{d\bar{f}(z)}{dz}+\frac{1}{2}\left(z\bar{f}(z)\right)=c \qquad \ldots(20)$$

Since we know that it is equally likely that the particles move left and right, i.e. the function is even, this implies.

$$\frac{d\bar{f}(z)}{dz}\ (z=0)=0 \qquad \ldots(21)$$

Therefore.

$$\frac{d\bar{f}(z)}{dz}+\frac{1}{2}\left(z\bar{f}(z)\right)=0 \qquad \ldots(22)$$

Solving this equation.

$$\bar{f}(z)=\bar{f}(0)e^{-\frac{1}{4}z^2} \qquad \ldots(23)$$

This function must satisfy that.

$$\int_{-\infty}^{+\infty} \bar{f}(0)e^{-\frac{1}{4}z^2}dz = n \qquad ...(24)$$

Making a change of variesle, to obtain theGaussian int egral, we can see what.

$$\bar{f}(0) = \frac{n}{\sqrt{4\pi}} \qquad ...(25)$$

Like this.

$$\bar{f}(z) = \frac{n}{\sqrt{4\pi}}e^{-\frac{1}{4}z^2} \qquad ...(26)$$

Rewriting in terms of and $.xt$

$$\tilde{f}(x,t) = \frac{n}{\sqrt{4\pi D}}\frac{e^{-\frac{1}{4}z^2}}{\sqrt{t}} \qquad ...(27)$$

The above expression is known as the fundamental solutionof the diffusion equation.

C. *Mean quadratic displacement, Langevin's method.*

Let's prove the final result of Einstein's paper, that the value of the mean square displacement depends linearly with time, using Langevin's method [1].

Langevin proposes that a Brownian particle experiences two forces, one due to Stokes friction.

$$f = -\alpha v = -6\pi\eta r v \qquad ...(28)$$

And another with completely random origin, because the particle is very small in relation$\xi(t)$ to the volume that contains it. Bybuttering Newton's second law for a Brownian particle.

$$m\frac{d^2x}{dt^2} = -\alpha\frac{dx}{dt} + \xi_x(t) \qquad ...(29)$$

Multiplying by and simplifying.x

$$x\frac{d^2x}{dt^2} = -\frac{\alpha x}{m}\frac{dx}{dt} + \frac{x}{m}\xi_x(t) \qquad ...(30)$$

Now using the next two identities.

$$x\frac{d^2x}{dt^2} = \frac{1}{2}\frac{d^2x^2}{dt^2} - \left(\frac{dx}{dt}\right)^2 \qquad ...(31)$$

$$\frac{1}{2}\frac{dx^2}{dt^2} = x\frac{dx}{dt} \qquad ...(32)$$

Substituting them into the equation.

$$\frac{1}{2}\frac{d^2x^2}{dt^2} - \left(\frac{dx}{dt}\right)^2 = -\frac{\alpha}{m}\frac{1}{2}\frac{dx^2}{dt^2} + \frac{x}{m}\xi_x(t) \qquad ...(33)$$

Now taken the total average of the particle set.

$$\frac{1}{2}\frac{d^2\langle x^2\rangle}{dt^2} - \left\langle\left(\frac{dx}{dt}\right)^2\right\rangle = -\frac{\alpha}{m}\frac{1}{2}\frac{d\langle x^2\rangle}{dt^2} + \frac{\langle x\xi_x(t)\rangle}{m} \quad ...(34)$$

Here we must assume $\langle x\xi_x(t)\rangle = 0$ that what means that the average trajectory is independent of the fluctuations, and assume valid the theorem of equipartition of the energy i.e. , rewriting the equation using this information.$\frac{1}{2}m\left\langle\left(\frac{dx}{dt}\right)^2\right\rangle = \frac{1}{2}k_BT$

$$\frac{d^2\langle x^2\rangle}{dt^2} + \frac{\alpha}{m}\frac{d\langle x^2\rangle}{dt^2} - \frac{2}{m}k_BT = 0 \qquad ...(35)$$

