ME 605 Computational Fluid Dynamics
Fall 2021-22

Instructor Prof. Dilip Sundaram

Project-1

Name - Devanshu Thakar

Roll no. – 18110174

Contents

Problem Statement

You are required to write a computer program to solve the 1-D steady convection-diffusion equation computationally:

$$\frac{d}{dx}(\rho u \varphi) = \frac{d}{dx}\left(\Gamma \frac{d\varphi}{dx}\right)$$

with a domain length $L = 1.0$, $\rho = 1.0$, $u = 1.0$, ϕ (x = 0) = 0, and ϕ (x = L) = 1.0. Choose a Peclet number, $\mathrm{Pe} = \frac{\rho u \mathrm{L}}{\Gamma}$, of 50. Perform the following exercises using your code.

1. Consider a uniform grid with 11 nodes (inclusive of the boundary nodes). Apply upwind (backward) differencing for the convective term and central differencing for the diffusive term.
2. Repeat part (1) above, except with central differencing for the convective term as well.
3. Plot φ vs. x separately for part 1 and for part 2. In each of these plots, compare the numerical solution with the exact analytical solution for Pe = 50. Also, in the part (1) plot, show the exact solution for Pe = 18. Discuss how the exact solution for Pe = 18 compares with the upwinded numerical solution.
4. Repeat parts (1) through (3) with 41 nodes.
5. Try out non-uniform grids and higher order schemes and compare your results with the exact solution.

Solution :

Analytical Solution -

$$\frac{d}{dx}(\rho u \phi) = \frac{d}{dx}\left(\Gamma \frac{d\phi}{dx}\right)$$

Given ρ, u and Γ to be constant, hence independent of x. We have

$$\rho u \frac{d\phi}{dx} = \Gamma \frac{d^2\phi}{dx^2}$$

Integrating on both sides

$$\rho u\, \phi(x) = \Gamma\, \frac{d\phi}{dx} + c_1$$

$$\therefore \frac{\rho u}{\Gamma}\, \phi(x) = \frac{d\phi}{dx} + \frac{c_1}{\Gamma}$$

The above equation is a linear differential equation, multiplying with Integrating factor $e^{\int -\frac{\rho u}{\Gamma} dx} = e^{-\frac{\rho u x}{\Gamma}}$

$$e^{-\frac{\rho u x}{\Gamma}}\, \frac{d\phi}{dx} - e^{-\frac{\rho u x}{\Gamma}} \frac{\rho u}{\Gamma}\, \phi(x) = \frac{-c_1}{\Gamma} e^{-\frac{\rho u x}{\Gamma}}$$

$$\therefore \frac{d\left(\phi e^{-\frac{\rho u x}{\Gamma}}\right)}{dx} = \frac{-c_1}{\Gamma} e^{-\frac{\rho u x}{\Gamma}}$$

Integrating on both sides with x

$$\therefore\ \phi(x)e^{-\frac{\rho u x}{\Gamma}} = \frac{c_1}{\rho u}e^{-\frac{\rho u x}{\Gamma}} + c_2$$

$$\phi(x)e^{-\frac{\rho u x}{\Gamma}} = c_1' e^{-\frac{\rho u x}{\Gamma}} + c_2$$

$$\phi(x) = c_1' + c_2 e^{\frac{Pe\,x}{\mathrm{L}}}$$

At $x = 0,\ \phi = \phi_o$ $\qquad \phi_o = c_1' + c_2$

At $x = L\ \phi{=}\phi_L$ $\qquad \phi_L{=}c_1' + c_2 e^{Pe}$

$c_2 = \frac{(\phi_L - \phi_o)}{e^{Pe}-1}$ and $c_1' = \phi_O - \frac{(\phi_L-\phi_o)}{e^{Pe}-1}$

Substituting c_2 and c_1' and $Pe = \rho u L/\Gamma$

$$\phi(x) = \phi_O - \frac{(\phi_L - \phi_o)}{e^{Pe} - 1} + \frac{(\phi_L - \phi_o)}{e^{Pe} - 1} e^{\frac{Pe\,x}{\mathrm{L}}}$$

Therefore we get the exact analytical solution as -

$$\frac{\phi - \phi_o}{\phi_L - \phi_o} = \frac{\exp(Pe\,x/L) - 1}{\exp(Pe) - 1}$$

Taylor Series expansion of $\boldsymbol{\phi}$

To obtain the approximations for the first and second order derivatives we use Tayler series expansion

$$\phi(x) = \phi(x_i) + \frac{(x - x_i)}{1!}\left(\frac{\partial \phi}{\partial x}\right)_i + \frac{(x - x_i)^2}{2!}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i + \frac{(x - x_i)^3}{3!}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_i + \cdots + \frac{(x - x_i)^n}{n!}\left(\frac{\partial^n \phi}{\partial x^n}\right)_i + H$$

Substituting x by x_{i-1} in above equation –

$$\phi(x_{i-1}) = \phi(x_i) + \frac{(x_{i-1} - x_i)}{1!}\left(\frac{\partial \phi}{\partial x}\right)_i + \frac{(x - x_i)^2}{2!}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i + H$$

Neglecting terms higher than 2nd order derivative we get –

$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{\phi(x_i) - \phi(x_{i-1})}{(x_i - x_{i-1})} - \frac{x - x_i}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i$$

Assuming uniform grids $x_i - x_{i-1} = \Delta x$. We get the approximation of the first order derivative by the upwind difference scheme

$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{\phi(x_i) - \phi(x_{i-1})}{(x_i - x_{i-1})} + O(\Delta x)$$

Approximating Taylor series at both ϕ_{i+1} and ϕ_{i-1} we get –

$$\phi_i = \phi_{i-1} + \frac{(x_{i-1} - x_i)}{1!}\left(\frac{\partial\phi}{\partial x}\right)_i + \frac{(x_{i-1} - x_i)^2}{2!}\left(\frac{\partial^2\phi}{\partial x^2}\right)_i$$

$$\phi_i = \phi_{i+1} + \frac{(x_{i+1} - x_i)}{1!}\left(\frac{\partial\phi}{\partial x}\right)_i + \frac{(x_{i+1} - x_i)^2}{2!}\left(\frac{\partial^2\phi}{\partial x^2}\right)_i$$

Combining both the above equations for a uniform grid we get –

$$\left(\frac{\partial\phi}{\partial x}\right)_i = \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}}$$

Polynomial fitting

For deriving a 2nd order approximation of the second order derivative $\left(\frac{\partial^2\phi}{\partial x^2}\right)$, let $\phi(x)$ be a polynomial of degree 2.

$$\phi(x) = a_o + a_1 x + a_2 x^2$$

Consider three grid points $i-1$, i and $i+1$. Let x_i=0 be at the origin. $\therefore$ $x_{i-1} = -\Delta x$ and x_{i+1}=Δx. Assuming x is increasing with i and grid is uniform.

