ME 605

Computational Fluid Dynamics

Project 1

Numerical Solution to 1-D Steady Convection Diffusion Equation

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Problem Statement

We are given a 2nd Order ODE,

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

where, $x \in [0, L]$

Since, this is a 2nd order differential equation in x, we require 2 boundary equations to solve the ODE. The boundary equations given,

i. $\varphi(x = 0) = 0$
ii. $\varphi(x = L) = 1$

In the equation,

i. The first order derivative in x, $\frac{d}{dx}(\rho u\varphi)$, is the convective term
ii. The second order derivative in x, $\frac{d}{dx}\left(\Gamma\frac{d\varphi}{dx}\right)$, is the diffusion term

For constant ρ, u and Γ, we can rewrite the equation as

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

Define

$$x' = \frac{x}{L} \Rightarrow \frac{dx'}{dx} = \frac{1}{L}$$

Then the equation becomes,

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

$$\Rightarrow \frac{\rho u}{L}\frac{d\varphi}{dx'} = \frac{\Gamma}{L^2}\frac{d^2\varphi}{dx'^2} \Rightarrow Pe\cdot\frac{d\varphi}{dx'} = \frac{d^2\varphi}{dx'^2}$$

where, Pe is the Peclet number, defined by

$$Pe = \frac{\rho u L}{\Gamma}$$

In the present scenario, we are given

i. $L = 1$
ii. $\rho = 1$
iii. $u = 1$

Hence, $x' = x$, and, the equation becomes

$$Pe\cdot\frac{d\varphi}{dx} = \frac{d^2\varphi}{dx^2}$$

Analytical Solution

Solving the following 2nd Order ODE analytically,

$$Pe \cdot \frac{d\varphi}{dx} = \frac{d^2\varphi}{dx^2}$$

$$\Rightarrow \frac{d^2\varphi}{dx^2} + p\frac{d\varphi}{dx} = 0$$

where, $p = -Pe$

Therefore, the characteristic equation for this ODE, is

$$r^2 + pr = 0$$

$$\Rightarrow r \cdot (r + p) = 0$$

Hence, the two roots of the characteristic equation are,

$$r = 0, -p$$

Therefore, the general solution to the above ODE is

$$\varphi(x) = C_1 + C_2 \cdot \exp(Pe \cdot x)$$

where, C_1 and C_2 are arbitrary constants.

Applying the boundary conditions, we get

i. $\varphi(x = 0) = 0$ $\quad \therefore C_1 + C_2 = 0$

ii. $\varphi(x = 1) = 0$ $\quad \therefore C_1 + \exp(Pe) \cdot C_2 = 1$

Solving the system of linear equations for C_1 and C_2, we get

$$C_1 = \frac{-1}{\exp(Pe) - 1}$$

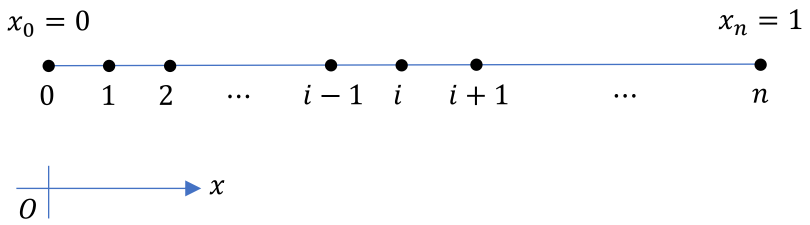
$$C_2 = \frac{1}{\exp(Pe) - 1}$$

Hence, the specific analytical solution to our 2nd Order ODE is

$$\varphi(x) = \frac{\exp(Pe \cdot x) - 1}{\exp(Pe) - 1}$$

Numerical Solution

Define $n+1$ grid points on the given interval $[0,1]$ for x



Define, $\forall\ i \in \{1, 2, \ldots n\}$

$$\Delta x_i = x_i - x_{i-1}$$

$$\varphi_i = \varphi(x = x_i)$$

$$\varphi_0 = \varphi(x = 0) = 0$$

For the discretized interval defined above, we can approximate

i. First derivative with respect to x, using upwind difference

We have, $u = 1 > 0$, the velocity is towards $+ve$ x-axis, hence we use backward difference

$$\frac{d\varphi}{dx}\Big|_{x=x_i} = \varphi_i' \approx \frac{\varphi_i - \varphi_{i-1}}{\Delta x_i}$$

