Exercise 2

Introduction

The diffusion-transport problem is a common type of partial differential equation that arises in many scientific and engineering applications. It involves the transport of a substance through a medium, which can be modeled by a diffusive term and a transport term. In this report, we consider the following diffusion-transport problem:

$$\begin{cases} -(\mu u' - \psi' u)' = 1, \quad 0 < x < 1 \\ u(0) = u(1) = 0 \end{cases}$$

Here, μ is a positive constant and $\psi = \alpha x$ is a given function, where α is a real constant. The problem is subject to homogeneous Dirichlet boundary conditions. In **Part 1**, we will calculate the exact solution of our problem using the symbolic toolbox in MATLAB and approximate the problem using three finite difference methods: centered, backward, and forward, for different values of μ and α. We will then analyze and comment on the results obtained on grids of step size $h = 0.1$ and $h = 0.01$. Finally, we will deduct the concept of *upwind*. In **Part 2**, we will operate the substitution $u(x) = \rho(t)e^{\frac{\psi(t)}{\mu}}$ and - after computing the exact solution ρ - we will utilize finite differences with a centered scheme to compute the exact approximated solutions. The obtained results will be remapped into the original variable u, and we will provide an analysis of our findings.

Part 1

Analysis

Exact Solution To obtain the exact solution, we first rewrite the problem in a more manageable form:

$$-\mu u'' + \alpha u' = 1$$

We now use the MATLAB symbolic toolbox and the `dsolve` command to find the exact solution to our Neumann problem. The algorithm can be found on the `exactsol.m` MATLAB script. We immediately obtain the exact solution to be:

$$u(x) = -\frac{x + e^{\frac{\alpha x}{\mu}} - x e^{\frac{\alpha}{\mu}} - 1}{\alpha e^{\frac{\alpha}{\mu}} - 1}$$

Numerical Solution We now turn our attention to approximating the solution using finite difference methods.
These methods will be applied to the discretized version of the problem, obtained by dividing the interval $[0, 1]$ into a uniform grid of $n + 1$ points ($x_0 < x_1 < ... < x_n < x_{n+1}$), with grid spacing $h = 1/n$. The discrete solution u_i at the i-th grid point will be approximated by the corresponding value of the unknown function $u(x_i)$.

Discretization with centered differences (CD) The centered differences method approximates the derivative $u'(x_i)$ by the central difference formula:

$$u'(x_i) \approx \frac{u(x_{i+1}) - u(x_{i-1})}{2h}$$

The second derivative $u''(x_i)$ is approximated by applying the central difference formula to $u'(x_i)$:

$$u''(x_i) \approx \frac{u'(x_{i+1}) - u'(x_{i-1})}{2h} \approx \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2}$$

Substituting these approximations into the differential equation, we obtain the following discrete equation:

$$-\frac{\mu}{h^2}(u_{j+1}-2u_j+u_{j-1})+\frac{\alpha}{2h}(u_{j+1}-u_{j-1})=1$$

Simplifying and rearranging, we get:

$$u_{j-1}\left(-\frac{\mu}{h^2}-\frac{\alpha}{2h}\right)+u_j\left(\frac{2\mu}{h^2}\right)+u_{j+1}\left(-\frac{\mu}{h^2}+\frac{\alpha}{2h}\right)=1 \quad (*)$$

for $1 \leq i \leq n$, with boundary conditions $u_0 = u_{n+1} = 0$.
The corresponding linear system is $\mathbf{Au} = \mathbf{1}$, where $\mathbf{A}$ is the matrix with elements:

$$\begin{bmatrix} 2\mu/h^2 & -\mu/h^2+\alpha/2h & 0 & \cdots & 0 \\ -\mu/h^2-\alpha/2h & 2\mu/h^2 & -\mu/h^2+\alpha/2h & 0 & \cdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \cdots & -\mu/h^2-\alpha/2h & 2\mu/h^2 & -\mu/h^2+\alpha/2h \\ 0 & \cdots & 0 & -\mu/h^2-\alpha/2h & 2\mu/h^2 \end{bmatrix}$$

The matrix $\mathbf{A}$ is symmetric diagonally dominant and tridiagonal, therefore $\mathbf{A}$ is invertible which ensures the existence of a unique solution to the linear system of equations, easily computable by using the \ MATLAB operator.
Hence, we obtain:

$$\mathbf{A}\cdot\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} 1+u_0\left(\frac{\mu}{h^2}+\frac{\alpha}{2h}\right) \\ 1 \\ \vdots \\ 1 \\ 1+u_{n+1}\left(\frac{\mu}{h^2}-\frac{\alpha}{2h}\right) \end{bmatrix}$$

First and last components of the known terms vector result from the incorporation of Dirichlet boundary conditions into our system of equations, using $(*)$ for $j = 1$ and $j = n$.