$\phi(x_i) = a_o$, $\phi(x_{i-1}) = a_o - a_1\Delta x + a_2\Delta x^2$ and $\phi(x_{i+1}) = a_o + a_1\Delta x + a_2\Delta x^2$

$\therefore \phi_i = a_o$ and $\Delta x^2 a_2 - \Delta x\, a_1 = \phi_{i-1} - \phi_i$ $a_2\Delta x^2 + a_1\Delta x = \phi_{i+1} - \phi_i$

On solving for a_2 and a_1 we get

$a_2 = \frac{\phi_{i+1}+\phi_{i-1}-2\phi_i}{2\Delta x^2}$ and $a_1 = \frac{\phi_{i+1}-\phi_{i-1}}{2\Delta x}$

$$\therefore \phi(x) = \phi_i + \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}x + \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{2\Delta x^2}x^2$$

On differentiating once we get CDS expression

$$\left(\frac{d\phi}{dx}\right) = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} = \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}}$$

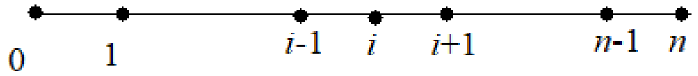
On differentiating twice we get CDS expression for second derivative

$$\left(\frac{d^2\phi}{dx^2}\right) = \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{\Delta x^2}$$

1. Uniform grid with UDS in convection

Uniform grid N=11 nodes, with upwind difference scheme in convective term and CDS in diffusive term

The uniform grid will have equal spacing between the grid points. The grid can be visualized as shown below –



Approximating convective term by upwind (backward)

$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}$$

CDS for diffusion term –

$$\left(\frac{d^2\phi}{dx^2}\right)_i = \frac{d}{dx}\left(\frac{d\phi}{dx}\right) = \frac{\left(\frac{d\phi}{dx}\right)_{i+\frac{1}{2}} - \left(\frac{d\phi}{dx}\right)_{i-\frac{1}{2}}}{x_{i+1/2} - x_{i-1/2}}$$

Approximating the first derivative $\left(\frac{d\phi}{dx}\right)_{i+\frac{1}{2}}$ and $\left(\frac{d\phi}{dx}\right)_{i-\frac{1}{2}}$ by a CDS scheme –

$\left(\frac{d\phi}{dx}\right)_{i+\frac{1}{2}} = \frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i}$ and $\left(\frac{d\phi}{dx}\right)_{i-\frac{1}{2}} = \frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}$

Since the grid is uniform. $\therefore \Delta x = x_i - x_{i-1} = x_{i+1} - x_i = x_{i+1/2} - x_{i-1/2}$

Substituting expression for $\left(\frac{d\phi}{dx}\right)_{i+\frac{1}{2}}$, $\left(\frac{d\phi}{dx}\right)_{i-\frac{1}{2}}$ and Δx in equation – **1**

$$\left(\frac{d^2\phi}{dx^2}\right)_i = \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{\Delta x^2}$$

Substituting the second and first order derivative approximations –

$$\rho u \frac{\phi_i - \phi_{i-1}}{\Delta x} = \Gamma \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{\Delta x^2}$$

$$\therefore \Gamma\, \phi_{i+1} + (\Gamma + \rho u \Delta x)\phi_{i-1} - (\rho u \Delta x + 2\Gamma)\phi_i = 0 \qquad (\mathbf{1})$$

Equation- (1) is the final form of the discretized equation using upwind (backward) difference scheme for convective term and central difference scheme for the advective term.

Using the notation of A_P to denote the principle diagonal, A_E (east of A_P) upper diagonal of the principle diagonal and A_W (west of A_P) as the lower diagonal from the principle diagonal.

$$\therefore A_P^i \phi_i + A_E^i \phi_{i+1} + A_W^i \phi_{i-1} = 0$$

Where $A_P^i = -(\rho u \Delta x + 2\Gamma)$; $A_E^i = \Gamma$ and $A_W^i = (\Gamma + \rho u \Delta x)$

At the first interior node (i.e $i = 2$) $\phi_1 = \phi(x = 0)$ (boundary condition) is known.

$\therefore A_P^i \phi_i + A_E^i \phi_{i+1} = -(\Gamma + \rho u \Delta x)\phi_1$

Similarly at the last interior node –

$\therefore A_P^i \phi_i + A_W^i \phi_{i-1} = -\Gamma \phi_L$

In terms on Matrix notation –

$$\boldsymbol{A}\,\boldsymbol{\Phi} = \boldsymbol{B}$$

$$\text{where } A = \begin{bmatrix} A_P^1 & A_E^1 & 0 & 0 & 0 \\ A_W^2 & A_P^2 & A_E^2 & 0 & 0 \\ 0 & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & A_E^{10} \\ 0 & . & . & A_W^{11} & A_P^{11} \end{bmatrix}, \quad \Phi = \begin{bmatrix} \phi_1 \\ \phi_2 \\ : \\ 0 \\ \phi_{11} \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} -(\Gamma + \rho u \Delta x)\phi_1 \\ 0 \\ : \\ 0 \\ -\Gamma \phi_L \end{bmatrix}$$

2. Uniform grid with CDS in convection

Uniform grid N=11 nodes, with CDS in convective term and CDS in diffusive term as well.