The error in this approximation is of the order: Δx_i

ii. First derivative with respect to x, using central difference

$$\frac{d\varphi}{dx}\Big|_{x=x_i} = \varphi_i' \approx \frac{\varphi_{i+1} - \varphi_{i-1}}{\Delta x_{i+1} + \Delta x_i}$$

The error in this approximation is of the order: $\Delta x_{i+1} - \Delta x_i$

However, for $\Delta x_{i+1} = \Delta x_i = \Delta x$, the error is of the order: $(\Delta x)^2$

iii. Second derivative with respect to x, using central difference

$$\frac{d^2\varphi}{dx^2}\Big|_{x=x_i} = \varphi_i'' \approx 2 \cdot \frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{(\Delta x_{i+1})^2 + (\Delta x_i)^2} + 2 \cdot \varphi_i' \cdot \frac{\Delta x_{i+1} - \Delta x_i}{(\Delta x_{i+1})^2 + (\Delta x_i)^2}$$

The error in this approximation is of the order: $\frac{(\Delta x_{i+1})^3 - (\Delta x_i)^3}{(\Delta x_{i+1})^2 + (\Delta x_i)^2}$

However, for $\Delta x_{i+1} = \Delta x_i = \Delta x$, the error is of the order: $(\Delta x)^2$

Now, we apply the above discretization schemes to convert the given ODE to an algebraic equation

1. Using upwind scheme for the convection term and central difference scheme for the diffusion term –

   For the convection term, we have

   $$Pe \cdot \frac{d\varphi}{dx} \Big|_{x=x_i} = Pe \cdot \varphi_i' \approx Pe \cdot \frac{\varphi_i - \varphi_{i-1}}{\Delta x_i}$$

   For the diffusion term, we have

   $$\frac{d^2\varphi}{dx^2} \Big|_{x=x_i} = \varphi_i'' \approx 2 \cdot \frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{(\Delta x_{i+1})^2 + (\Delta x_i)^2} + 2 \cdot \varphi_i' \cdot \frac{\Delta x_{i+1} - \Delta x_i}{(\Delta x_{i+1})^2 + (\Delta x_i)^2}$$

   $$= 2 \cdot \frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{(\Delta x_{i+1})^2 + (\Delta x_i)^2} + 2 \cdot \frac{\varphi_i - \varphi_{i-1}}{\Delta x_i} \cdot \frac{\Delta x_{i+1} - \Delta x_i}{(\Delta x_{i+1})^2 + (\Delta x_i)^2}$$

   The differential equation becomes,

   $$2 \cdot \frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{(\Delta x_{i+1})^2 + (\Delta x_i)^2} + 2 \cdot \frac{\varphi_i - \varphi_{i-1}}{\Delta x_i} \cdot \frac{\Delta x_{i+1} - \Delta x_i}{(\Delta x_{i+1})^2 + (\Delta x_i)^2} = Pe \cdot \frac{\varphi_i - \varphi_{i-1}}{\Delta x_i}$$

   Define

   $$\delta_i = (\Delta x_{i+1})^2 + (\Delta x_i)^2$$

   $$\gamma_i = \Delta x_{i+1} - \Delta x_i$$

   Thus, rewriting the equation as

   $$\frac{2}{\delta_i} \cdot (\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}) + \frac{2\gamma_i}{\delta_i \Delta x_i} \cdot (\varphi_i - \varphi_{i-1}) = \frac{Pe}{\Delta x_i} \cdot (\varphi_i - \varphi_{i-1})$$

   $$\Rightarrow 2\Delta x_i \cdot \varphi_{i+1} + (2\gamma_i - 4\Delta x_i - Pe \cdot \delta_i) \cdot \varphi_i + (2\Delta x_i - 2\gamma_i + Pe \cdot \delta_i) \cdot \varphi_{i-1} = 0$$