Discretization with forward differences (FD) We now iterate the same process using the forward finite differences schemes. The derivative $u'(x_i)$ is therefore approximated by the forward difference formula:

$$u'(x_i) \approx \frac{u(x_{i+1})-u(x_i)}{h}$$

We will keep adopting a central differences formula for the second derivative $u''(x_i)$, which will be approximated again by:

$$u''(x_i) \approx \frac{u'(x_{i+1})-u'(x_{i-1})}{2h} \approx \frac{u(x_{i+1})-2u(x_i)+u(x_{i-1})}{h^2}$$

Substituting these approximations into the differential equation, simplifying and rearranging, we get:

$$u_{j-1}\left(-\frac{\mu}{h^2}\right)+u_j\left(\frac{2\mu}{h^2}-\frac{\alpha}{h}\right)+u_{j+1}\left(-\frac{\mu}{h^2}+\frac{\alpha}{h}\right)=1 \quad (**)$$

for $1 \leq i \leq n$. The corresponding linear system is $\mathbf{Bu} = \mathbf{1}$, where $\mathbf{A}$ is the matrix with elements:

$$\begin{bmatrix} 2\mu/h^2-\alpha/h & -\mu/h^2+\alpha/h & 0 & \cdots & 0 \\ -\mu/h^2 & 2\mu/h^2-\alpha/h & -\mu/h^2+\alpha/h & 0 & \cdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \cdots & -\mu/h^2 & 2\mu/h^2-\alpha/h & -\mu/h^2+\alpha/h \\ 0 & \cdots & 0 & -\mu/h^2 & 2\mu/h^2-\alpha/h \end{bmatrix}$$

The matrix **B** has the same properties as the matrix **B**, thus we have the existence of a unique solution to the linear system of equations. We obtain:

$$\mathbf{B} \cdot \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} 1 + u_0 \left(\frac{\mu}{h^2}\right) \\ 1 \\ \vdots \\ 1 \\ 1 + u_{n+1} \left(\frac{\mu}{h^2} - \frac{\alpha}{h}\right) \end{bmatrix}$$

Again, first and last components of the known terms vector result from the incorporation of Dirichlet boundary conditions into our system of equations, using $(**)$ for $j = 1$ and $j = n$.

Discretization with backward differences (BD) Finally, we approximate the derivative $u'(x_i)$ using the backward difference formula:

$$u'(x_i) \approx \frac{u(x_i) - u(x_{i-1})}{h}$$

while $u''(x_i)$ will be still approximated by:

$$u''(x_i) \approx \frac{u'(x_{i+1}) - u'(x_{i-1})}{2h} \approx \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2}$$

Substituting these approximations into the differential equation, simplifying and rearranging, we get:

$$u_{j-1} \left(-\frac{\mu}{h^2} - \frac{\alpha}{h}\right) + u_j \left(\frac{2\mu}{h^2} + \frac{\alpha}{h}\right) + u_{j+1} \left(-\frac{\mu}{h^2}\right) = 1 \quad (***)$$

for $1 \leq i \leq n$. The corresponding linear system is $\mathbf{Cu} = \mathbf{1}$, where $\mathbf{C}$ is the matrix with elements:

$$\begin{bmatrix} 2\mu/h^2 + \alpha/h & -\mu/h^2 & 0 & \cdots & 0 \\ -\mu/h^2 - \alpha/h & 2\mu/h^2 + \alpha/h & -\mu/h^2 & 0 & \cdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \cdots & -\mu/h^2 - \alpha/h & 2\mu/h^2 + \alpha/h & -\mu/h^2 \\ 0 & \cdots & 0 & -\mu/h^2 - \alpha/h & 2\mu/h^2 + \alpha/h \end{bmatrix}$$