Solving for , and doing $\frac{d\langle x^2\rangle}{dt^2}\gamma = \frac{t}{\tau_r}$.

$$\frac{d\langle x^2\rangle}{dt^2} = \frac{2K_BT}{m\alpha} + C\gamma e^{-\frac{t}{\tau_r}} \qquad ...(36)$$

The last physical consideration that is made is that the relaxation time of the particles is and therefore the observation time, so we have that the second term is practically zero.$\tau_r \approx 10^{-8}st \gg \tau_r$

$$\frac{d\langle x^2\rangle}{dt} = \frac{2K_BT}{m} \qquad ...(37)$$

Integrating again.

$$\langle x^2\rangle - \langle x^2(0)\rangle = \frac{2K_BT}{\alpha}t \qquad ...(38)$$

So we have shown that the value of the mean square displacement depends linearly with time.

III. RESULTS

It has been assumed that the particlesdo not interact with the others, so the simulation has been done without considering some kind of clash between them, for this the python random library was used, which generates the random steps of the movement of the particles.

The first part of the program simulates a movement in three dimensions, pair a set of 200 particles with 500 steps in time in figures 1 and 2, you can see the final position of the particles after this process with different perspectives.

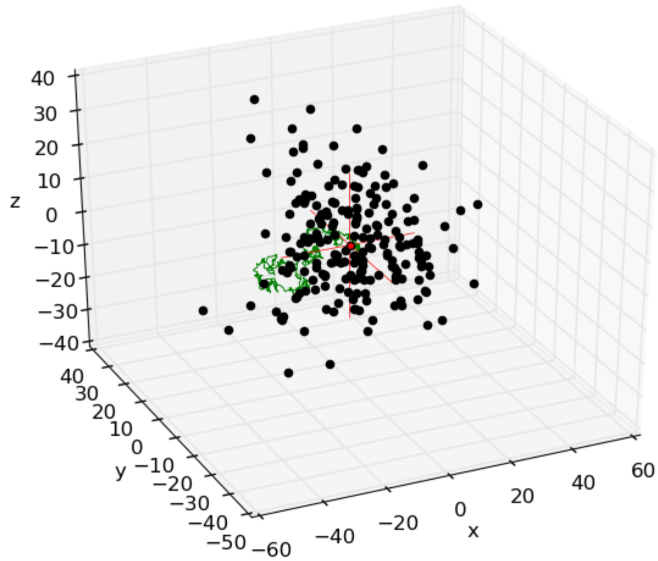

Fig. 1. Brownian motion of a set of 200 particles with 200 steps in time, the red dot shows the common origin to , of the 500 particles $t = 0$

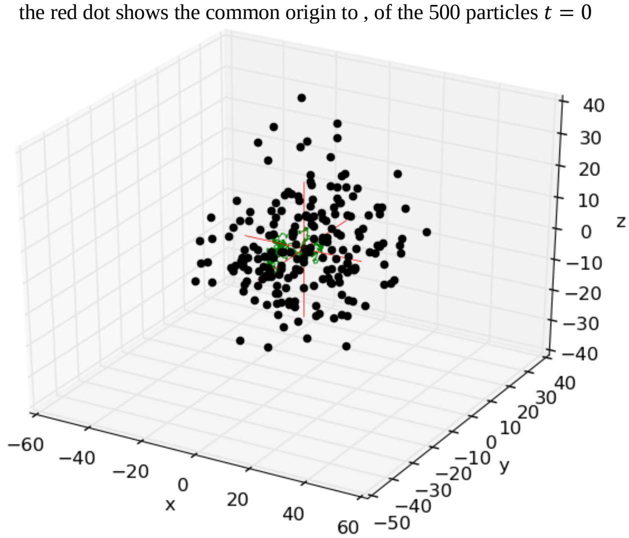

Fig. 2. Different perspective of figure 1, in green you can see the path of one of these particles, the program includes a section that visualizes the path of all the particles, the red lines mark the coordinate axis at zero.

