Theoretical Foundations and Simulation of Diffusion Processes by use of Finite Differences

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Task 1.1: Fick's 1st Law

It states that the flux is proportional to the concentration gradient and the proportionality constant.

$$J = -D\frac{\partial \phi}{\partial t}$$

where,

- J = diffusion flux
- D = Proportionality constant

Lets consider a case:

we can define the local concentration and diffusion flux through a unit area, A at position x as:

$c(x,t),\ J(x)$

we have

$$\frac{dc(x,t)}{dt} = -\frac{\partial J}{\partial x}$$

$$\frac{\partial c(x,t)}{\partial t} = -\frac{\partial J}{\partial x}$$

Substituting first law of Fick's, we get

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

Task 1.2

When the concentration / diffusion of particles remain unchanged. Diffusion process has reached the state of equilibrium means flux J = 0 and from Fick's 1st law,

$$J = -D\frac{\partial \phi}{\partial t} = 0$$

$$\frac{\partial \phi}{\partial t} = 0$$

i.e, Conc. gradient = 0

that means

$$D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} = 0$$

$$\frac{\partial^2 C}{\partial x^2} + D_y/D_x\frac{\partial^2 C}{\partial y^2} = 0$$

$let D_y/D_x = P$

$$\frac{\partial^2 C}{\partial x^2} + P\frac{\partial^2 C}{\partial y^2} = 0$$

$$P\frac{\partial^2 \rho(x,y)}{\partial x^2} + \frac{\partial^2 \rho(x,y)}{\partial y^2} = 0$$

$$\frac{\partial c(x)}{\partial t} = 0 \quad \text{(for stationary diffusion)}$$

As, Concentration does not change with time.

$$\frac{\partial^2 \rho(x,y)}{\partial x^2} + \frac{\partial^2 \rho(x,y)}{\partial y^2} = 0$$

when we multiply diffusivity (P) in above equation,

$$P\left[\frac{\partial^2 \rho(x,y)}{\partial x^2} + \frac{\partial^2 \rho(x,y)}{\partial y^2}\right] = 0$$

As given, process is anistropic diffusion process, all the parameters depending on direction not the position

$$P\frac{\partial^2 \rho(x,y)}{\partial x^2} + \frac{\partial^2 \rho(x,y)}{\partial y^2} = 0$$

Firstly, we have to know about diffusion tensor and their relavant equations. We can consider matrix of diffusivity: When we consider 2-Dimensional, x and y can be consider as different position and direction. P is considered as Diffusivity.

$$(P_{ij}) = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix}$$

$$J_1 = -P_{11}\frac{\partial P}{\partial x_1} - P_{12}\frac{\partial P}{\partial x_2} = 0$$

$$J_2 = -P_{22}\frac{\partial P}{\partial x_2} - P_{21}\frac{\partial P}{\partial x_1} = 0$$

Diffusivity can be affected by chossing different direction when providing different symmetry and their independent elements.

Task 1.3

The Laplace equation can be proved as follows:

$$let \quad \widetilde{x} = x \quad and \quad \widetilde{y} = \sqrt{P}y$$

$$\partial\widetilde{x} = \partial x \qquad \Longrightarrow \qquad \partial\widetilde{x}/\partial x = 1$$

$$\partial\widetilde{y} = \sqrt{P}\partial y \qquad \Longrightarrow \qquad \partial\widetilde{y}/\partial y = 1/\sqrt{P}$$

$$\rho(\widetilde{x},\widetilde{y}) = \rho(x, \sqrt{P}y)$$

$$\frac{\partial^2}{\partial x^2}\rho(\widetilde{x},\widetilde{y}) = \frac{\partial^2}{\partial x^2}\rho(x,y)$$

$$\frac{\partial^2}{\partial y^2}\rho(\widetilde{x},\widetilde{y}) = p\frac{\partial^2}{\partial y^2}\rho(x,y)$$

We know that, Concentration does not change with time.

$$\text{i.e, } \frac{\partial^2}{\partial x^2}\rho(x,y) + P\frac{\partial^2}{\partial y^2}\rho(x,y) = 0$$

$$\implies \frac{\partial^2}{\partial x^2}\rho(\widetilde{x},\widetilde{y}) + P * \frac{1}{P} * \frac{\partial^2}{\partial x^2}\rho(\widetilde{x},\widetilde{y}) = 0$$

