Diffusion and Random Walks

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Purpose

This activity uses a simple “random walk” computational model to teach students about the process of diffusion. Mathematics, experiential knowledge-based reasoning, and particle-based simulations are combined to enhance conceptual understanding and to connect microscopic phenomena with experimental observations.

Overview

The lesson begins with a background lecture on diffusion and Brownian motion and their significance. Then a guided NetLogo simulation of a single particle executing a random walk is observed and discussed with the class. Students then pair up and use the NetLogo software to independently simulate hundreds of particles and observe their collective behavior, e.g. the shape of their distribution, their average position, and the average distance from the center; and answer questions on the attached worksheets. Students are brought back together for discussion at the end of class, followed by a brief demonstration of diffusion in different temperature samples of water.

Student Outcomes

Students will be able to:

- Define a random walk and state some reasons it is important to science.
- Describe step-by-step how random walks are modeled in NetLogo.
- Use appropriate averages (position, distance) to understand the behavior of a collection of particles.
- Explain how Brownian motion results in random walks.
- Explain how Brownian motion leads to diffusion on a large scale.
- Change the parameters of the random walk (e.g. step frequency, step size).
- Observe the effects of variation of these parameters.
- Relate these parameters to the properties of a solvent (e.g. temperature, density).

Standards Addressed

HS-LS2-4.

Time

Two class periods of 45 minutes.

Level

AP Chemistry

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Materials and Tools

Computers (one per two students and one for the instructor)
NetLogo (download at https://ccl.northwestern.edu/netlogo/)
Excel or other spreadsheet program
Projector
Attached NetLogo simulation, Random Walk Bernie
Attached worksheet, Diffusion Worksheet

Preparation

Pre-assess mathematical knowledge. Students should know or be taught the following:

- How to take an average.
- What a square root is and how it looks on a graph
- The difference between distance and position.

Pre-assess knowledge of Excel. Students should know or be taught the following:

- Entry of *x–y* data into a spreadsheet.
- Plotting of *x–y* data from spreadsheet.

Install NetLogo on all computers.
Make sure students can download the attached NetLogo model.
3 beakers filled with different temperatures of water (for instance, 20˚C, 50˚C, and 80˚C).

Prerequisites

Before the lesson, students must:

- Complete the pre-assessments as above.
- Understand that solutions contain solute particles dispersed in a solvent.
- Understand that particles in a stationary solution are not stationary themselves, but are moving with an average kinetic energy proportional to their temperature, colliding frequently.
- Understand that entropy is related to the probability of finding particles in a given configuration.

Background

Historical background:
In 1905 Albert Einstein published four papers of monumental importance. One established quantum mechanics and won him the Nobel Prize in Physics, another introduced special relativity and a third introduced the famous equation $E = mc^2$. But perhaps his most important paper from this year was a paper he wrote on pollen in water. To help us understand how a paper about pollen could be anywhere near as important as any of these others, each of which is of no less than cosmic significance, let's set the stage. Amazingly, scientists in 1905 were still not convinced that atoms even existed. Atomic theory was seen as useful but not fact, not by a long shot. Some of the greatest physicists of the time would actively speak out against the atomic theory, to the extent that it drove Ludwig Boltzmann, one of the greatest physicists who ever lived, to suicide, tragically right around this time, and I say tragically because this perception about atomic theory is going to change overnight with the publication of this seemingly simple paper on pollen and the experiments that followed.

The subject of the paper was not pollen itself but something that had been observed about 80 years before by a botanist named Robert Brown.

[show video of Brownian motion - https://www.youtube.com/watch?v=ygiCHALySmM or https://www.youtube.com/watch?v=cDcprgWiQEY and discuss. Ask students what they think is going on, and lead them to the question: Why are these particles moving?]