The second part of the program makes a simulation for the movement of a particle in a dimencion, and its variation over time is graphed, this simulation is important because the results obtained by Eintein and Langevin are in a spatial dimension.

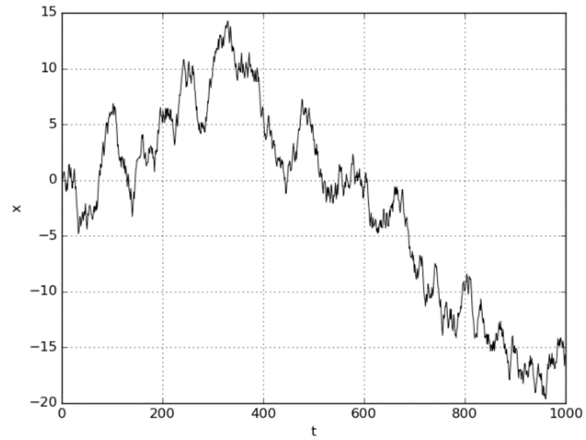

Fig. 3. Brownian motion of a Brownian particle for 1000 steps in time.

The last part of the program thirty simulations are made for each n number of steps in time from to $t = 1$, the average is obtained $t = 100$that is equal to the average quadratic displacement[3] of each n and is plotted with its corresponding n.

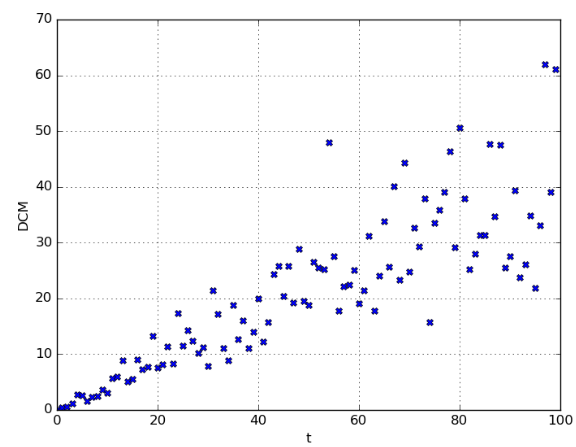

Fig. 4. Simulation that checks the linear behavior of the expected value over time

IV. Discussion

The simulation requires a large number of calculations to make the graph in 3D and this makes it difficult to manipulate the graph to have different perspectives of the simulation even when it has been done with relatively few particles, because to have a more real result it is necessary to do the simulation for a number of particles close to the number of Avogadro, and also model the clashes that exist between them.

At thetime for the movement in one dimension we can see that even though the Brownian is a stochastic process that is to say that it is a function of random variables we can characterize at least the expected valuer of its displacement.

As we verified in the third part of the program, to verify this result and the most important of Einstein's article, a total of 30 simulations were made for a Brownian motion in 1 dimension, with t steps in time, for each of the simulations the value of its final displacement is obtained with respect to the origin, now it is averaged over the 30 simulations that average value coincides with the DCM of the Brownian particles and using a shekel for, we vary the value of t so for each we t will have a DCM value, this is what is shown in figure 4, we can see that it follows a linear behavior but that it begins to disperse with form the time continues to increase, But we can see a more uniform behavior from 0 to 60 steps in time.

V. Conclusions

We have managedor simulated an "approximation" to Brownian motion, as many restrictions have been made on the particles.

It has been verified the most important result of the article of Einstein, without having made experimental measurements, because as we have said it is an approximation, therefore strictly what has been shown is a property of the stochastic process calling a browniano, therefore what we have is an approximation for any stochastic phenomenon that follows its characteristics this is of vital importance, It has a large number of applications in many areas of science.

Programmes

p1.py

p2 p3.py

References

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