Task 2.1: Central finite difference scheme

Step 1:

Discretizing the domain into uniformly partitioned time mesh

Step 2:

Differential Equation must be satisfied at all points

Step 3:

Replace second order derivative as $u''(t_n) = \frac{u^{n+1} - 2u^n + u^{n-1}}{\delta t^2}$

Now we need to discretize the equation:

$$\frac{\partial^2}{\partial x^2}\rho(x,y) + P\frac{\partial^2}{\partial y^2}\rho(x,y) = 0$$

s

$$\implies \frac{\partial^2}{\partial x^2}\rho_{i,j}(x,y) + P\frac{\partial^2}{\partial y^2}\rho_{i,j}(x,y) = 0$$

let us consider P = 1 (for isotropic materials) and $h_x = h_y = 1$

Now , we get

$$4\rho_{i,j} - \rho_{i+1,j} - \rho_{i-1,j} - \rho_{i,j+1} - \rho_{i,j-1} = 0$$

Task 2.2:

Applying central finite difference scheme to each node in innner domain.

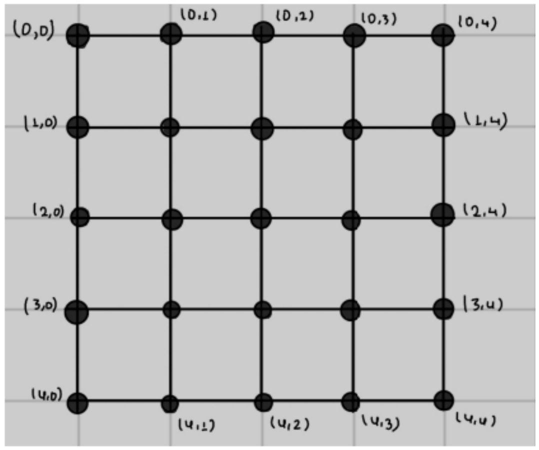


Figure 1: sketch of the mapping from the (i, j) notation

Discretized scheme as a linear system of equations is as follows:

$$
\begin{gathered}
-4\rho_1 + \rho_{0,1} + \rho_{1,0} + \rho_2 + \rho_4 = 0 \\
-4\rho_2 + \rho_{0,2} + \rho_1 + \rho_3 + \rho_5 = 0 \\
-4\rho_3 + \rho_{0,3} + \rho_{1,4} + \rho_2 + \rho_6 = 0 \\
-4\rho_4 + \rho_{2,0} + \rho_1 + \rho_5 + \rho_7 = 0 \\
-4\rho_5 + \rho_2 + \rho_4 + \rho_6 + \rho_8 = 0 \\
-4\rho_6 + \rho_{2,4} + \rho_5 + \rho_3 + \rho_9 = 0 \\
-4\rho_7 + \rho_{4,1} + \rho_{3,0} + \rho_4 + \rho_8 = 0 \\
-4\rho_8 + \rho_{4,2} + \rho_5 + \rho_7 + \rho_9 = 0 \\
-4\rho_9 + \rho_6 + \rho_8 + \rho_{4,3} + \rho_{3,4} = 0
\end{gathered}
$$

$$
AX = \begin{bmatrix}
4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\
0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\
0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\
0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4
\end{bmatrix}
\begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \\ \rho_4 \\ \rho_5 \\ \rho_6 \\ \rho_7 \\ \rho_8 \\ \rho_9 \end{bmatrix}
=
\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}
$$

Task 3.1: Dirichlet boundary conditions

At node 3, we can have the equation from below given figure: Derivation of the discrete (linear) equation for this node:

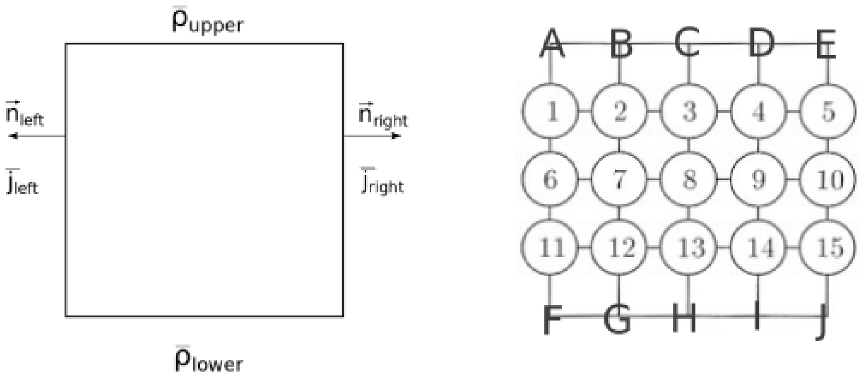
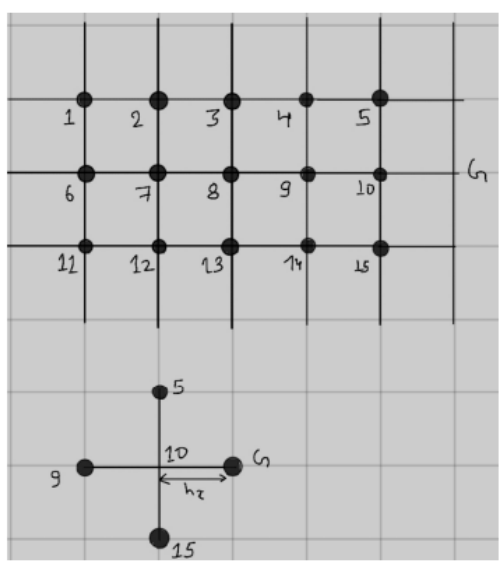


Figure 2: System and discretization

$$
\begin{aligned}
-4\rho_3 + \rho_c + \rho_2 + \rho_4 + \rho_8 &= 0 \\
-4\rho_3 + \rho_2 + \rho_4 + \rho_8 &= -\rho_c
\end{aligned}
$$

Task 3.2: Neumann boundary conditions

The Neumann boundary condition specifies the normal derivative at a boundary to be zero or a constant. Let, Ghost node will be G.



When we look at the picture. Discretize Fick's equation,

$$\frac{\partial\rho_{10}}{\partial x} = \frac{\rho_c-\rho_g}{2h_x}$$
$$\rho_G = \rho_g - 2h_x\frac{\partial\rho_{10}}{\partial x}$$
$$\rho_5+\rho_g+\rho_{15}+\rho_g+(-4\rho_{10}) = 0$$
$$\rho_5+2\rho_g+\rho_{15}-4\rho_{10} = -2h_x\frac{\partial\rho_{10}}{\partial x}$$

Task 4.1: Assemble the the linear system of equations

For balancing the below matrix equation, we have to multiply left hand side by following ρ matrix

$$\begin{bmatrix}
-4 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 2 & -4 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & -4 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0\\
0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0\\
0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0 & 0\\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 1 & 0\\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 2 & -4 & 0 & 0 & 0 & 0 & 1\\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -4 & 2 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -4 & 1\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 2 & -4
\end{bmatrix} = \begin{bmatrix}
\frac{2h}{D}J_{left}\\ 0\\ 0\\ 0\\ \frac{2h}{D}(-J_{right})\\ \frac{2h}{D}J_{left}\\ 0\\ 0\\ 0\\ \frac{2h}{D}(-J_{right})\\ \frac{2h}{D}J_{left}\\ 0\\ 0\\ 0\\ \frac{2h}{D}(-J_{right})
\end{bmatrix} - \begin{bmatrix}
\rho_A\\ \rho_B\\ \rho_C\\ \rho_D\\ \rho_E\\ 0\\ 0\\ 0\\ 0\\ 0\\ \rho_F\\ \rho_G\\ \rho_H\\ \rho_I\\ \rho_J
\end{bmatrix}$$

Task 4.2:

1. We can see most of the elements on coefficient matrix is zero, i.e Sparse matrix and it is bounded too
2. The shape of the coefficient matrix is influenced by number of nodes in each length of domain