   Again, define

   $$e_i = 2\Delta x_i - 2\gamma_i + Pe \cdot \delta_i$$

   $$f_i = 2\gamma_i - 4\Delta x_i - Pe \cdot \delta_i$$

   $$g_i = 2\Delta x_i$$

2. Using central differencing schemes for both convection and diffusion terms –

   For the convection term, we now have

   $$Pe \cdot \frac{d\varphi}{dx} \Big|_{x=x_i} = Pe \cdot \varphi_i' \approx Pe \cdot \frac{\varphi_{i+1} - \varphi_{i-1}}{\Delta x_{i+1} + \Delta x_i}$$

   For diffusion term, we have

$$\frac{d^2\varphi}{dx^2}\Big|_{x=x_i} = \varphi_i'' \approx 2\cdot\frac{\varphi_{i+1}-2\varphi_i+\varphi_{i-1}}{(\Delta x_{i+1})^2+(\Delta x_i)^2} + 2\cdot\varphi_i'\cdot\frac{\Delta x_{i+1}-\Delta x_i}{(\Delta x_{i+1})^2+(\Delta x_i)^2}$$
$$= 2\cdot\frac{\varphi_{i+1}-2\varphi_i+\varphi_{i-1}}{(\Delta x_{i+1})^2+(\Delta x_i)^2} + 2\cdot\frac{\varphi_{i+1}-\varphi_{i-1}}{\Delta x_{i+1}+\Delta x_i}\cdot\frac{\Delta x_{i+1}-\Delta x_i}{(\Delta x_{i+1})^2+(\Delta x_i)^2}$$

Hence, the differential equation is converted into an algebraic one –

$$2\cdot\frac{\varphi_{i+1}-2\varphi_i+\varphi_{i-1}}{(\Delta x_{i+1})^2+(\Delta x_i)^2} + 2\cdot\frac{\varphi_{i+1}-\varphi_{i-1}}{\Delta x_{i+1}+\Delta x_i}\cdot\frac{\Delta x_{i+1}-\Delta x_i}{(\Delta x_{i+1})^2+(\Delta x_i)^2} = Pe\cdot\frac{\varphi_{i+1}-\varphi_{i-1}}{\Delta x_{i+1}+\Delta x_i}$$

Define

$$\delta_i = (\Delta x_{i+1})^2 + (\Delta x_i)^2$$
$$\gamma_i = \Delta x_{i+1} - \Delta x_i$$
$$\lambda_i = \Delta x_{i+1} + \Delta x_i$$

Thus, rewriting the equation as

$$\frac{2}{\delta_i}\cdot(\varphi_{i+1}-2\varphi_i+\varphi_{i-1}) + \frac{2\gamma_i}{\delta_i\lambda_i}\cdot(\varphi_{i+1}-\varphi_{i-1}) = \frac{Pe}{\lambda_i}\cdot(\varphi_{i+1}-\varphi_{i-1})$$
$$\Rightarrow (2\lambda_i + 2\gamma_i - Pe\cdot\delta_i)\cdot\varphi_{i+1} - 4\lambda_i\cdot\varphi_i + (2\lambda_i - 2\gamma_i + Pe\cdot\delta_i)\cdot\varphi_{i-1} = 0$$

Again, define

$$e_i = 2\lambda_i - 2\gamma_i + Pe\cdot\delta_i$$
$$f_i = -4\lambda_i$$
$$g_i = 2\lambda_i + 2\gamma_i - Pe\cdot\delta_i$$

In both cases, we finally arrive at a system of linear equations,

$$g_i\cdot\varphi_{i+1} + f_i\cdot\varphi_i + e_i\cdot\varphi_{i-1} = 0$$
$$\forall\ i \in \{1, 2, \dots n-1\}$$

