Modeling Random Walks of Particles in Porous Media

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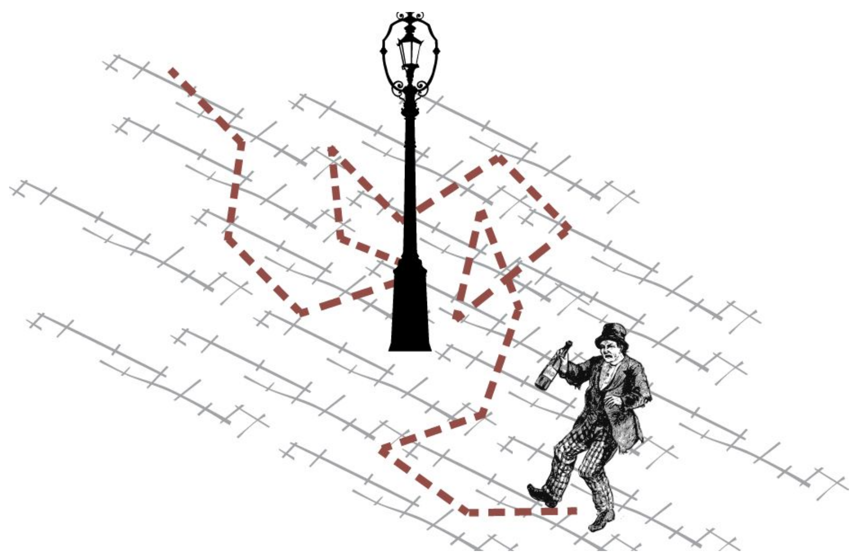
Introduction

- Theory of random walk (brownian motion, drunken man problem)
- Sentence or more about phd thesis of einstein (relates to 3d)
- Brownian motion in practice (in porous media)

The random walk theory is based on describing a path that consists of taking random steps in random directions in a grid, lattice, etc. The random walk model is a very simple concept but can be used in places outside such as in finance, in math, the Brownian motion, and other areas. The random walk theory is used in Brownian motion, which describes the movement of particles in a fluid or gas due to collisions with other molecules/atoms. The Brownian motion was originally founded by Robert Brown in 1827, but then it became part of Einstein's Ph. D. research paper in 1905, proving the existence of atoms.

Brownian motion applies to porous media. For instance, in permeable concrete, water molecules spread out and fill the pore spaces. Diffusion occurs within the concrete. Understanding how particles move in porous media is valuable to researchers delving into this field of study. Brownian motion can also be used in a mathematical model known as geometric Brownian motion. This model is used in the Black-Scholes option pricing formula which can be used to help predict asset price movement, assess risks, and aid investment decisions.

Some analytical aspects of the Brownian motion include probability distribution, mean and variety, time increments, random walks, etc. The probability distribution describes the likelihood of multiple outcomes. The Brownian motion has an average rate of change and a measure of dispersion.