Numerical Implementation

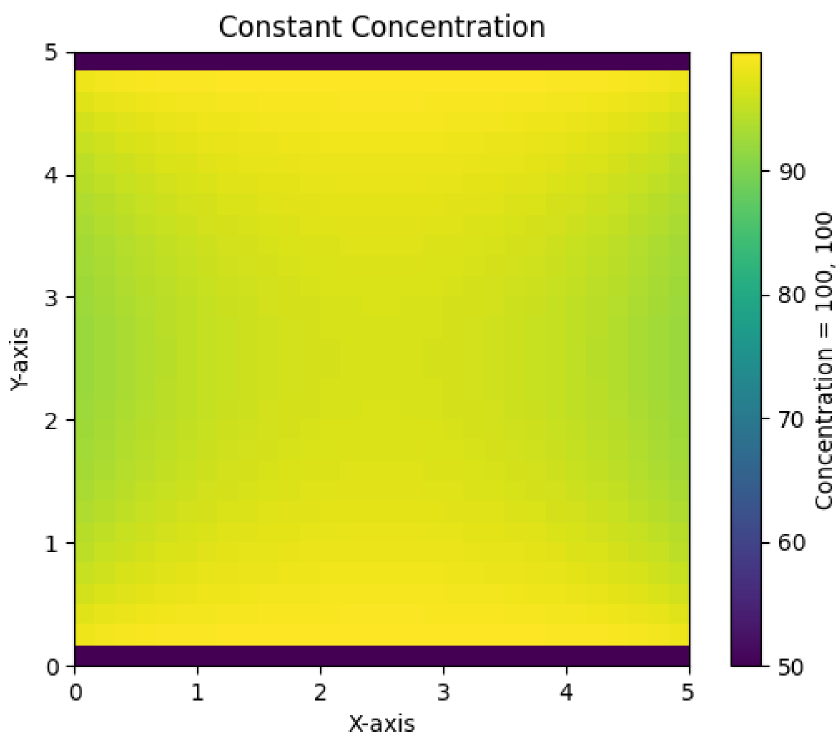
Task 5.1:

The solution for a system with specified width (lx), height (ly), and the given number of nodes (Nx and Ny) with arbitrary values assigned to the boundaries for j and has been implemented using either Python(Please check the script provided).

Task 5.2:

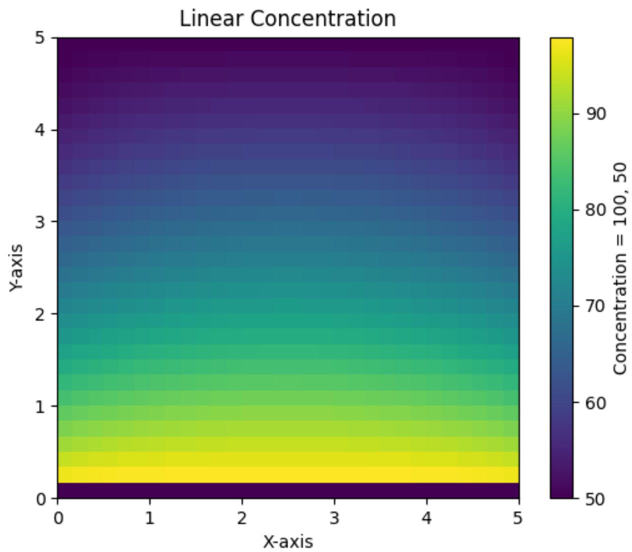
Task 5.2(1):

After applying jleft = jright = upper = 100 mol ·m3 , lower = 100 mol·m3, we can see that concentration is constant everywhere



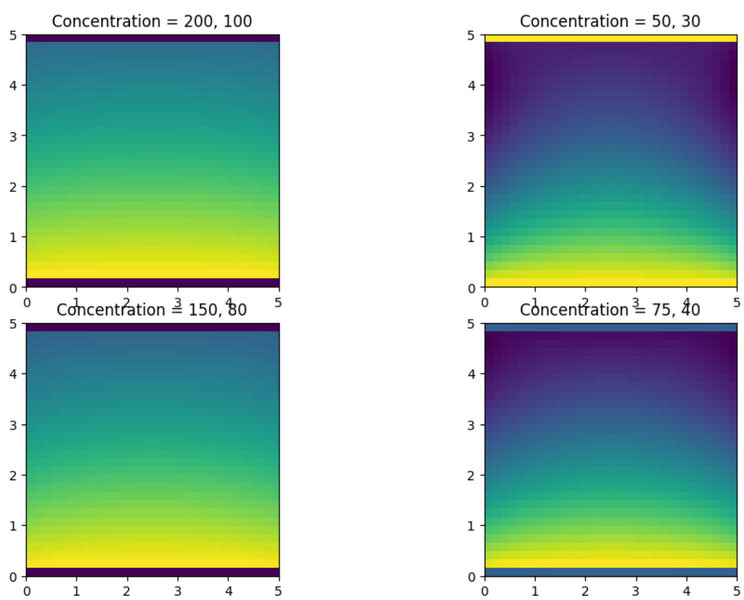
Task 5.2(2):

After applying upper = 100 mol · m3 , lower = 50 mol · m3, we can now see in the plot that concentration is linear.