Also, for $i = 1$

$$g_1\cdot\varphi_2 + f_1\cdot\varphi_1 = -e_1\cdot\varphi_0$$

And, for $i = n-1$

$$f_{n-1}\cdot\varphi_{n-1} + e_{n-1}\cdot\varphi_{n-2} = -g_{n-1}\cdot\varphi_n$$

Representing the system of $n-1$ linear equations in matrix form

$$A = \begin{pmatrix} f_1 & g_1 & 0 & & & 0 & 0 & 0 \\ e_2 & f_2 & g_2 & \cdots & & 0 & 0 & 0 \\ 0 & e_3 & f_3 & & & 0 & 0 & 0 \\ & \vdots & & \ddots & & & \vdots & \\ 0 & 0 & 0 & & f_{n-3} & g_{n-3} & 0 & \\ 0 & 0 & 0 & \cdots & e_{n-2} & f_{n-2} & g_{n-2} & \\ 0 & 0 & 0 & & 0 & e_{n-1} & f_{n-1} & \end{pmatrix} b = \begin{pmatrix} -e_1\cdot\varphi_0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ -g_{n-1}\cdot\varphi_n \end{pmatrix} \phi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \vdots \\ \varphi_{n-3} \\ \varphi_{n-2} \\ \varphi_{n-1} \end{pmatrix}$$

Thus, we need to solve the matrix equation,

$$A \cdot \phi = b$$

Since, A is a banded matrix, we can use Thomas' algorithm to find the solution in the order of n iterations.

Tridiagonal Matrix Algorithm or Thomas' Algorithm

Given a matrix equation, $A \cdot x = b$, with a banded matrix, $A_{m \times m}$, we can find the solution in order of m time, using the following algorithm –

1. Define

$$e_i = a_{i,i-1} \quad , \forall\ i \in \{2,3,4 \dots m\}$$
$$f_i = a_{i,i} \quad , \forall\ i \in \{1,2,3 \dots m\}$$
$$g_i = a_{i,i+1} \quad , \forall\ i \in \{1,2,3 \dots m-1\}$$

   where $a_{i,j}$ is the element at ith row and jth column of A.

2. Build upper, $U_{m \times m}$, and lower, $L_{m \times m}$, triangular matrices, such that $A = L \cdot U$
    a. $u_{1,1} = f_1, \qquad u_{1,2} = g_1$
    b. $l_{1,1} = 1$
    c. $For\ i \leftarrow 2\ to\ m$
        i. $u_{i,i} = f_i - g_{i-1} \cdot {e_i}/{u_{i-1,i-1}}$
        ii. $u_{i,i+1} = g_i$
        iii. $l_{i,i} = 1$
        iv. $l_{i,i-1} = {e_i}/{u_{i-1,i-1}}$
3. Solve the matrix equation $L \cdot d = b$
    a. $d_1 = {b_1}/{l_{1,1}}$
    b. $For\ i \leftarrow 2\ to\ m$
        i. $d_i = {b_i - d_{i-1} \cdot l_{i,i-1}}/{l_{i,i}}$
4. Solve the matrix equation $U \cdot x = d$
    a. $x_m = {d_m}/{u_{m,m}}$
    b. $For\ i \leftarrow m-1\ to\ 1, step = -1$
        i. $x_i = {d_i - x_{i+1} \cdot u_{i,i+1}}/{u_{i,i}}$

1. Numerical solution using Upwind Difference for Convective Term and Central Difference for Diffusive Term

Using, $Pe = 50$ and $n = 10$ and uniform grid for the general numerical method derived previously, we have

$$\Delta x_i = \Delta x = \frac{1}{n}$$
$$\delta_i = \delta = 2 \cdot (\Delta x)^2$$
$$\gamma_i = 0$$
$$\forall\ i \in \{1,2 \dots\ 10\}$$