Objectives and Impact of Pr. Sahimi's Research

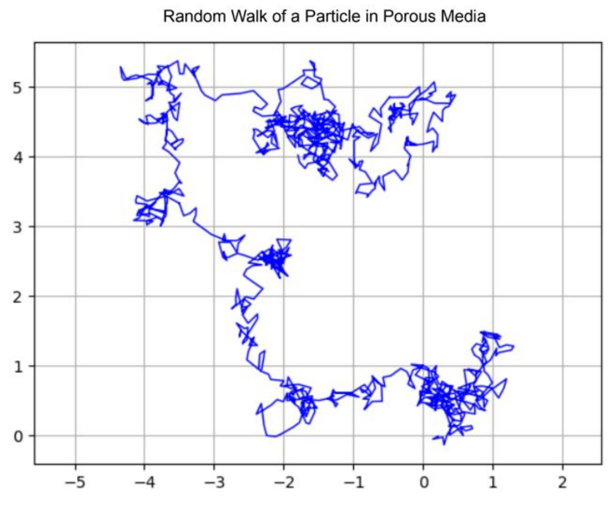


Figure 1: Example of Random Walk of a Particle in Actual Porous Media

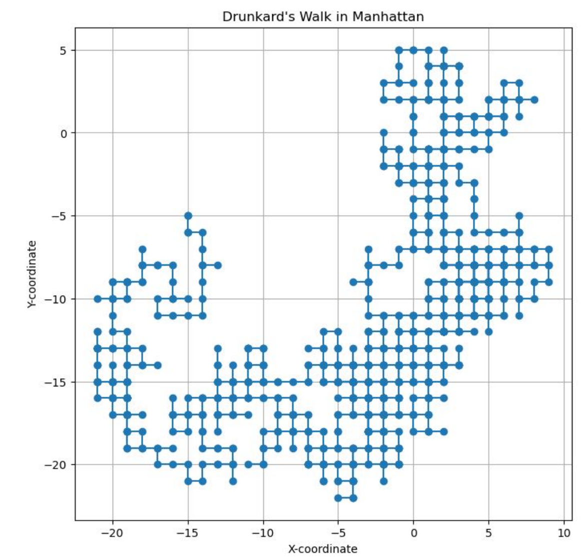


Figure 2: Illustration of a Random Walk of a Particle Resembling a Drunken Person

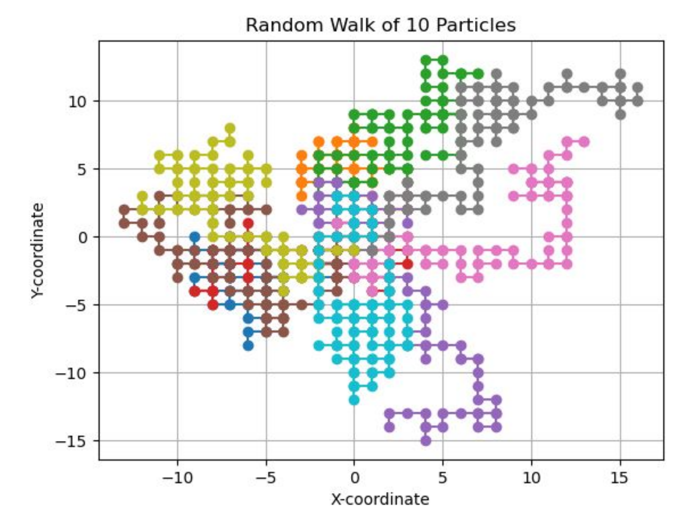


Figure 3: Illustration of Multiple Particles' Random Walk in a Grid Space

"A drunken man will always find his way home but a drunken bird will get lost forever" - Shizuo Kakutani.

In this research, we want to simulate the distance of the particles in a porous media. When modeling the random walks for our study, a 2D grid will be used. In a one-dimensional grid, there are only 2 possible directions , while in a 2D grid, there are 4 possible directions . For every dimension higher, 2 directions will be added. Normally, all 4 directions would have an equal probability of movement if modeling a simple random walk, but since we are also accounting for porous media, we want to simulate some boundaries in the model, one of them being unequal probabilities of movement . Since we want an accurate distance, we will track all the distances of all the random walks of multiple particles, namely at least 1000 particles. Then we get all the average distances for each step taken and plot them on a grid.

