PHY407 Final Project
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Physics Background

Diffusion is a motion of particles from regions of higher concentration moving to regions of lower concentration. The 3-dimensional diffusion equation is given as：

$$\frac{\partial U}{\partial t} = D\nabla^2 U = D\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2}\right) \qquad \text{[Eq 1]}$$

Where D is the diffusion coefficient, U(x, y, z, t) is the particle density at a given location (x, y, z) and time t. This equation describes the random motion of particles in fluid, every individual particle follows Brownian motion, but the motion of many particles will follow the motion described by the diffusion equation. The boundary conditions are that the particle density is zero at the container's walls.

The square root of mean square displacement is given as:

$$d = \sqrt{2nDt} \qquad \text{[Eq 2]}$$

where n is dimension.

Computational Background

Diffusion equation can be approximated using FTCS method:

$$U_{i,j,k}^{n+1} = U^n_{i,j,k} + \Delta t * D\left[\frac{U^n_{i+1,j,k} - 2U^n_{i,j,k} + U^n_{i-1,j,k}}{(\Delta x)^2} + \frac{U^n_{i,j+1,k} - 2U^n_{i,j,k} + U^n_{i,j-1,k}}{(\Delta y)^2} + \frac{U^n_{i,j,k+1} - 2U^n_{i,j,k} + U^n_{i,j,k-1}}{(\Delta z)^2}\right]$$

[Eq 3]

We discretize time and position, where x=iΔx, y=jΔy, z=kΔz, t=nΔt. By repeating this equation n times, we will be able to simulate how the system of particles evolve in time t.

This FTCS method is stable if:

$$\Delta t \le \frac{1}{2D}\left(\frac{(\Delta x \Delta y \Delta z)^2}{(\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2}\right) \qquad \text{[Eq 4]}$$

Diffusion can also be modelled by random walk. The probability of moving in x, y, z direction are the same, and each step has the same width Δ d. Therefore, after N steps, the total displacement should be:

$$d(N) = \sum_{i=1}^{N} \left(\Delta d \cdot u_i \right) \qquad \text{[Eq 5]}$$

where u_i is the probability of moving in each direction:

$$u_i = \begin{cases} +x, \ p = \frac{1}{6} \\ -x, \ p = \frac{1}{6} \\ +y, \ p = \frac{1}{6} \\ -y, \ p = \frac{1}{6} \\ +z, \ p = \frac{1}{6} \\ -z, \ p = \frac{1}{6} \end{cases} \qquad \text{[Eq 6]}$$

This can be accomplished by creating a list of numbers of 0 to 5, and assign each value to a direction, then pick a random element from the list using *random.choice()*. Repeat this calculation for every particle in the system.

Square root of mean square displacement can be calculated by random walk model, by calculating the average displacement of multiple particles:

$$d = \frac{\sum_{j=1}^{n} \sqrt{\left(\left(x_j - x_0 \right)^2 + \left(y_j - y_0 \right)^2 + \left(z_j - z_0 \right)^2 \right)}}{n} \qquad \text{[Eq 7]}$$

Where x_0, y_0, z_0 are initial position of particles, and x_j, y_j, z_j are the final position.

Questions

1. Use the diffusion equation to simulate a diffusion model. Pick a small space and measure its density and make a time vs density graph.
   The conditions for this question can be set as followings:
   - D = 1
   - Initial condition: $U^0_{x_0 y_0 z_0} = 10{,}000$, for $-\frac{\Delta x}{2} < x_0 < \frac{\Delta x}{2}, -\frac{\Delta y}{2} < y_0 < \frac{\Delta y}{2}, -\frac{\Delta z}{2} < z_0 < \frac{\Delta z}{2}$, and $U^0_{x_i y_i z_i} = 0 \ everywhere\ else$
   - The container walls are at x = y = z = [-10 cm, 10 cm]
   - Let $\Delta x = \Delta y = \Delta z = 0.1cm$ and $\Delta t = 10^{-5} s$
   - Measurement Time: 0.01 s

2. Use random walk to simulate diffusion in the same space as in question 1 and make a time vs density graph. Compare the graph from Question 1. Do they have the same shape? For this questions, use the values specified in question 1, but with $U^0_{x_0 y_0 z_0} = 100{,}000$.