The arrangement for the grid points will be the same as in part-1. CDS for the convective term as well. The derivative can be approximated as -

$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}}$$

Since the grid is uniform , $x_{i+1} - x_{i-1} = (x_{i+1} - x_i) + (x_i - x_{i-1}) = 2\Delta x$

Substituting the approximations for the convective and the diffusive terms

$$\rho u \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} = \Gamma \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{\Delta x^2}$$

$$\therefore \rho u \Delta x(\phi_{i+1} - \phi_{i-1}) = 2\Gamma(\phi_{i+1} + \phi_{i-1} - 2\phi_i)$$

$$\therefore -(\rho u \Delta x + 2\Gamma)\phi_{i-1} + 4\Gamma\phi_i + (\rho u \Delta x - 2\Gamma)\phi_{i+1} = 0 \qquad (\mathbf{2})$$

Equation- (2) is the final form of the discretized equation using central difference scheme for convective term and central difference scheme for the advective term.

$$\therefore A_P^i \phi_i + A_E^i \phi_{i+1} + A_W^i \phi_{i-1} = 0$$

where $A_P^i = 4\Gamma$; $\quad A_E^i = (\rho u \Delta x - 2\Gamma)$ $\quad$ and $\quad A_W^i = -(\rho u \Delta x + 2\Gamma)$

At the first interior node (i.e $i = 2$) $\phi_1 = \phi(x = 0)$ (boundary condition) is known.

$\therefore A_P^i \phi_i + A_E^i \phi_{i+1} = (\rho u \Delta x + 2\Gamma)\phi_1$

Similarly at the last interior node, ($\phi(x = L)$ =1) boundary condition

$\therefore A_P^i \phi_i + A_W^i \phi_{i-1} = -(\rho u \Delta x - 2\Gamma)\phi_L$

In terms on Matrix notation –

$$\boldsymbol{A\ \Phi = B}$$

$$\text{where } A = \begin{bmatrix} A_P^1 & A_E^1 & 0 & 0 & 0 \\ A_W^2 & A_P^2 & A_E^2 & 0 & 0 \\ 0 & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & A_E^{10} \\ 0 & . & . & A_W^{11} & A_P^{11} \end{bmatrix}, \Phi = \begin{bmatrix} \phi_1 \\ \phi_2 \\ : \\ 0 \\ \phi_{11} \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} (\rho u \Delta x + 2\Gamma)\phi_1 \\ 0 \\ : \\ 0 \\ -(\rho u \Delta x - 2\Gamma)\phi_L \end{bmatrix}$$

3. Plot of $\boldsymbol{\phi}$ vs. $\boldsymbol{x}$

3.1 Plot for part-1

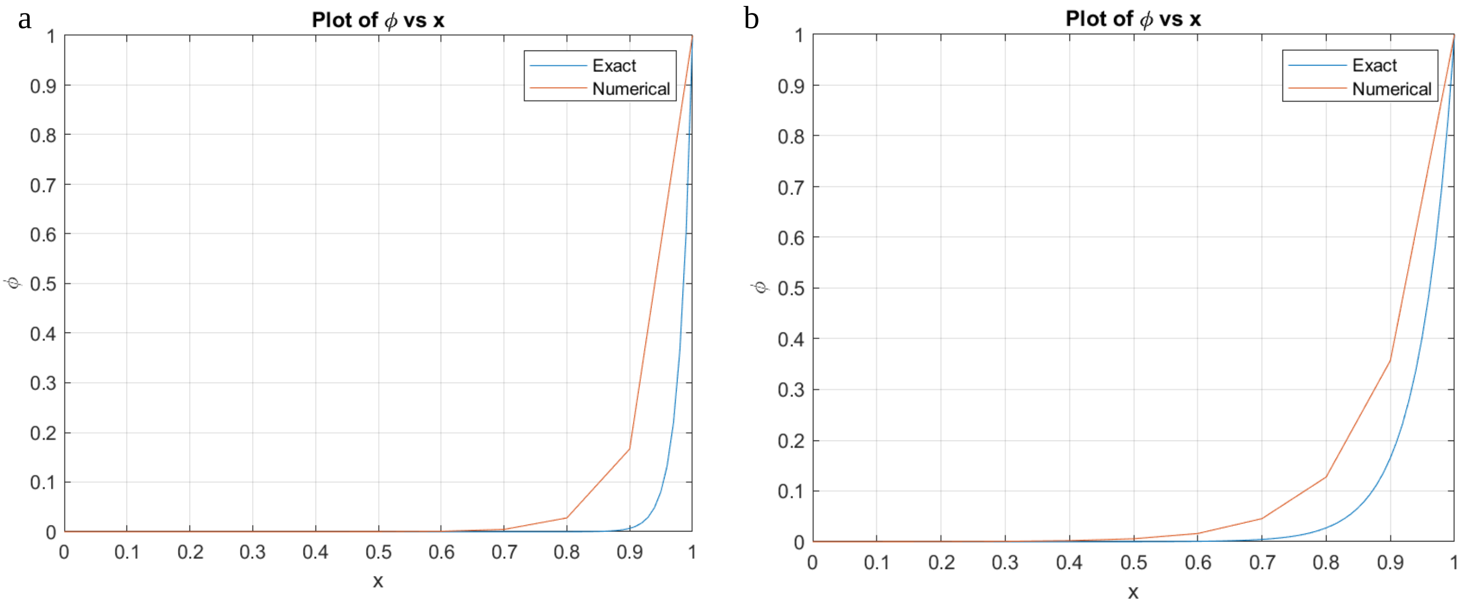


Figure 1 Plot of ϕ vs. x computed using **11 uniform nodes** (a) with upwind (backward) scheme in convective term, with **Pe=50** (b) with upwind (backward) scheme in convective term, with **Pe=18**