Results and Discussion

- Analytical results for **Diffusion** (Derivative for Distance and Time) **Fick's 2nd Law**
- Diffusion constant is related to slope of distance squared and time

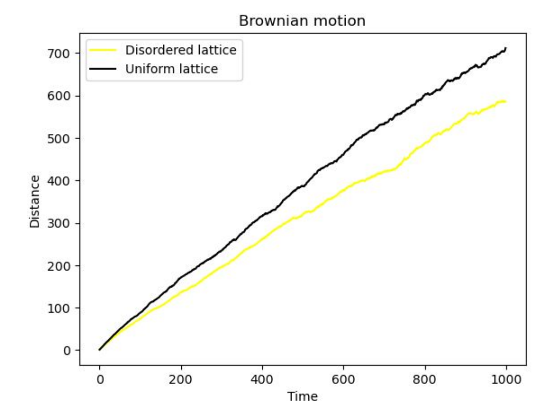


Figure 5: Difference between equal and unequal distribution

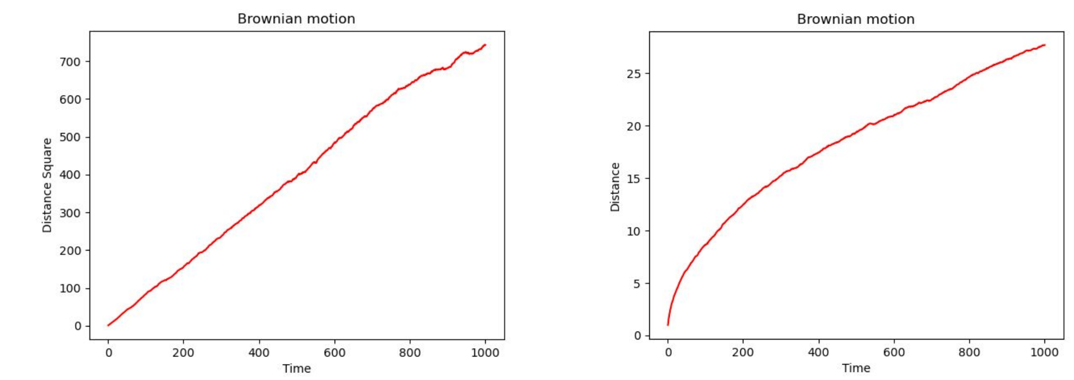


Figure 4: Distance in respect to time in Brownian Motion of a Particle

Fick's second law mathematically describes how fast diffusion happens. It also says the rate at which the concentration changes over time is proportional to how much the concentration changes concerning distance. The grid on the right shows a logarithmic function while the grid on the left shows a linear function. What do they represent you may ask? Starting with the right grid, it represents how each particle diffuses. As you can see, the distance starts to slow down as time passes. This is because it is easy to get a certain distance, but harder to get further due to the properties of diffusion. In Figure 5, the left grid plot represents the linear correlation of distance square and time. Also, the slope of this line represent the diffusion coefficient.The diffusion coefficient describes the rate of diffusion, which indicates how fast particles move across specific areas. The way to get that is by squaring the distance of the diffusion plot . That way, we can get the relationship between distance squared and time, which is linear. This ensures that we get an accurate indication of how fast particles move across specific areas.

$$\frac{\partial C}{\partial t} = \chi \frac{\partial^2 C}{\partial x^2}$$

in which the accumulation, dC/dt [cm^{-3} s^{-1}], is proportional to the diffusivity [cm^2/s] and the 2nd derivative (or curvature) of the concentration, [cm^{-3} cm^{-2}] or [cm^{-5}].

Next steps

- Next will be delving into other aspects of Brownian motion
- Next will be some different distributions of numbers, such as poisson or levy

What I plan to do next is to delve into a computer science major along with delving into exercise science and maybe materials science as well when I get to college. Thanks to SHINE, I already got better at coding and learned a bit more about materials science and on top of that, I got to experience what research is like. I am not completely sure what I'm going to do after college, but I will continue to strive for better.

Acknowledgements

Thank you to Prof. Sahimi for taking me in as part of his team and choosing two amazing graduate students to create and help me through my project. Also, thank you Shayan Jalalmanesh and Shayan Rahimi for guiding me through the entire project and taking it upon themselves to teach me a language in half a month. An additional thanks to Code.org for funding my scholarship to the SHINE program. Lastly, special thanks to Monica Lopez, and Marcus Gutierrez for setting up the SHINE program and making this experience come alive.