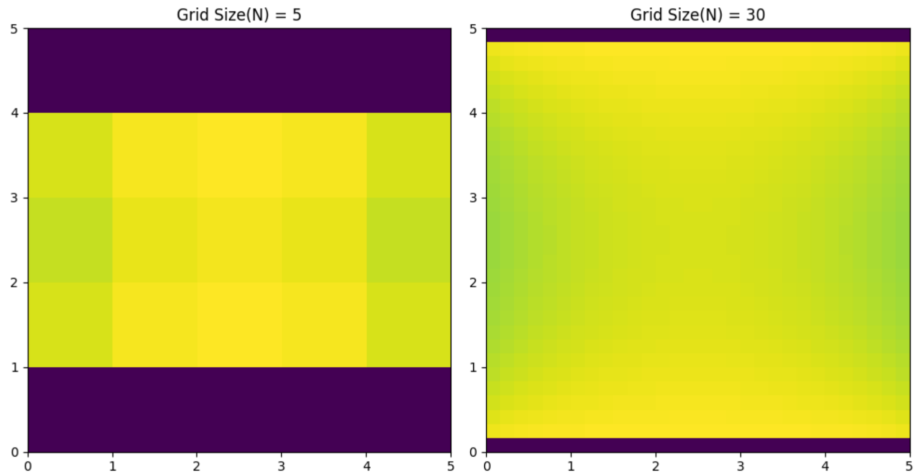
Task 5.2(3):

After changing the Dirichlet BC to different pairs of concentrations, we can see that all the plots are linear.



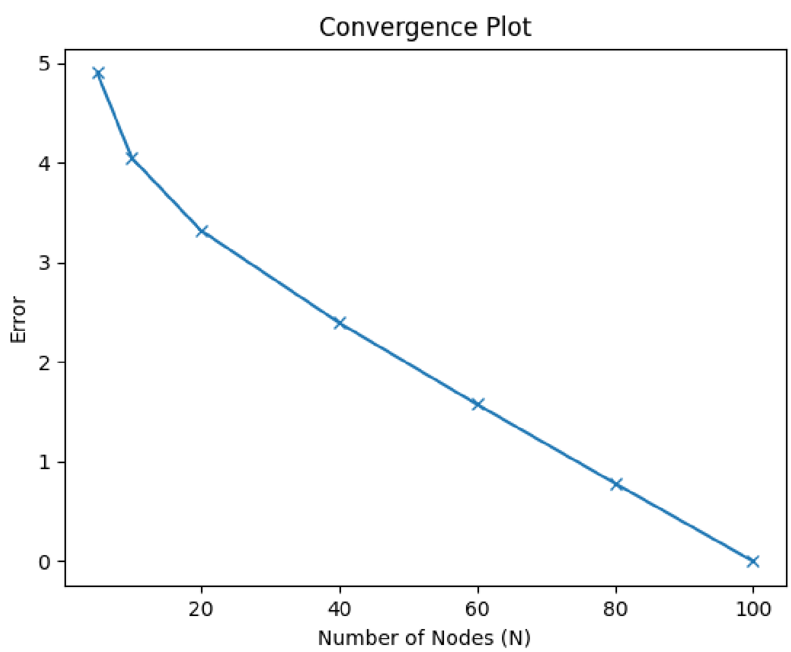
Task 5.2(4):

By comparing the numerical solution of a coarse grid (e.g.,, 5x5) with the analytical solution, we can clearly see that the number of nodes i.e, grid resolution is the biggest discrepancy in the coarse grid.



Task 5.2(5):

When the number of nodes (N) is smaller The computation cost is lower. When the number of nodes increases, the error comes down as well, which is evident in the convergence plot. Also, a smaller norm indicates a closer match between the numerical and analytical solutions



Task 5.2(6):

When both jleft and jright are zero, the coefficients in the matrix A become constant and do not depend on the specific grid size(N). Therefore, we can precompute the constant part of the matrix outside the loop, avoiding redundant calculations.

Task 5.2(7):

For number of nodes = 30 and for different boundary conditions, we can see that Jleft and Jright are equal, and rhoupper and rholower are same. The distribution of flux is also same on both side of boundary condition.