Below are my class notes of a topic called Random Diffusion. The coding for this assignment should graph like a mountain while (like a bulge) and settling flat over time.

Based on below class notes, please provide the following:

1) Graph (IF you can, show the graph settling over time; can it have colors).

2).Please provide the variables and values in a word.doc

3) Provide all relevant equations (save as word.doc)

4) *** Important*** Describe how you solved the equation. (ex: If you are solving differential equation, describe Euler Method showing how it was simplified by using Taylor approximation.).

5). The stability of the numerical method (ex: if you change the delta or delta x, does your result change.) Change something and see the effect it has.

Please save all above separately so that I can follow it, and add comments to coding so that I can understand and explain it.

Thank you so much.

7.4 RANDOM WALKS AND DIFFUSION

We have mentioned several times that random walks are equivalent to diffusion. In this section we will explore this connection in a little more detail. We will again adopt the cream-in-your-coffee analogy in which we have a large number of particles (cream) moving in solution (coffee). The goal is to calculate how these particles are spatially distributed as a function of time. In our discussion of random walkers we have, up to this point, focused on the motion of individual walkers. An alternative way to describe the same physics involves the density of particles, $\rho(x, y, z, t)$, which can be conveniently defined if the system contains a large number of particles (walkers). The idea, known as *coarse graining*, is to consider regions of space that are big enough to contain a large number of particles so that the density ($\equiv$ mass/volume) can be meaningfully defined. The density is then proportional to the probability per unit volume per unit time, denoted by $P(x, y, z, t)$, to find a particle at (x, y, z) at time t. Thus, ρ and P obey the same equation.

To find this equation, we focus back on an individual random walker. We assume that it is confined to take steps on a simple-cubic lattice, and that it makes one "walking step" each time step. $P(i, j, k, n)$ is the probability to find the particle at the site (i, j, k) at time n. Since we are on a simple cubic lattice, there are 6 different nearest neighbor sites. If the walker is on one of these sites at time $n-1$, there is a probability of $1/6$ that it will then move to site (i, j, k) at time n. Hence, the total probability to arrive at (i, j, k) is

$$P(i,j,k,n) = \frac{1}{6}\,[P(i+1,j,k,n-1) + P(i-1,j,k,n-1) + P(i,j+1,k,n-1) + P(i,j-1,k,n-1) + P(i,j,k+1,n-1) + P(i,j,k-1,n-1)]. \quad (7.15)$$

Rearranging this equation, we get

$$\begin{aligned} P(i,j,k,n) - P(i,j,k,n-1) \;=\; & \\ \frac{1}{6}\,\{&[P(i+1,j,k,n-1) - 2P(i,j,k,n-1) + P(i-1,j,k,n-1)] \\ &+ [P(i,j+1,k,n-1) - 2P(i,j,k,n-1) + P(i,j-1,k,n-1)] \\ &+ [P(i,j,k+1,n-1) - 2P(i,j,k,n-1) + P(i,j,k-1,n-1)]\}\,. \end{aligned} \tag{7.16}$$

Apart from a constant factor $(1/\Delta t)$, the left side of this equation is just the finite difference approximation for the time derivative of P, while the right-hand side is proportional to a second order space derivative. This suggests taking the continuum limit, which leads to

$$\frac{\partial P(x,y,z,t)}{\partial t} \;=\; D\,\nabla^2 P(x,y,z,t)\,, \tag{7.17}$$

where $D = (1/6)(\Delta x)^2/\Delta t$ in this approximation.[17] Equation (7.17) is the diffusion equation, and our derivation shows the close connection between the random walks and diffusion. The density ρ obeys the same equation

$$\frac{\partial \rho}{\partial t} \;=\; D\,\nabla^2 \rho\,. \tag{7.18}$$

We encountered a similar differential equation in our studies of waves in Chapter 6, and the numerical approach we used there can be extended to treat the diffusion equation. For ease of notation we will assume that ρ is a function of only one spatial dimension, x, although everything we do below can readily be extended to two or three dimensions. We can then write $\rho(x,t) = \rho(i\Delta x, n\Delta t) = \rho(i,n)$, so that the first index corresponds to space and the second to time. Converting (7.18) to one dimension yields

$$\frac{\partial \rho}{\partial t} \;=\; D\,\frac{\partial^2 \rho}{\partial x^2}\,, \tag{7.19}$$

and the finite-difference version of this (as in (7.16)) is

$$\frac{\rho(i,n+1) - \rho(i,n)}{\Delta t} \;=\; \frac{\rho(i+1,n) - 2\rho(i,n) + \rho(i-1,n)}{(\Delta x)^2}\,. \tag{7.20}$$