And hence

$$e_i = e = 2 \cdot \Delta x + Pe \cdot \delta$$
$$f_i = f = -4 \cdot \Delta x - Pe \cdot \delta$$
$$g_i = g = 2 \cdot \Delta x$$
$$\forall\ i \in \{0,1,2 \dots\ 10\}$$

The numerical solution is computed using the script P1_Q1_18110166.py.

i	x_i	φ_i	φ_i'	φ_i''
0	0.0	0.00E+00	-	-
1	0.1	8.27E-08	8.27E-07	4.13E-05
2	0.2	5.79E-07	4.96E-06	2.48E-04
3	0.3	3.56E-06	2.98E-05	1.49E-03
4	0.4	2.14E-05	1.79E-04	8.93E-03
5	0.5	1.29E-04	1.07E-03	5.36E-02
6	0.6	7.72E-04	6.43E-03	3.22E-01
7	0.7	4.63E-03	3.86E-02	1.93E+00
8	0.8	2.78E-02	2.31E-01	1.16E+01
9	0.9	1.67E-01	1.39E+00	6.94E+01
10	1.0	1.00E+00	8.33E+00	-

Table 1: Numerical Solution using upwind and central difference for convection and diffusion term respectively.

2. Numerical solution using Central Difference for both Convective and Diffusion terms

Using $Pe = 50$ and $n = 10$, and uniform grid for the general numeric method derived previously, we have

$$\Delta x_i = \Delta x = \frac{1}{n}$$
$$\delta_i = \delta = 2 \cdot (\Delta x)^2$$
$$\gamma_i = 0$$
$$\lambda_i = \lambda = 2 \cdot \Delta x$$
$$\forall\, i \in \{1,2 \ldots\ 10\}$$

And hence,

$$e_i = e = 2 \cdot \lambda + Pe \cdot \delta$$
$$f_i = f = -4 \cdot \lambda$$
$$g_i = g = 2 \cdot \lambda - Pe \cdot \delta$$
$$\forall\, i \in \{0,1,2 \ldots\ 10\}$$

The numerical solution is computed using the script P1_Q2_18110166.py.

i	x_i	φ_i	φ_i'	φ_i''
0	0.0	0.00E+00	-	-
1	0.1	3.89E-02	4.65E-03	2.32E-01
2	0.2	8.56E-02	-1.08E-02	-5.42E-01
3	0.3	1.41E-01	2.53E-02	1.26E+00
4	0.4	2.08E-01	-5.90E-02	-2.95E+00
5	0.5	2.89E-01	1.38E-01	6.89E+00
6	0.6	3.85E-01	-3.21E-01	-1.61E+01
7	0.7	5.00E-01	7.50E-01	3.75E+01
8	0.8	6.37E-01	-1.75E+00	-8.75E+01
9	0.9	8.02E-01	4.08E+00	2.04E+02
10	1.0	1.00E+00	-	-

Table 2: Numerical Solution using central difference for both convection and diffusion term.