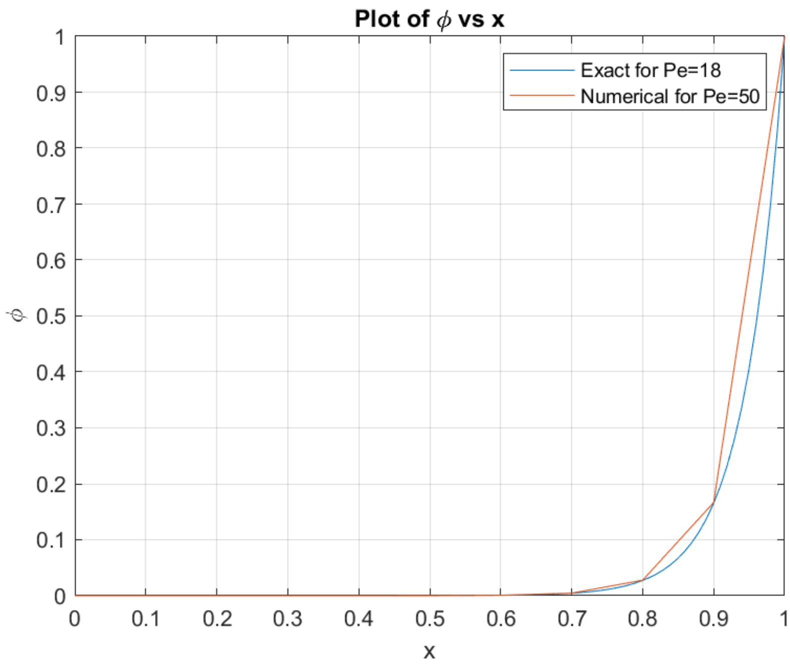


Figure 2 Plot of ϕ vs. x computed using **11 uniform nodes** upwind (backward) scheme in convective term. Exact solution for $Pe = 18$ with numerical solution for $Pe = 50$

3.1.1 Discussion

From the Figure-1 it can be observed that for both the values of Pe=50 and 18 the numerically calculated solution is showing high error beyond $x = 0.6$ or 0.7. This is because the ϕ undergoes a sudden change in derivative as x is increased. Also with the increase in Pe

it can be seen that ϕ is changing more rapidly for higher x. The Peclet number (Pe) is a ratio of convection ($\rho u L$) and diffusion (Γ diffusivity). Therefore, by reducing Pe we get more diffusion dominated solution. Due to this there is less error for Pe=18 compared to Pe=50.

From Figure-2 it can be seen that the numerical solution for $Pe = 50$ (part-1) is matching very closely to the exact solution with Pe=18. In other words the numerical solution for $Pe = 50$ corrosponds to the exact solution of Pe=18. A lesser value of Pe indicates a diffusion dominated solution. Therefore, it can be said that the upwind (backward) difference scheme (UDS) produces a solution which is having excess diffusion. Thus, the first order UDS is giving over-diffusive solution.

3.2 Plot for part-2

The numerical solution by using CDS in diffusive term is shown in Figure-3.

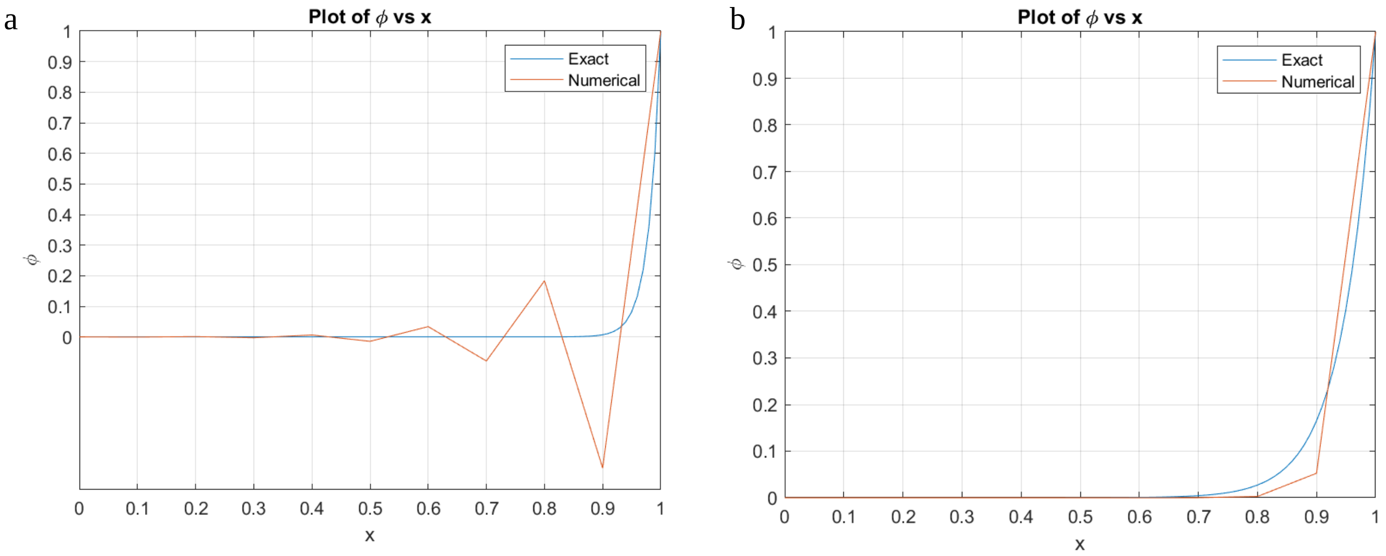


Figure 3 Plot of ϕ vs. x computed using **11 uniform nodes** with CDS scheme in convective term (a) **Pe=50** (b) **Pe=18**

3.2.1 Discussion

It can be observed that for Pe=50 the Central difference scheme in convective term is showing oscillatory nature. By decreasing Pe the oscillatory nature of solution is reduced to a certain extent. However, still the solution is slightly oscillatory as for x=0.7 to x=0.9 the numerical solution is less than analytical solution and after x=0.9 the numerical solution is higher than exact solution. The oscillatory solution in CDS can be attributed to the fact that CDS takes into account the differences from both sides equally. In most of the physical problem there is some sense of direction in which a particular quantality is flowing. CDS is unable to consider the direction of the flow.