3. How long will it take for oxygen in the air to diffuse 1 cm below the surface of a cup of water. Suppose the diffusion constant of water is D = 1cm^2/s. How does travel time vary with the value of D?

4. Make a plot of square root of mean square displacement for the random walk model. Does it have the same shape as Equation 2? Suppose bacteria have the shape of a sphere and need to get oxygen to the centre of their bodies within 10 seconds. What is the largest size of their bodies, given D = 1 * 10^{-5} cm^2/s

Answers

Question 1)

Particles obey the diffusion equation when they move from regions of high concentration to those of lower concentration. The diffusion equation is expressed in a form of partial differential equation, whose 3D version can be found in Equation 1. In this report, the diffusion equation in 3D was computationally simulated by applying the numerical analysis method called FTCS (Forward Time Centred Space), which can be found in Equation 3.

The initial condition states that the density is 100,000 at the centre of the box and 0 elsewhere. Moreover, the box has the dimension of [-10,10] x [-10,10] x [-10,10], which was then divided into 200 grid points on each side with the interval of 0.1. Then the density of particles at the grid point right above the centre of the box, which is represented in coordinates as (x, y, z) = (0, 0, 0.1), was recorded over time and plotted in Figure 1 below. The total measurement time was 0.01 seconds with the interval of Δt = 10^{-5} seconds, which was chosen based on the stability condition of FTCS in Equation 4.

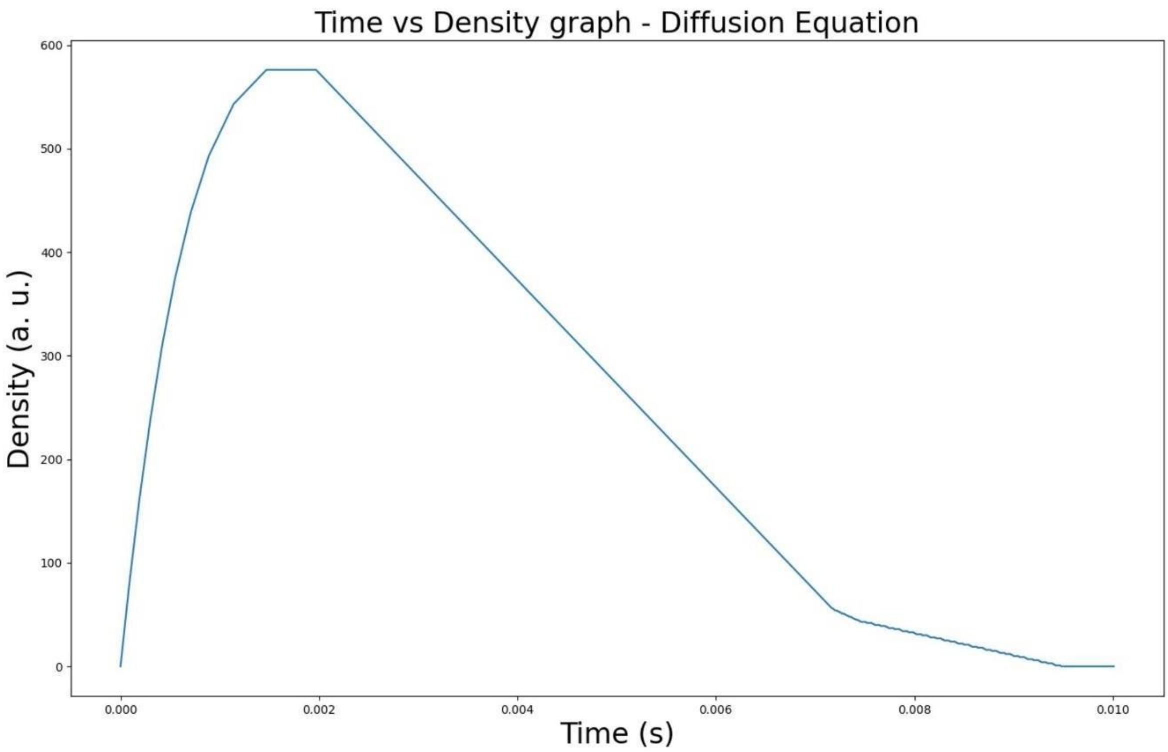

Figure 1: The density of particles at (x,y,z) = (0, 0, 0.1) as a result of solving diffusion equation by FTCS method was plotted over time. Note that the units of time and density are seconds and arbitrary, respectively.