3. Comparing the Solutions

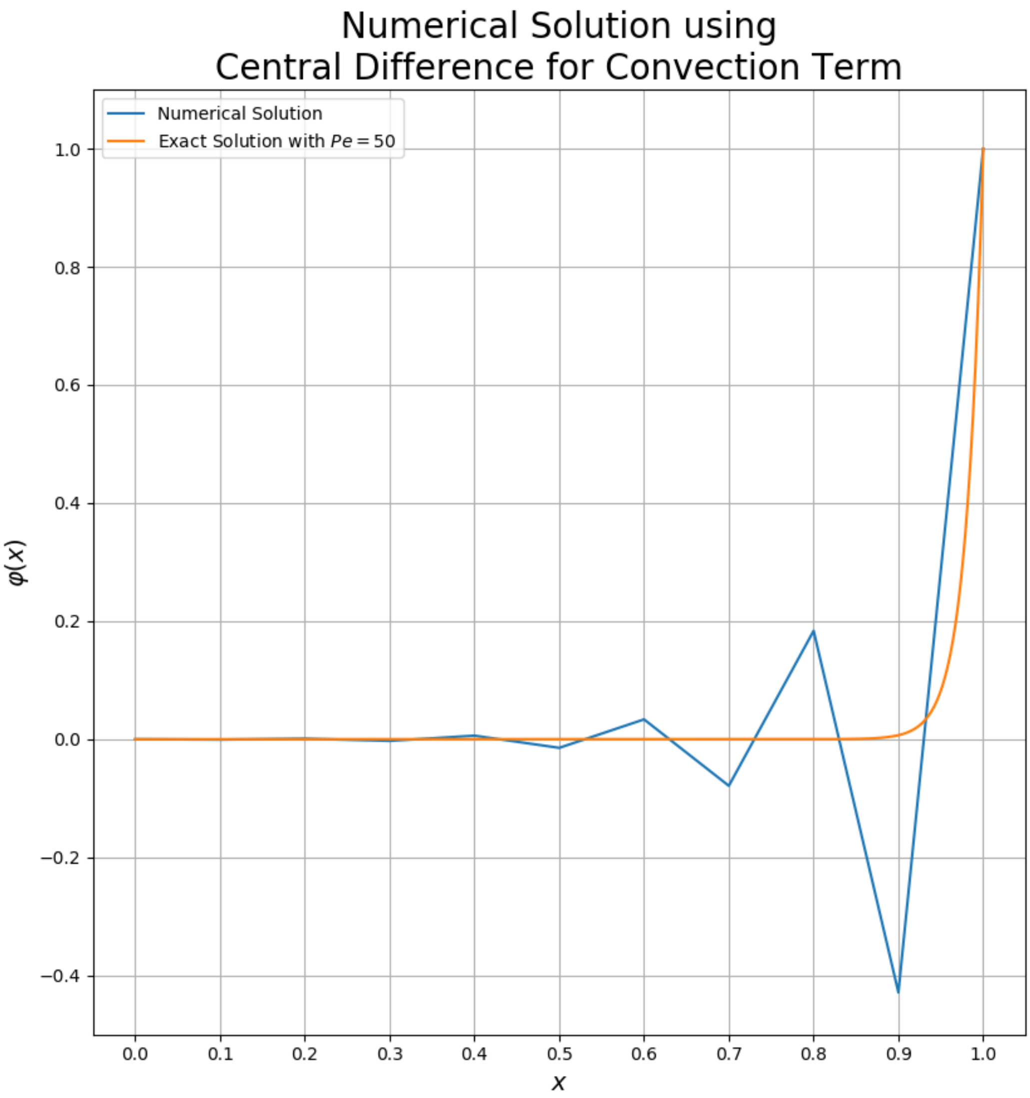


Figure 1

In figure 1, we can observe the oscillating nature of numerical solution using central difference scheme. The solution using upwind scheme is much more stable in this regard.

In order to explain this behavior mathematically, we can reason from the ODE that a big value of Peclet number (Pe), will result in a large magnitude of second derivative compared to the first derivative. This means the magnitude of change in slope is greater than the magnitude of slope itself. For $u > 0$, this would mean magnitude of first derivative using forward difference is much larger than that using backward difference. Since first derivative using central difference can be expressed as average of first derivatives using forward and backward difference schemes, the net difference in φ between consecutive grid points is large when using central difference scheme. Hence, the numerical solution using central difference scheme overshoots the exact solution, and we observe alternatingly positive and negative errors in the solution.

There is also a correctness associated with using the upwind difference scheme from the physics of the equation. A boundary value problem can be interpreted as some information fixed at the boundary, that is being transferred throughout the space. In case of diffusion the transfer is in all directions whereas in convection it is in the direction of the flow. A big Peclet number implies the problem is mostly influenced by the convection term. Hence, the information on the upwind side provides better approximate for the information in the current grid point.