Rearranging to express the density at time step $n+1$ in terms of ρ at step n we find

$$\rho(i,n+1) \;=\; \rho(i,n) \;+\; \frac{D\,\Delta t}{(\Delta x)^2}\,[\rho(i+1,n) \;+\; \rho(i-1,n) \;-\; 2\,\rho(i,n)]\,. \tag{7.21}$$

If we are given the initial distribution of the cream particles, $\rho(x, t=0)$, we can use (7.21) to solve for ρ at future times. A program to implement this can be constructed along the lines we developed in Chapter 6 to deal with waves on a string, so we will leave the details to the exercises. While the programming is

[17] This particular value of D is for a simple cubic lattice, and is not universal.

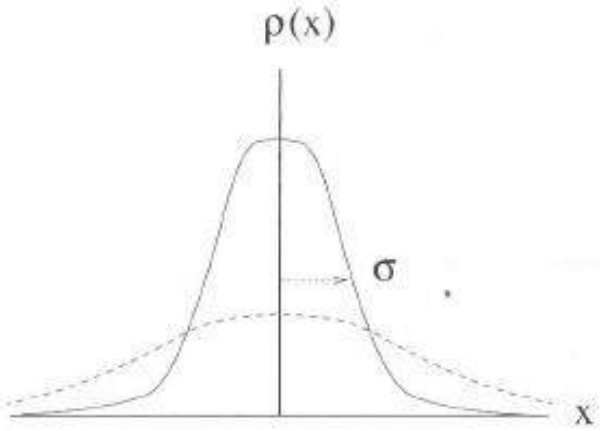

FIGURE 7.8: Schematic solutions of the diffusion equation at two different times. The solid curve shows the density at an early time, while the dashed curve shows it at some time later. The Gaussian distribution broadens with time, but the area under the curve, which is equal to the total number of particles, does not change.

straightforward, there remains the choice of spatial and temporal step sizes. As you might have guessed, the numerical instabilities we encountered when solving the wave equation can also arise here.

While it is not easy to provide a general analytic solution to the diffusion equation, one special case is very instructive. You can verify by substitution that the function

$$\rho(x,t) = \frac{1}{\sigma} \exp\left[-\frac{x^2}{2\,\sigma^2}\right] , \tag{7.22}$$

satisfies (7.19), provided that σ is *time dependent*, with $\sigma = \sqrt{2Dt}$. This result can be understood intuitively from Figure 7.8, which shows sketches of the density at two different times. At any particular time the spatial distribution has a Gaussian form whose half-width σ is, roughly speaking, the spatial size occupied by the clump of particles. As time passes, the density maintains a Gaussian form with the only change being that the width increases as $\sigma \sim \sqrt{t}$. That this is also just the root-mean-square distance traveled by an average particle can be seen as follows. At $t = 0$ the clump of particles will, according to our assumptions concerning how the drop is deposited, be very small ($\sigma \sim 0$). At a later time the cream distribution will be of order σ in extent, so this must also be the distance traveled by a typical diffusing cream particle. Hence, the distance traveled by a particle as it diffuses varies as $t^{1/2}$. This behavior[18] is precisely what we found in our studies of random walkers (7.1).

[18]This result is also an example of the central-limit theorem, which is mentioned in Appendix G in connection with the distribution functions associated with random processes. In the present problem many random values (steps in the diffusion/random-walk process) combine to yield a Gaussian distribution. The width of this distribution is proportional to $N^{1/2}$, where N is the number of steps. Here $N \sim t$.