Note that the density at (0, 0, 0.1) was initially zero, as all particles were concentrated at the centre at t = 0, and quickly peaked as soon as the particles started diffusive motion out of the centre. However, as the diffusion continued and particles spread into much lowly concentrated regions, the density at (0, 0, 0.1) gradually decreased as expected. Lastly, the small fluctuation was detected in the last quarter of the time.

Question 2)

In addition to solving partial differential equation with FTCS method as done in question 1, the diffusion of particles can also be simulated by a random walk process, which has been covered in one of the previous labs. However, since the particles are confined to 3D box, the random walk was simulated in 3 dimensions instead of 2 dimensions as in the lab. The probability of each move was defined in equation 7. Similar to Question 1, the density of particles at the nearest neighbour of the centre, or (x, y, z) = (0.1, 0.1, 0.1) was then observed and plotted in Figure 2.

The random walk of a single particle and multi particles in 3 dimensions, or “3D Brownian motion”, has also been simulated and can be found in the video file “3D_Brownian_SingleParticle.mp4” and “3D_Brownian_MultiParticles.mp4”.

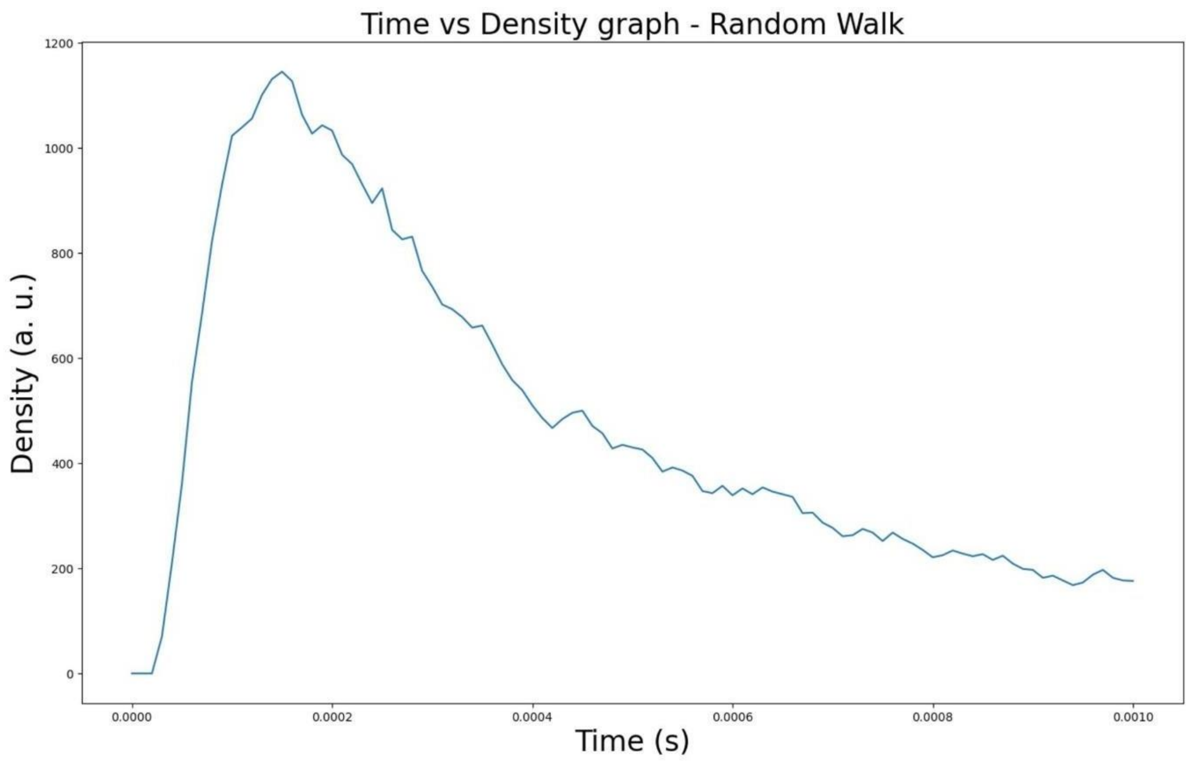

Figure 2: The density of particles at (x,y,z) = (0.1, 0.1, 0.1) as a result of simulating random walk in 3D was plotted over time. Note that the units of time and density are seconds and arbitrary, respectively.

Note that there is a similarity between Figure 1 and Figure 2, as Figure 2 also started at zero and peaked immediately after the particles start to diffuse from the centre. Then the density decreased gradually over time as particles spread more into empty spaces of the box.

Question 3)

The travel time of an oxygen molecule in penetrating 1 cm into the water was also estimated by computationally solving the diffusion equation using FTCS method. Then, the travel time at different diffusion coefficients was investigated and plotted in Figure 3.

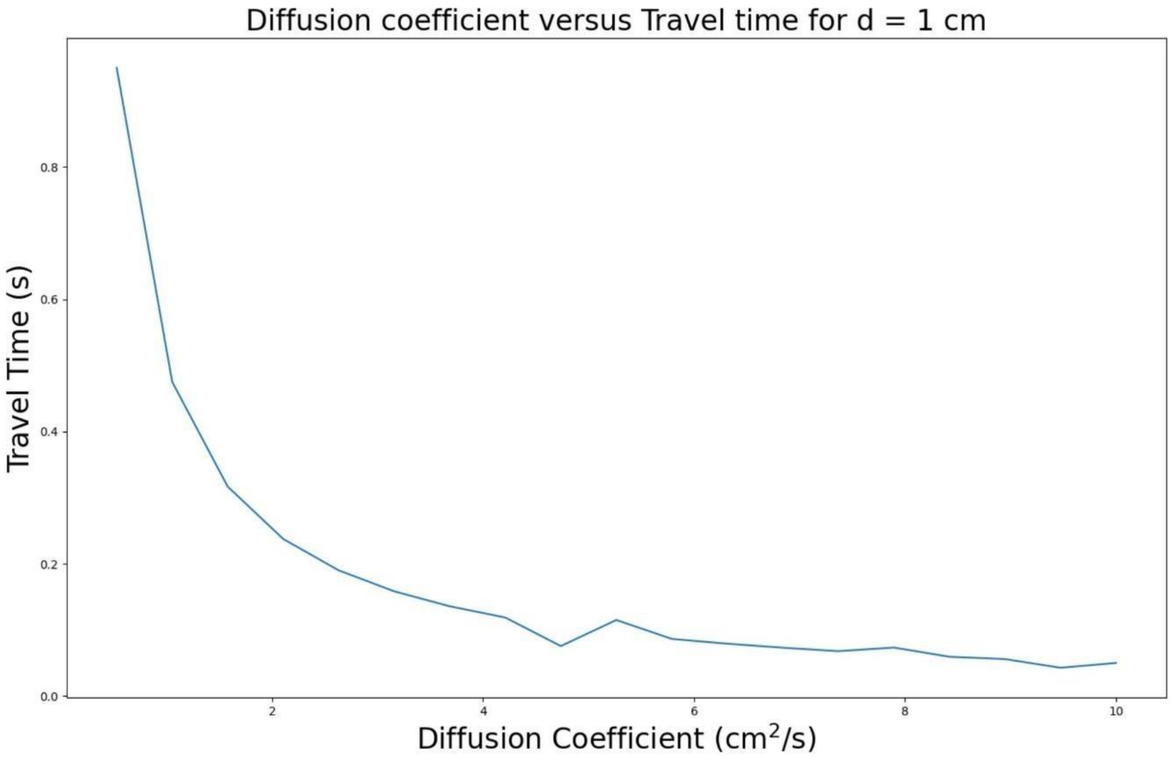

Figure 3: The time travel of an oxygen molecule to penetrate 1cm of water was plotted against diffusion coefficients.