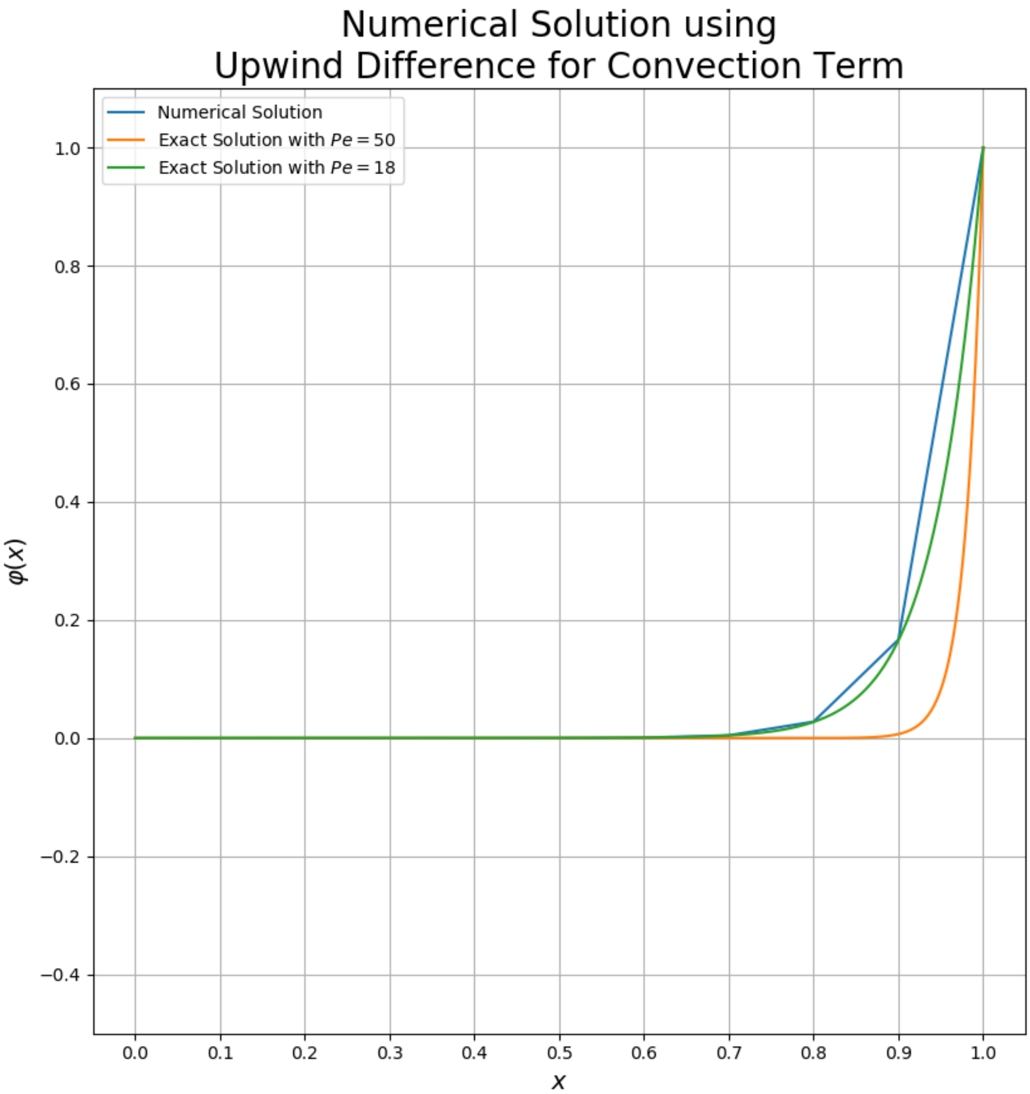


Figure 2

In figure 2, we notice even though the numerical solution matches the trend of the exact solution for $Pe = 50$, the values of the numerical solution exactly match that of the exact solution for $Pe = 18$.