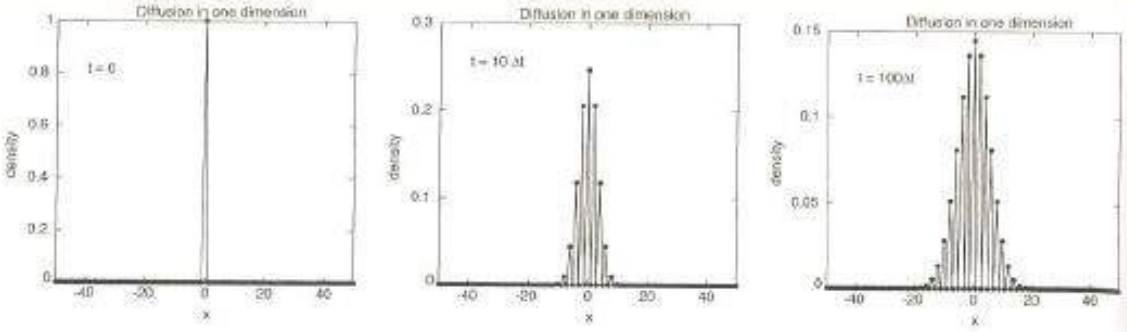

FIGURE 7.9: Time evolution calculated from the diffusion equation in one dimension at $t = 0$ (left), $t = 10\Delta t$ (center), and $t = 100\Delta t$ (right). The spatial step was $\Delta x = 1$ so the density was calculated only at the locations $x = 0, \pm 1, \pm 2$, etc. The lines are simply drawn to connect these points. We chose $D = 1$ and $\Delta t = 0.5$ so as to satisfy the stability condition (7.23) as an equality. Note that the vertical scales are different in the different plots; the maximum value of the density decreased as t increased, so as to keep the total number of particles fixed.

This analytic result tells us that a disturbance such as our particle distribution can be expected to spread by an amount as large as $\sim \sqrt{2D\tau}$ during time τ, or equivalently, it takes the distribution a time of order $\ell^2/(2D)$ to spread a distance of ℓ. Thus, to guarantee numerical stability we must make sure that the space and time steps satisfy

$$\Delta t \;\leq\; (\Delta x)^2/(2D)\;, \tag{7.23}$$

since larger values of the time step size would not allow the computed distribution to spread as quickly as we know that it must. This potential instability is similar to that found in connection with waves on a string, which should not be surprising since we are dealing with a similar equation.

A numerical solution of the diffusion equation obtained using (7.21) is shown in Figure 7.9. Here we have assumed that the initial density is zero everywhere except at the origin, $x = 0$; thus, our drop of cream is all initially located in one very small region. At $t = 10\Delta t$ the density profile has broadened, as the particles have spread over the range $x \approx \pm 6$. The amount of spreading has increased further at $t = 100\Delta t$. Qualitatively this distribution has spread out an additional factor of ≈ 3 for a tenfold increase in time, which is what we expect for diffusion.

A curious feature of the results for $t > 0$ is that the density alternates between zero and nonzero values. This behavior is due to the initial density profile which we assumed. Our initial profile had all of the density situated at a *single* grid site. This violates our usual rule-of-thumb that step sizes should always be smaller than any of the characteristic scales in the problem. Here one characteristic length scale is the spatial extent of the density profile. By allowing all of the density to be located at a single grid site we are effectively taking the density distribution to be a singular function.[19] The price we pay for this is that the finite difference equation (7.21) produces these spurious zeros.[20]

[19] This is much like a Dirac delta function or a "point" charge.

[20] This can be appreciated by evaluating $\rho(i, 1)$ by hand, using (7.21), for the initial profile