The lower the diffusion coefficient, the oxygen molecule took the longer time to penetrate the same length into the water. This phenomenon can also be predicted theoretically by Equation 2, as the diffusion coefficient 'D' and time 't' are inversely proportional when rearranged as below:

$$d = \sqrt{2nDt}$$

$$\Rightarrow \quad d^2 = 2nDt$$

$$\Rightarrow \quad t = \frac{d^2}{2nD}$$

where 'd' refers to the penetration length in this case.

Question 4)

Displacement of a particle is the distance away from the initial position after a certain time, and the square root of mean square displacement can be calculated by taking the average of displacement for multiple particles. The relationship between square root of mean square displacement and time is shown as following:

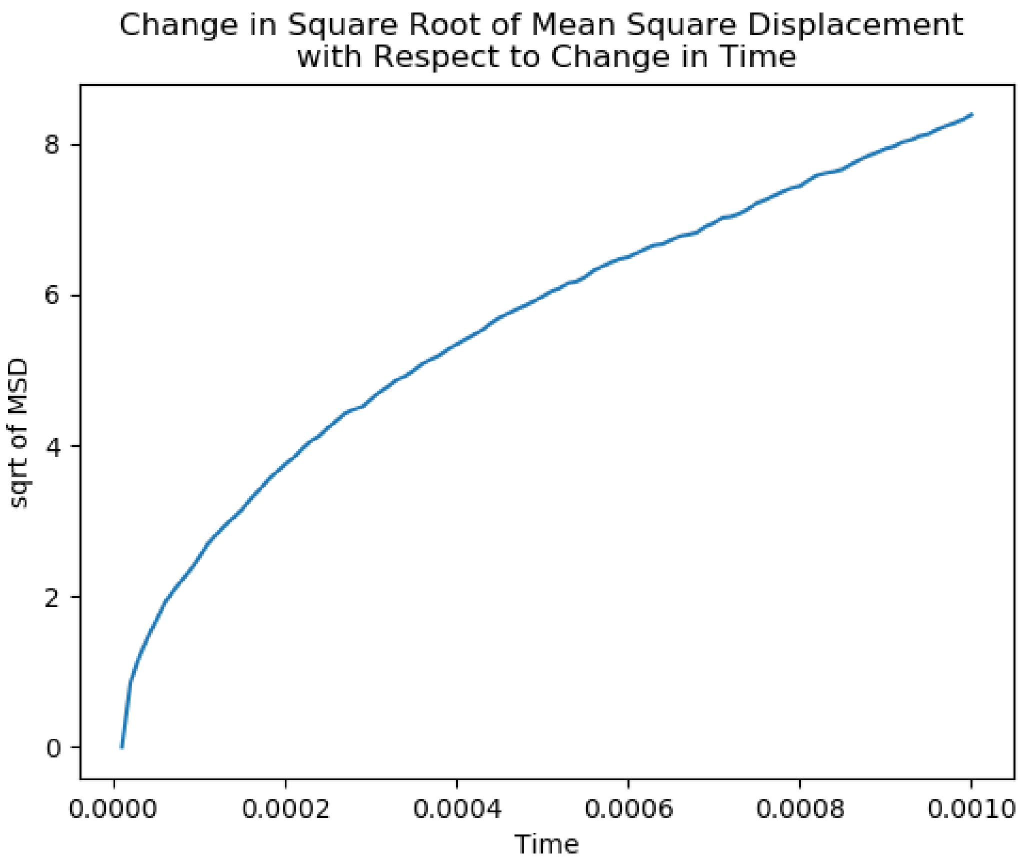

Figure 4: Square root of mean square displacement vs time in 3-d space, calculated using 1,000 particles.

When using the random walk model, the square root of the mean square displacement vs time graph has the shape as a square root function, the square root of the mean square displacement grows proportional to square root of time. This confirms that the square root of the mean square displacement of diffusion can be predicted by equation $d = \sqrt{2nDt}$. Using this equation, we can calculate that if a bacterias has D=0.00001cm^2/s, and if oxygen needs to get to the center of its body within 10 s, then the largest size it can be is 0.014 cm.

References

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