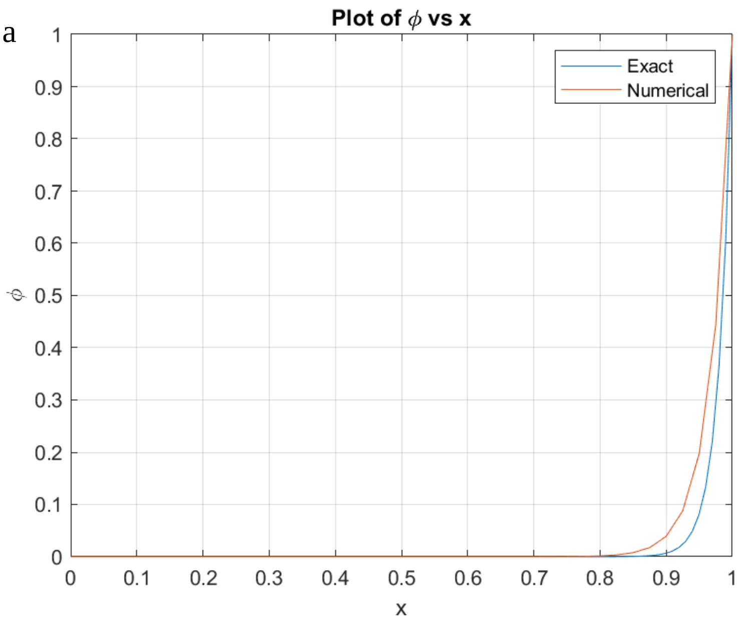
Assuming that the flow is from node $i - 1$ to i a backward difference scheme is used. Upwind difference scheme (UDS) is sometimes better than CDS, as it takes into account the direction of the quantity. Moreover, UDS considers the direction in which information is propagating. The upwind (backward) difference scheme is able to capture a sense of direction of the flow, however, it is giving over diffusive solution.

4. With 41 nodes

For uniform grid by increasing the number of grid points, the grid becomes more finer. However, the derivation of the discretized equations remains the same. The only thing that needs to be changed is the value of number of grid points in code Q1.m and Q2.m for part-1 and part-2 respectively. Both the codes were run for 41 uniform grid points with value of Pe=50 and 18. The plots showing ϕ calculated numerically with the analytical ϕ are shown as follows:

4.1 Using BDS in convective term

a



b

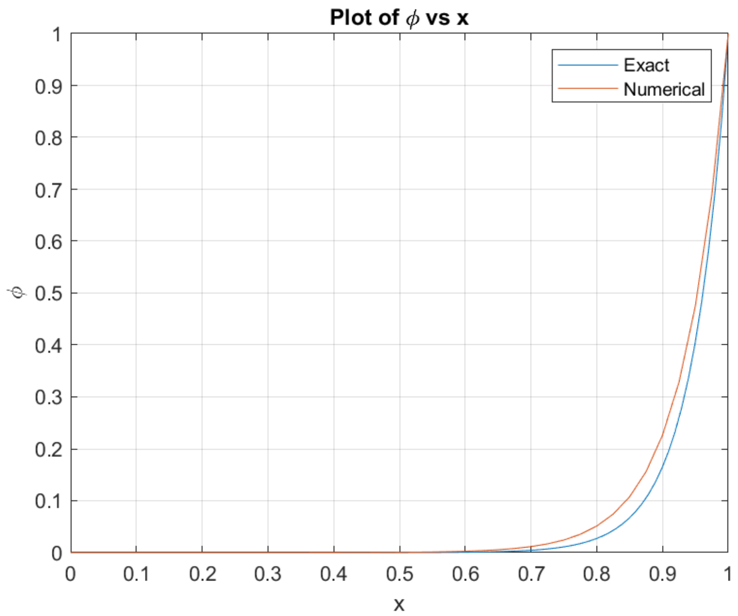


Figure 4 Plot of ϕ vs. x using upwind (backward) scheme in convection term and total **grid nodes=41** (a) For $\boldsymbol{Pe = 50}$ (b) For $\boldsymbol{Pe = 18}$