A, **B** and **C** share the same properties. We obtain:

$$\mathbf{C} \cdot \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} 1 + u_0 \left(\frac{\mu}{h^2} + \frac{\alpha}{h}\right) \\ 1 \\ \vdots \\ 1 \\ 1 + u_{n+1} \left(\frac{\mu}{h^2}\right) \end{bmatrix}$$

Code summary The MATLAB code `RunFD.m` computes numerical solutions for the given problem using different finite difference schemes: backward, centered, and forward.
The code first defines some functions and sets up parameters for the problem, then iterates through different combinations of parameters and computes the numerical solution using the various finite differences schemes. Finally, it plots the results and calculates the error with respect to the exact solution.
The main script consists of the following steps:

1. Clear variables and close all figures.

2. Define the functions `f` and `uex` for the problem.

3. Set up the problem parameters (`L`, `u0`, `uL`, `hh`, `alfaa`, and `muu`).
4. Loop through the different combinations of parameters and compute the numerical solution using the different finite differences schemes (we will use the functions `FDbackward.m`, `FDcentr.m`, and `FDforward.m` which implement the backward, centered, and forward finite differences schemes, respectively.).
5. Plot the results and calculate the *infinity norm* of the error with respect to the exact solution.

Each of the three functions at point 4. takes the parameters `alfa`, `h`, `mu`, `n`, `u0`, and `uL`, and returns a numerical solution `Uh` for the given problem. A comparison of the solution graphs is also shown. We run our tests for `alfa = 1,-1` and `mu = 0.1,0.01`, using as a step length `h = 0.1,0.01`.

Results The following tables show how the *infinity norm* of the error of the exact solution with respect to the exact solution may vary, using different finite differences schemes and changing the step length `h`. The result of the various graph plots is ultimately displayed.

$\alpha = 1 \quad \mu = 0.1$

`h`	`err` **(BD)**	`err` **(CD)**	`err` **(FD)**
0.1	1.316e-01	3.4528e-02	3.6785e-01
0.01	1.7647e-02	3.0667e-04	1.9189e-02

$\alpha = 1 \quad \mu = 0.01$

`h`	`err` **(BD)**	`err` **(CD)**	`err` **(FD)**
0.1	9.0863e-02	6.9612e-01	1.1111e+00
0.01	1.3212e-01	3.4546e-02	3.6787e-01

$\alpha = -1 \quad \mu = 0.1$

`h`	`err` **(BD)**	`err` **(CD)**	`err` **(FD)**
0.1	3.6785e-01	3.4528e-02	1.3166e-01
0.01	1.9189e-02	3.0667e-04	1.7647e-02

$\alpha = -1 \quad \mu = 0.01$

`h`	`err` **(BD)**	`err` **(CD)**	`err` **(FD)**
0.1	1.1111e+00	6.9612e-01	9.0863e-02
0.01	3.6787e-01	3.4546e-02	1.3212e-01

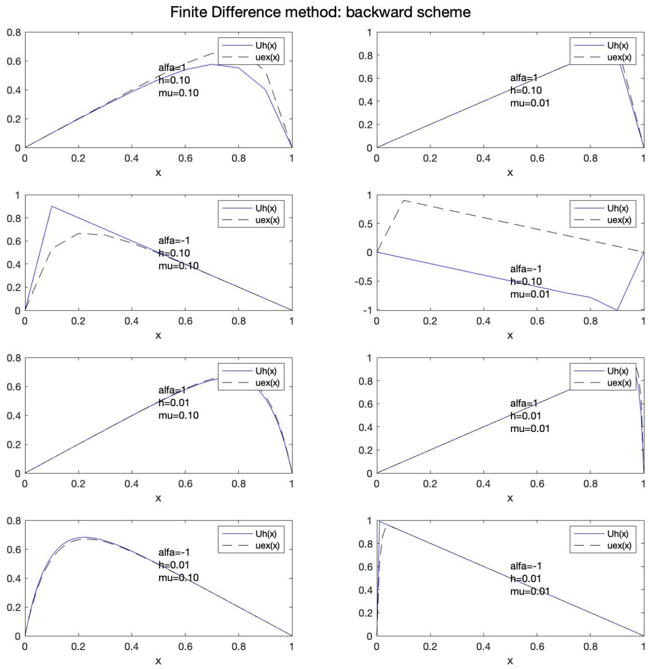

Figure 3: Comparison between exact and approximated solutions, BD.