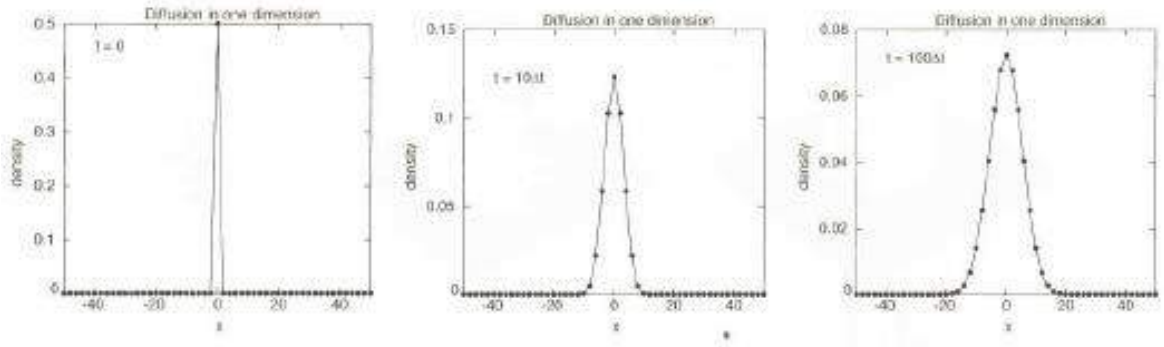

FIGURE 7.10: Time evolution calculated from the diffusion equation in one dimension at $t = 0$ (left), $t = 10\Delta t$ (center), and $t = 100\Delta t$ (right). Here we have averaged the values from Figure 7.9 at adjacent spatial grid sites to minimize discreteness effects.

One way to overcome this problem would be to use a smaller spatial step size so that the initial density profile is spread out over many grid sites. We will explore this approach in the exercises. Another, perhaps a bit more expedient (but equivalent) solution is to simply average the results in Figure 7.9 over adjacent grid elements. That is, we can average the results for adjacent spatial sites so as to "smooth over" the points where the density was zero. Doing this yields the results in Figure 7.10. The density profiles at $t = 10\Delta t$ and $100\Delta t$ now have the expected Gaussian shapes. The amplitude of the Gaussian distribution decreases and its width increases as we follow the motion to larger times. We will leave it for the reader to show that the width of the distribution, which is the scale over which the particles are spread, varies as $\sqrt{t}$. This is, of course, a defining feature of diffusion.

This numerical approach to the diffusion equation is very general and can be used just as well in two or three dimensions. We will explore the derivation of the corresponding finite difference equations (which are analogous to (7.21)) in the exercises. The stability condition becomes somewhat more restrictive on Δt as the dimensionality increases, a topic we will leave for the references. Figure 7.11 shows some results for a two-dimensional case. Here we have assumed initial conditions as in the cream-in-your-coffee problem, with all of the particles confined to a square region surrounding the origin. The density profile then spreads with time in an approximately spherical manner. This numerical approach can also be used to study other types of problems. All that is needed is the initial density profile. The finite difference algorithm (7.21) can then be used to calculate the profile at all future times.

To make the connection between the diffusion equation and random walks even more explicit, we now consider the same cream-in-your-coffee problem using a random-walk approach. We do this by considering a large number of walkers

in Figure 7.9. If you do this you will also see that in order to get a density of precisely zero at alternating grid sites, the spatial and temporal grid sizes must be chosen according to the stability condition, as we have done in our simulation. Other choices of the grid sizes would not necessarily lead to such exact cancellations of the density, but would still yield values that alternate in magnitude.

FIGURE 7.11: Time evolution calculated from the diffusion equation in two dimensions. At $t = 0$ (left) all of the particles were confined to "clump" at the center of the system. The distributions at $t = 6\Delta t$ (center), and $t = 20\Delta t$ (right) are also shown. The parameters used in the calculation were $\Delta x = 1$, $D = 1$, and $\Delta t = 0.25$. The region shown here covers the range $|x, y| \leq 10$.

that all start at the origin. This corresponds to the cream particles just after they have been deposited into the coffee. To obtain the density profile at time $t = n\Delta t$, we calculate the *probability distribution* of the walkers after n steps. That is, we let every walker take n steps, each of length unity, and record their positions. A histogram of the number of walkers that end up at location x, as a function of x, is then constructed. This is the desired probability distribution, or equivalently, density profile.

Some results for the one dimensional case are shown in Figure 7.12, and at first sight they might seem a bit strange as the probability of finding a walker at the odd-numbered grid sites is zero. However, this can be understood by recognizing that if a walker that starts from the origin and takes an even number of steps, it must end up at an even numbered site. Thus, we should really average the results over adjacent grid sites, much as we did with the diffusion-equation results.[21] In any case, the random-walk results exhibit the Gaussian spreading of the particle distribution that we have come to expect. Indeed, our derivation of (7.17) shows that the analogy with diffusion is exact. The general approach is to consider a large number of walkers distributed in space according to the particular initial conditions of the problem. Each walker is then allowed to move and the distribution of walkers is monitored as a function of step number, that is, time. We will employ this approach to bring out another aspect of the cream-in-your-coffee problem in Section 7.7.