

1.1 1-D Diffusion

1.1.2 The final values of probabilities at any time remain same independent of the change in values of Δt or Δx . However, the curve becomes more smooth or less smooth depending upon the change.

1.2 - 2-D Diffusion

1.2.1 Write down the two dimensional diffusion equation (axes: x and y) for a metal with diffusivity D.

$$\frac{\partial U}{\partial t} = D \left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} \right)$$

where, D is the diffusivity

U is the temperature of metal

1.2.2 Apply finite difference approximations to discretize the two dimensional diffusion equation.

We show that a double derivative can be written in a discrete form as:

$$\frac{d^2 f(x)}{dx^2} = \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x))}{(\Delta x)^2}$$

$$\text{Let } g(x) = \frac{df(x)}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x+\Delta x) - f(x)}{\Delta x} = \lim_{\Delta x \rightarrow 0} \frac{f(x) - f(x-\Delta x)}{\Delta x}$$

(By the definition of derivative)

$$\begin{aligned} \frac{dg}{dx} &= \frac{d^2 f}{dx^2} = \lim_{\Delta x \rightarrow 0} \frac{g(x) - g(x - \Delta x)}{\Delta x} = \lim_{\Delta x \rightarrow 0} \frac{g(x + \Delta x) - g(x)}{\Delta x} \\ &= \lim_{\Delta x \rightarrow 0} \frac{\frac{df(x+\Delta x)}{dx} - \frac{df(x)}{dx}}{\Delta x} \\ &= \lim_{\Delta x \rightarrow 0} \frac{\frac{f(x+\Delta x) - f(x)}{\Delta x} - \frac{f(x) - f(x-\Delta x)}{\Delta x}}{\Delta x} \end{aligned}$$

Therefore,

$$\frac{d^2 f(x)}{dx^2} = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x))}{(\Delta x)^2}$$

Hence, a double partial derivative can be written in discretized form as:

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{f(x + \Delta x, t) - 2f(x, t) + f(x - \Delta x, t)}{(\Delta x)^2}$$

Therefore, the two dimensional diffusion equation in discrete form can be written as:

$$\frac{U(x, y, t + \Delta t) - U(x, y, t)}{\Delta t} = D \left(\frac{U(x + \Delta x, y, t) - 2U(x, y, t) + U(x - \Delta x, y, t)}{(\Delta x)^2} - \frac{U(x, y + \Delta y, t) - 2U(x, y, t) + U(x, y - \Delta y, t)}{(\Delta y)^2} \right)$$

1.2.3 Write down the maximum time step you can allow without the process becoming unstable. Comment on how you formulated the expression.

The maximum timestep Δt allowed without the process becoming unstable is:

$$\Delta t = \frac{1}{2D} \frac{(\Delta x \Delta y)^2}{(\Delta x)^2 + (\Delta y)^2}$$

The growth factor is given by:

$$G = 1 - 2D \frac{\Delta t}{(\Delta x)^2} \cdot (1 - \cos(k\Delta x)) - 2D \frac{\Delta t}{(\Delta y)^2} (1 - \cos(l\Delta y))$$

The minimum value occurs when $k\Delta x = \pi = l\Delta y$.

$$G = 1 - 4D \left(\frac{\Delta t}{(\Delta x)^2} + \frac{\Delta t}{(\Delta y)^2} \right)$$

For growth factor to be ≥ 0 (stability)

$$\frac{\Delta t}{(\Delta x)^2} + \frac{\Delta t}{(\Delta y)^2} \leq \frac{1}{2}$$

$$\implies \Delta t \leq \frac{1}{2} \left(\frac{(\Delta x)^2 (\Delta y)^2}{(\Delta x)^2 + (\Delta y)^2} \right)$$

1.2.4 We will apply the 2-D diffusion equation to study the heat spread in a 2-dimensional metal plate. The initial temperature of the metal plate (T_i) is 300 K. The metal plate is kept aside a heat conducting material (circular disc) with temperature (T_j) 700 K. Assume that the size of the metal plate is 10 mm (width and height). Consider intervals in each direction (dx and dy) as 0.1 mm. Consider the dimensions of the circular disc as 2 mm centred at (5, 5) relative to the metal plate. Use the following information to quantify the initial conditions for the recurrence relation formed above. Vectorize your code properly.

Initial Conditions (i.e. at $t = 0$) : Let $U(i, j, t)$ denote the temperature of the cell (i,j) at time t. The centre of the disk is denoted by $(C_x, C_y) = (5, 5)$. The radius of the disk is $r = 2\text{mm}$. The initial conditions are:

- $\Delta x = 0.1\text{mm}$, $\Delta y = 0.1\text{mm}$
- $n_x = 10/0.1 = 100$, $n_y = 10/0.1 = 100$
- All the points which are not inside the area of the circular disk have $T=300\text{K}$ i.e.
 $U(i, j, 0) = 300\text{K}$ such that $(i\Delta x - C_x)^2 + (j\Delta y - C_y)^2 \geq r^2, 1 \leq i, j \leq 100$
- All points which are inside the area of circular disk have $T=700\text{K}$ i.e.
 $U(i, j, 0) = 700\text{K}$ such that $(i\Delta x - C_x)^2 + (j\Delta y - C_y)^2 < r^2, 1 \leq i, j \leq 100$

Using the above conditions and the discrete form of heat equation, we can calculate the temperature of the metal for any number of timesteps.

1.2.5 We will consider 101 time steps. Using the stability condition formulated from Question 1.2.3, calculate the time interval between two time steps. Write a function to use this information to solve the recurrence relation for 101 time steps.

Considering $D = 4$,

$$\Delta t = \frac{1}{2D} \frac{(\Delta x \Delta y)^2}{(\Delta x)^2 + (\Delta y)^2} = \frac{1}{2 \times 4} \frac{(0.1 \times 0.1)^2}{(0.1)^2 + (0.1)^2} = 6.25 \times 10^{-4} \text{ s}$$

1.2.6 Using the recurrence relation obtained above, create a heat map animation to show the evolution of time steps for each of 20 time steps. Conduct the experiments for two different values of diffusivity (4.0 and 6.0) and comment your observations.

Observations: When we increase the diffusivity from 4 to 6, the timestep decreases. Therefore, the metal with diffusivity 6 shows the same diffusion as metal with diffusivity 4 in less time (since no of timesteps is same).