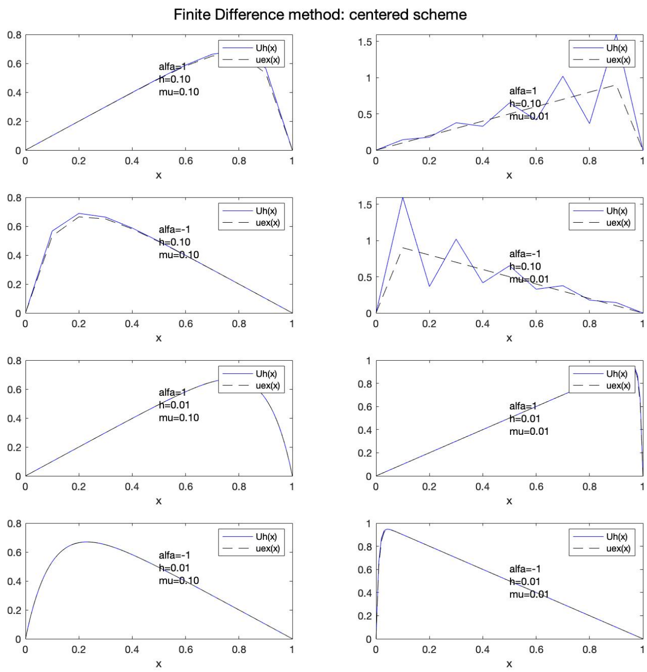

Figure 4: Comparison between exact and approximated solutions, CD.

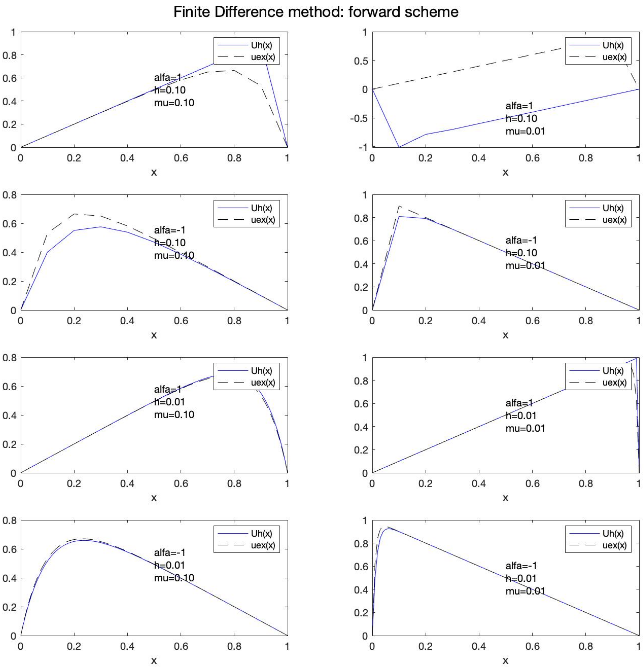

Figure 5: Comparison between exact and approximated solutions, FD.

Conclusions

In conclusion, we can easily notice how different finite differences schemes lead to different approximations of the exact solution.
In particular, the finite difference method with a backward scheme is found to be more accurate in approximating the diffusion problem proposed for $\alpha = 1$, compared to the forward scheme. For $\alpha = -1$, on the other hand, we have the opposite situation. We observe that these results are perfectly in line with the concept of *upwind*: to obtain better results, the finite difference approximation of the unknown function is computed with values from the upwind direction. This is because the transport of information occurs in the direction of convection, and hence the upwind direction is the direction from which information is coming.
In the simple upwind scheme, the second-order approximation of the first derivative - using the centered scheme - is replaced by the first-order approximation - using either the backward scheme or the forward scheme. Hence, especially for small values of `h`, it is possible to appreciate the greater accuracy of the centered approximation.