1 Problem Statement

Consider the diffusion equation

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{1}$$

$$D = \text{Const} > 0$$

in a rectangular domain

$$R = [0, l_x] \times [0, l_y] \tag{2}$$

with Neumann boundary conditions

$$\begin{aligned} u(0, y, t) &= L, \\ u(l_x, y, t) &= R, \\ u(x, 0, t) &= B, \\ u(x, l_y, t) &= T \end{aligned} \tag{3}$$

where L, R, B, T are constants. The initial condition is given by

$$u(x, y, 0) = u_0(x, y). \tag{4}$$

2 Numerical Method

The scheme used for the problem (1)–(4) is the implicit Euler scheme on a uniform grid with $n_x \times n_y$ cells

$$\frac{u^n_{i,j} - u^{n-1}_{i,j}}{\tau} = D\left(\frac{u^n_{i+1,j} - 2u^n_{i,j} + u^n_{i-1,j}}{h_x^2} + \frac{u^n_{i,j+1} - 2u^n_{i,j} + u^n_{i,j-1}}{h_y^2}\right) \tag{5}$$

where τ is the time step and h_x, h_y are the uniform grid spacings. The scheme (5) is stable for any τ. To determine $u^n_{i,j}$ in the boundary nodes, we use so-called virtual nodes. For instance, the value on the left boundary of a one-dimensional domain is

$$\frac{u_1 - u_{-1}}{2h} = \frac{du}{dz}(0) \quad \Rightarrow \quad u_{-1} = u_1 - 2h\frac{du}{dz}(0).$$

Using the scheme (5), we may write the resulting system of algebraic equations as

$$A\mathbf{u}^n = \mathbf{u}^{n-1} + \mathbf{B} \tag{6}$$

where A is a sparse matrix and $\mathbf{B}$ is the vector resulting from the boundary conditions. This system can be solved by a direct method based on LU decomposition.

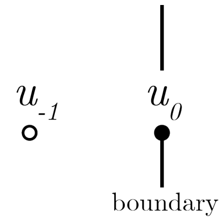
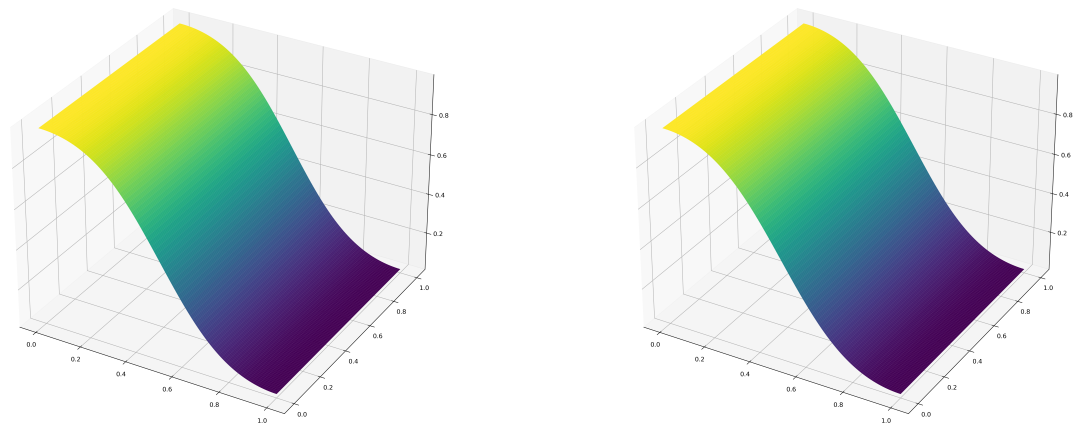


Figure 1: A virtual node of index -1



(a) Numerical solution

(b) Analytical solution

Figure 2: Solution to the diffusion problem with zero Neumann boundary conditions

3 Test Cases

To verify the code, solve the problem (1)–(4) with parameters $D = 1/4$, $l_x = l_y = 1$, $L = R = B = T = 0$, and

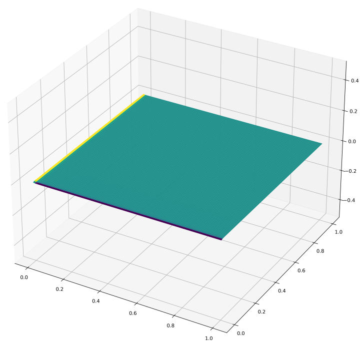
$$u_0(x, y) = \begin{cases} 1, & x \leq 1/2 \\ 0, & x > 1/2 \end{cases}.$$

The exact solution to this problem reads

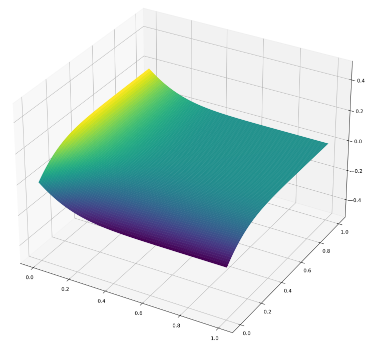
$$u(x, y, t) = \frac{1}{2} + \sum_{n=1}^{\infty} \frac{2}{\pi n} \sin \frac{\pi n}{2} \exp\left(-\frac{(\pi n)^2}{4} t\right) \cos(\pi n x). \tag{7}$$

Figure 2 shows the numerical and analytical solutions at $t = 1$.

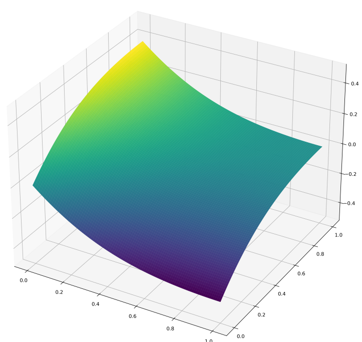
Another test case is (1)–(4) with $D = 1/4$, $l_x = l_y = 1$, $L = -1$, $B = 1$, $R = T = 0$, and zero initial condition $u_0(x) = 0$. The evolution of $u(x, y)$ is shown in Figure 3.



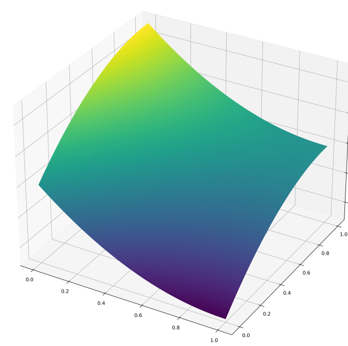
(a) $t = 10^{-4}$



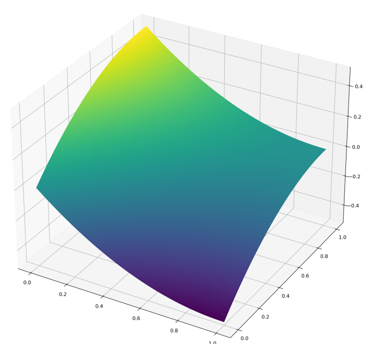
(b) $t = 0.1$



(c) $t = 0.5$



(d) $t = 5$



(e) $t = 50$

Figure 3: Solution to the diffusion problem with non-zero Neumann boundary conditions