4.2 Using CDS in convective term

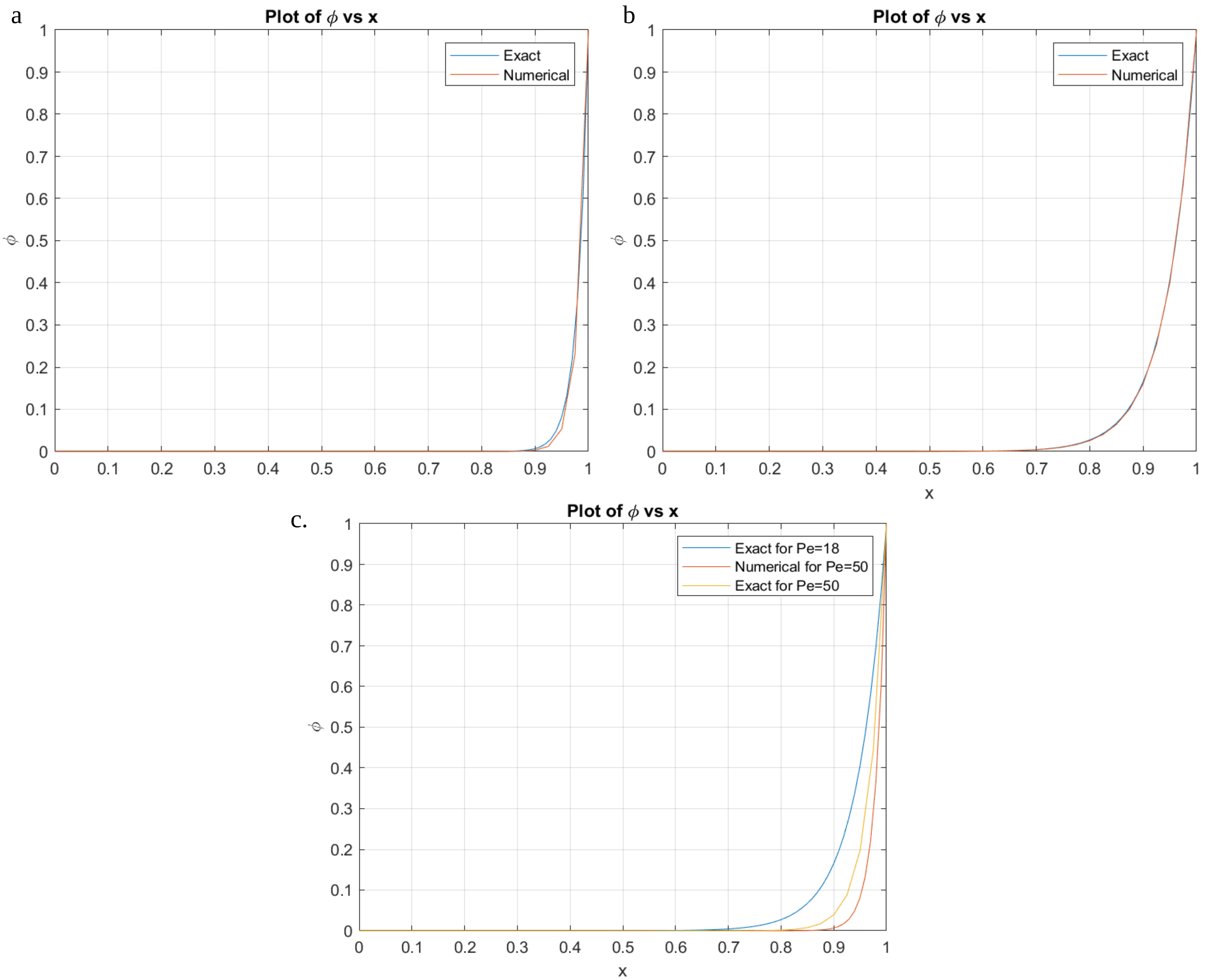


Figure 5 Plot of ϕ vs. x computed using CDS in convection term and total **grid nodes=41** (a) For $\mathbf{Pe} = \mathbf{50}$ (b) For $\mathbf{Pe} = \mathbf{18}$ (c) Plot numerical $Pe = 50$ with UDS in convection and exact for Pe=50 and 18

From Figure-5c it can be seen that by refining the grid to 41 points the numerical solution for Pe=18. not matching the exact solution of Pe=18 which was the case for 11 node points. In fact, the numerical solution is more close to the exact solution of Pe=50.

4.3 Discussion

From Figure-4 it can be seen that by increasing the number of node points the error in the upwind difference scheme has reduced. Though the numerical solution is still over-diffusive but the extent of over-diffusiveness is reduced. By making the grid finer more points are taken which reduces the error to some extent. However, the numerical solution still have error in regions where there is sharpen increase in derivative of ϕ (for larger x>0.7). From Figure-5, by refining the grid for CDS in convective term the solution is oscillation free. Therefore refining the grid helps to reduce the error and increases the accuracy of numerical solution.

5 Non-uniform and higher order scheme

5.1 Non-uniform grids

Truncation error depends not only on the grid spacing but also on the value of the derivative. Therefore, in uniform grid if the value of derivative is high the error would rise. In that situation using a non-uniform grid would be advantageous.

From the plot of ϕ vs. x from previous sections it can be observed that the value of slope remains approximately zero until x=0.7 or 0.8. After that there is a sudden increase in ϕ and its slope. Therefore using coarse grids near x=0 and finer grids near x=1 will help to reduce the error. Let Δx_{max} be the largest spacing between the two grid points, and r be the expansion factor. In total there are N non-uniform grid points. The summation of all the Δx_i s should be equal to L. Let Δx_1=Δx_{max}

$$\Delta x_1 + \Delta x_1 r + \Delta x_1 r^2 + \; \ldots . + \Delta x_1 r^{N-1} = L = 1$$

$$\Delta x_1 \frac{r^N - 1}{r - 1} = 1$$

Since the grid is contracting r<1. Let us choose $r = 0.7$ arbitrarily and N=10 for 11 grid points. Therefore Δx_1 can be computed from the above equation. For $r = 0.7$ we get Δx_1=0.306

5.1.1 Using FDS to discretize the diffusion term

Let the second derivative of the diffusive term be expanded using a FDS (Forward difference scheme). For the inner derivatives, a BDS (backward difference scheme) is used -

$$\left(\frac{d^2\phi}{dx^2}\right)_i = \frac{d}{dx}\left(\frac{d\phi}{dx}\right) = \frac{\left(\frac{d\phi}{dx}\right)_{i+1} - \left(\frac{d\phi}{dx}\right)_i}{x_{i+1} - x_i}$$

$$\left(\frac{d^2\phi}{dx^2}\right)_i = \frac{\frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} - \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}}{x_{i+1} - x_i}$$

$$\left(\frac{d^2\phi}{dx^2}\right)_i = \frac{\phi_{i+1}(x_i - x_{i-1}) + \phi_{i-1}(x_{i+1} - x_i) - \phi_i(x_{i+1} - x_{i-1})}{(x_{i+1} - x_i)^2(x_i - x_{i-1})}$$

Approximating the convective term using a BDS

$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}$$

Therefore the final discretized equation can be represented as

$$\therefore A_P^i \phi_i + A_E^i \phi_{i+1} + A_W^i \phi_{i-1} = 0$$

$A_P^i = \frac{\rho u}{x_i - x_{i-1}} + \frac{\Gamma(x_{i+1} - x_{i-1})}{(x_{i+1} - x_i)^2 (x_i - x_{i-1})}$ $\qquad$ $A_E^i = -\frac{\Gamma\,(x_i - x_{i-1})}{(x_{i+1} - x_i)^2 (x_i - x_{i-1})}$

$A_W^i = -\frac{\rho u}{x_i - x_{i-1}} - \frac{\Gamma(x_{i+1} - x_i)}{(x_{i+1} - x_i)^2 (x_i - x_{i-1})}$

MATLAB code Q5_non_uniform.m was used to solve using non-uniform grid.

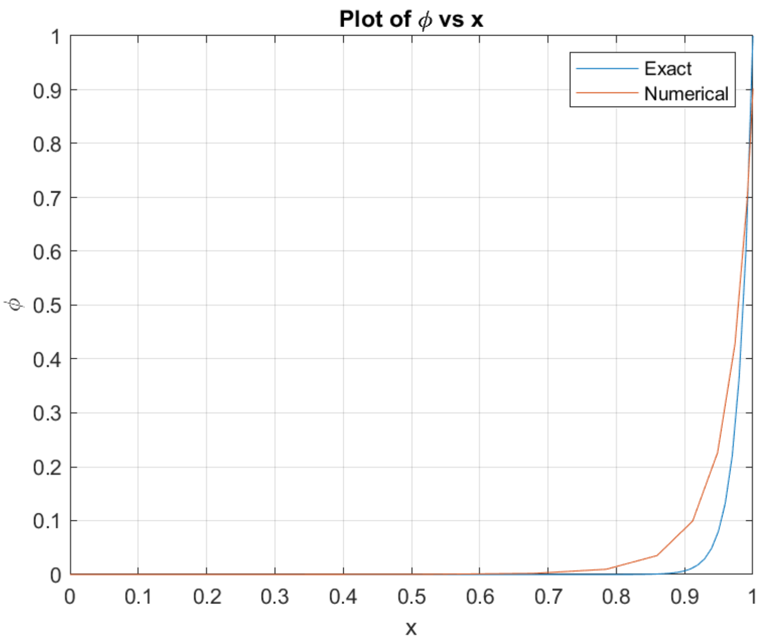


Figure 6 Plot of ϕ vs. x computed using **11 non-uniform nodes** with upwind (backward) scheme in convective term and FDS in diffusive term, with $\mathbf{Pe = 50}$