Brown observed that microscopic pollen particles in water were "in motion". That's as much as he describes their movements, so his descriptive abilities leave something to be desired, but we can tell he is a great scientist because he immediately tries to figure out a very important question: is the motion being driven by something living, or is something else going on entirely? To that effect he starts with dead flowers, but he still isn't convinced, so he tries petrified wood, then dozens of different minerals from ash to metal and even a piece of the Sphinx (oy vey, the Brits) and crushes them down to microscopic pieces. He observes that "in every mineral which I could reduce to a powder, sufficiently fine to be temporarily suspended in water, I found these molecules more or less copiously." The fact that no matter what you started with, animal, vegetable, or mineral, if you crushed it down small enough you would obtain these particles that seem to move of their own accord (what is now called "Brownian motion") is a complete mystery to people at the time, and 80 years later Einstein sets out to solve this mystery. What he says is that in order to execute this jittery "agitated" motion, even without being alive, particles must be bombarded by other particles (according to Newton, a particle in motion tends to stay in motion, so the fact that these particles keep changing direction means they must be hitting something) and those other particles, Einstein argues, are the water molecules themselves. So Einstein found a way to see the effects of individual water molecules even though scientists could not see them individually. In doing so, he not only proved once and for all that matter is atomic (something that people had been trying to do literally for *millennia*), vindicating Ludwig Boltzmann, he also provides a method to measure the size of a water molecule and the all-important (as you know) Avogadro number. These advances represented a crucial step not just for physics, but areas of study from biology and chemistry to even such things as history and finance, where people use diffusion and random walks to study the spread of culture and money, respectively.

Today we will use computer simulations to see what Robert Brown saw in 1837, we will analyze it knowing what Einstein knew in 1905, and as a result you will understand how the molecular world works still now in 2015.

Teaching Notes

First give all handouts, instructing students to fill out the Anticipation Worksheet. Then, after students have had a chance to discuss this in pairs, deliver the background lecture. Then distribute laptops and have students open the attached NetLogo model and follow along with you. Explain that this model is comprised of "turtles" that move according to a set of rules that are executed by the computer when the user clicks a button or moves a slider. These turtles can be used to represent anything that moves, from people to leaves in the wind; here they represent solute molecules in a stationary (i.e., not flowing) solvent. Demonstrate the rules of the simulation in the following order:

1. Simulate 1 turtle.
    a. Set the [num-turtles] slider to 1, then click [setup], then [go once].
    b. Describe that the turtle takes one step of size [step-size] in the direction it faces, then bumps into a solvent molecule, thus reorienting randomly.
    c. Click [go once] and describe that the turtle again takes a step in the direction it faces and reorients. Do this a few more times.
    d. Adjust the [step-size] slider and show a few more steps. (Note: the fact that each step is represented by two lines at right angles rather than one straight diagonal line does not affect the simulation.)

   e. Now set [ring-radius] to 10, [step-size] to 1, click [setup] and [go] and see how long it takes the random walker to leave the innermost circle (like a turtle falling off a lily pad). While doing this you may also explain what the different graphs depict.
   f. Press [setup] and [go] a few more times, each time measuring how many ticks it takes the turtle to fall off the lily pad. You should see that some turtles fall off quickly while some remain on for a long time.
2. Have the students simulate many turtles while completing the Activity Worksheet.
3. Bring students together and guide them through the calculation of the diffusion coefficient:
   a. Allow the system to evolve for some number of ticks t.
   b. Measure the MSD at that value of t.
   c. Change [step-size] to 2 and repeat steps (a) and (b).
   d. Let students repeat this procedure for 3 more step sizes, recording their values in a spreadsheet.
   e. Have students plot their results as a plot of diffusion coefficient D vs. step size t.
4. Discuss with students if this makes sense. Discuss with students what might affect the step size in an experiment. Ask students what else they could change to change the diffusion coefficient (this is a tough question – the only real answer I can think of is to change the time between collisions, which is fixed at 1 in the simulation).
5. As a final demonstration, fill three beakers with different temperatures of water (say, 20˚C, 50˚C, and 80˚C), and drop one drop of dye into each. The difference in rates of diffusion should be clear. Be sure to note that convection also plays a part in spreading the dye, and that is why there are trails and billows of dye in the water. However, the trails spread due to diffusion, and the effect of temperature should be clear.

Assessment

Student learning will be assessed via the attached worksheets as well as informally and with clicker questions during the final wrap-up.

Additional Information

The attached NetLogo model is a modified version of the model titled “Random Walk 360”.