5.1.2 Using CDS to discretize the diffusion term

Applying a Central Difference scheme for the diffusive terms and also for the first order derivatives occurring in it.

$$\left(\frac{d^2\phi}{dx^2}\right)_i = \frac{d}{dx}\left(\frac{d\phi}{dx}\right) \approx \frac{\left(\frac{d\phi}{dx}\right)_{i+\frac{1}{2}} - \left(\frac{d\phi}{dx}\right)_{i-\frac{1}{2}}}{\frac{1}{2}(x_{i+1} - x_{i-1})} = \frac{\frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} - \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}}{\frac{1}{2}(x_{i+1} - x_{i-1})}$$

$$\left(\frac{d^2\phi}{dx^2}\right)_i \approx \frac{\phi_{i+1}(x_i - x_{i-1}) + \phi_{i-1}(x_{i+1} - x_i) - \phi_i(x_{i+1} - x_{i-1})}{\frac{1}{2}(x_{i+1} - x_{i-1})(x_{i+1} - x_i)(x_i - x_{i-1})}$$

Approximating the convective term using a BDS

$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}$$

Therefore the final discretized equation can be represented as

$$\therefore A_P^i \phi_i + A_E^i \phi_{i+1} + A_W^i \phi_{i-1} = 0$$

$$A_P^i = \frac{\rho u}{x_i - x_{i-1}} + \frac{\Gamma(x_{i+1} - x_{i-1})}{\frac{1}{2}(x_{i+1} - x_{i-1})(x_{i+1} - x_i)(x_i - x_{i-1})} \qquad A_E^i = -\frac{\Gamma\,(x_i - x_{i-1})}{\frac{1}{2}(x_{i+1} - x_{i-1})(x_{i+1} - x_i)(x_i - x_{i-1})}$$

$$A_W^i = -\frac{\rho u}{x_i - x_{i-1}} - \frac{\Gamma(x_{i+1} - x_i)}{(x_{i+1} - x_i)^2 (x_i - x_{i-1})}$$

The same MATLAB program i.e. Q5_non_uniform.m can be used to generate the plot shown below :

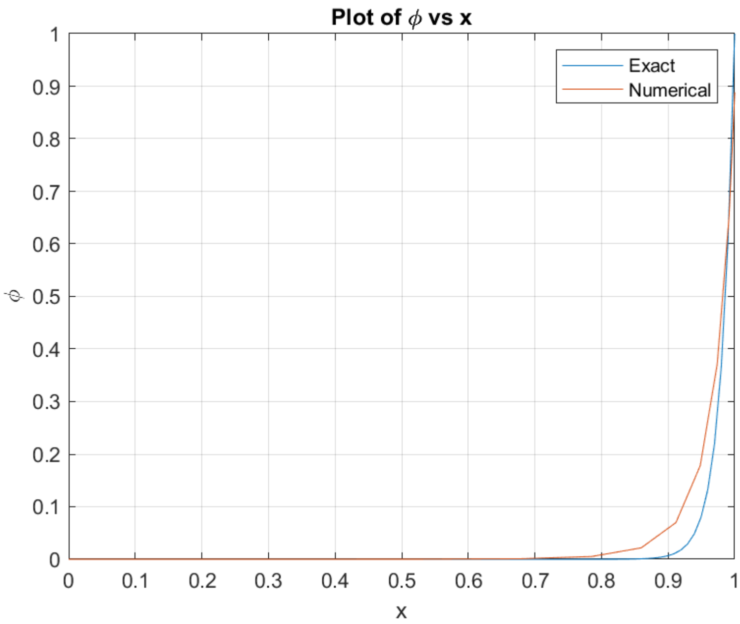


Figure 7 Plot of ϕ vs. x computed using **11 non-uniform nodes** with upwind (backward) scheme in convective term and CDS in diffusive term, with $\mathbf{Pe = 50}$

5.2 Higher Order Schemes

5.2.1 Using a fourth order polynomial for diffusive term

The second order diffusion term can be discretized by using a higher order central difference scheme. The second order derivative can be obtained by deriving a polynomial of degree four using five points i.e. ϕ_{i-2}, ϕ_{i-1}, ϕ_i, ϕ_{i+1} and ϕ_{i+2} over a uniform grid. Using a 4th order polynomial to get ϕ

$$\phi_x = a_o + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4$$

The coefficients a_o, a_1, a_2, a_3 and a_4 can be obtained by substituting ϕ_{i-2}, ϕ_{i-1}, ϕ_{i+1} and ϕ_{i+2} into the polynomial expression.

$$\left(\frac{d^2\phi}{dx^2}\right)_i = \frac{-\phi_{i+2} + 16\phi_{i+1} - 30\phi_i + 16\phi_{i-1} - \phi_{i-2}}{12(\Delta x)^2}$$

Approximating the convective term using a upwind backward (BDS)

$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} = \frac{\phi_i - \phi_{i-1}}{\Delta x}$$

Substituting into the 1D convective diffusion equation -

$$\rho u \frac{\phi_i - \phi_{i-1}}{\Delta x} = \Gamma \frac{-\phi_{i+2} + 16\phi_{i+1} - 30\phi_i + 16\phi_{i-1} - \phi_{i-2}}{12(\Delta x)^2}$$

$$\Gamma\phi_{i-2} - (12\rho u\Delta x + 16\Gamma)\phi_{i-1} + (12\rho u\Delta x + 30\Gamma)\phi_i - 16\Gamma\phi_{i+1} + \Gamma\phi_{i+2} = 0$$

However to use the above expression, the value of ϕ at the second and second last node is required. Therefore using a unwind backward difference scheme to approximate first order derivative and a CDS to approximate second order derivative. From the part-1 we have

$$\therefore \Gamma\, \phi_{i+1} + (\Gamma + \rho u\Delta x)\phi_{i-1} - (\rho u\Delta x + 2\Gamma)\phi_i = 0$$

The values of ϕ_2 and ϕ_{n-2} obtained in part-1 are used in this higher order scheme

From the expression we can evaluate ϕ_2 and ϕ_{n-1}. Note $\phi_1 = \phi(x = 0)$ and $\phi_n = \phi(x = L)$. The final Matrix will look like the following –

where $A =$

$$\begin{bmatrix}
-(\rho u\Delta x + 2\Gamma) & \Gamma & 0 & 0 & 0 & 0 & . & \\
-(12\rho u\Delta x + 16\Gamma) & (12\rho u\Delta x + 30\Gamma) & -16\Gamma & \Gamma & 0 & 0 & . & 0 \\
\Gamma & -(12\rho u\Delta x + 16\Gamma) & (12\rho u\Delta x + 30\Gamma) & -16\Gamma & \Gamma & 0 & . & 0 \\
0 & \Gamma & -(12\rho u\Delta x + 16\Gamma) & (12\rho u\Delta x + 30\Gamma) & -16\Gamma & \Gamma & . & . \\
0 & 0 & . & . & . & . & . & 0 \\
\vdots & . & . & . & . & . & . & 0 \\
\vdots & . & . & . & . & . & 0 & 0 \\
\vdots & 0 & . & . & \Gamma & -(12\rho u\Delta x + 16\Gamma) & (12\rho u\Delta x + 30\Gamma) & -16\Gamma \\
0 & 0 & 0 & 0 & 0 & 0 & (\Gamma + \rho u\Delta x) & -(\rho u\Delta x + 2\Gamma)
\end{bmatrix}$$

, $\Phi = \begin{bmatrix} \phi_2 \\ \phi_3 \\ \phi_4 \\ \vdots \\ \vdots \\ \phi_{n-2} \\ \phi_{n-1} \end{bmatrix}$ and $B = \begin{bmatrix} -(\Gamma + \rho u\Delta x)\phi_1 \\ -\Gamma\phi_1 \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \\ -\Gamma\phi_n \\ -\Gamma\phi_n \end{bmatrix}$

The MATLAB code Q5_higher_order.m is developed to solve the above matrix equation. The plot of ϕ vs. x for 11 uniform node points for Pe=50 and Pe=18 are shown in Figure--8

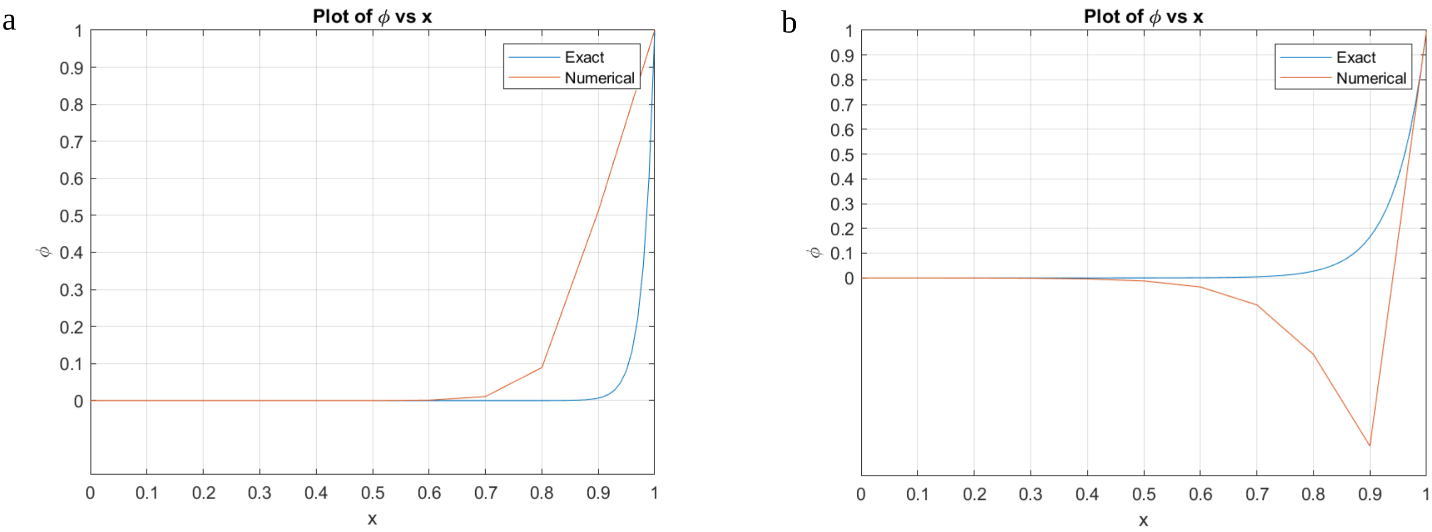


Figure 8 Plot of ϕ vs. x computed using **11 uniform nodes** with higher order scheme in diffusive term (a)For $\mathbf{Pe = 50}$ (b) For **Pe**-18

5.3 Discussion

From Figure-6 and Figure-7 it can be observe that using a non-uniform grid has reduced the error to some extent. The numerical solution is still having errors for larger x and also since an upwind scheme is used for discretizing the convective term the numerical solution is over-diffusive.

By using a higher order scheme for the diffusive term the results are showing very high deviation from actual value. Here a polynomial of degree-5 is used to approximate the second order derivative. Using 5 points might have produced more error because the second derivative is rapidly changing from x=0.7 to x=1.0. As a result the higher order scheme in diffusive term is showing large errors.

6. Conclusion

This project provided many valuable insights into the application of different approximation schemes, grid structure in solving a real world physical problem. For this particular problem the upwind difference scheme produced a over-diffusive solution, whereas the CDS produced an oscillatory solution for lesser grid points. On refining both the scheme their errors get reduced, however the grid need to be more finer (more than 41 points) for the upwind scheme solution to match the exact solution. The CDS solution is very close to the exact solution for 41 grid points.

A non-uniform grid with expansion factor of 0.7 and total 11 grid points, with upwind (backward) difference scheme and FDS and CDS scheme for the diffusion term was experimented. Though the error was reduced there was still a significant difference between the numerical solution and analytical solution. Therefore, using a non-uniform grid with small number of grid points does not provide significant accuracy in this problem. A higher order scheme produces more error because the total number of grid points are less and there is a large increase in derivatives for higher x.