4. Numerical solutions for denser Uniform Grids

Using $Pe = 50$ and $n = 40$, the numerical solutions using upwind difference and central difference schemes are plotted below –

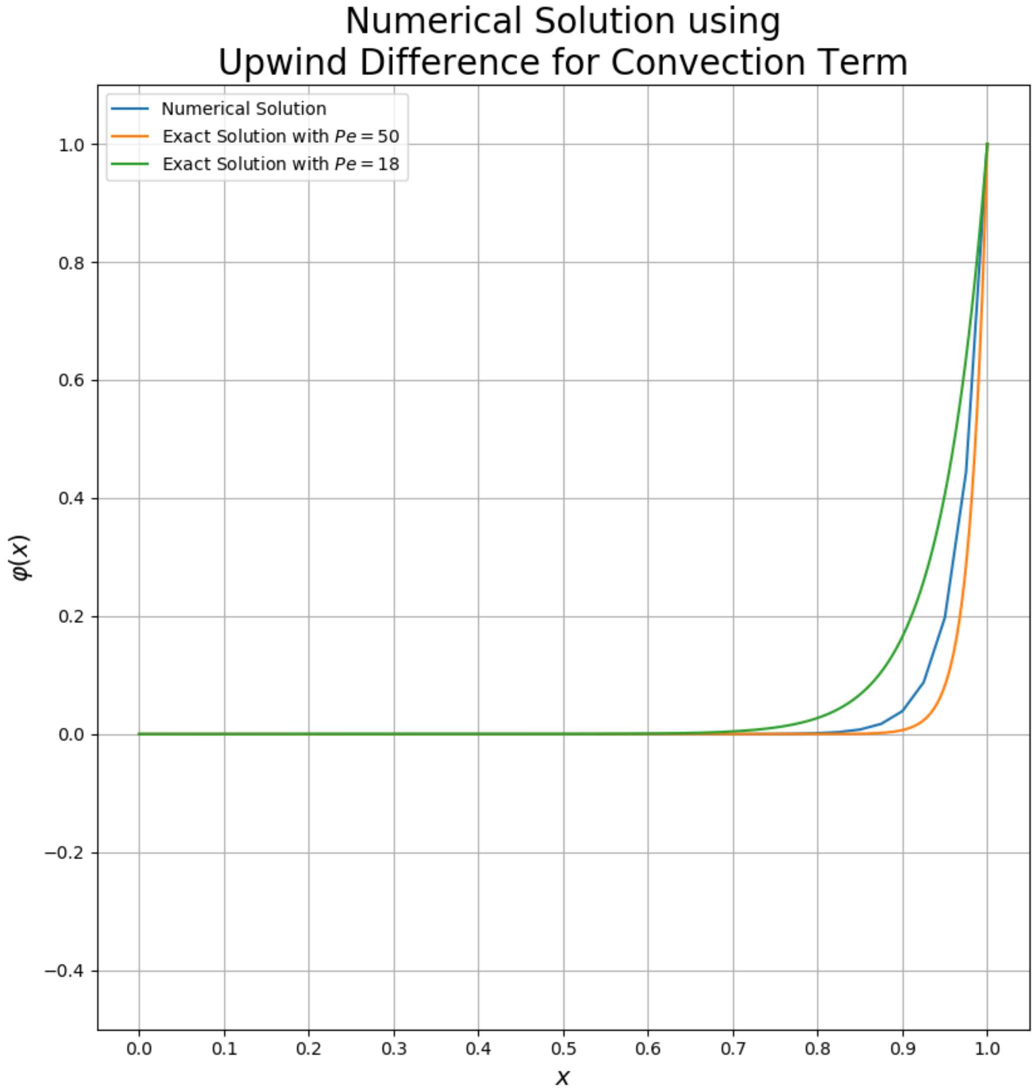


Figure 3

In figure 3, we can observe the numerical solution using upwind scheme is gradually approaching the exact solution with $Pe = 50$, as the number of grid points increase. But still the numerical solution seems to match the exact solution with some $Pe \in (18, 50)$ rather than the exact solution for $Pe = 50$.

In figure 4, we see the error in numerical solution using central scheme for convection term is much smaller compared to that using upwind scheme after increasing the grid density. This is due to the fact that the central difference scheme used here is a second order scheme while the upwind scheme used is only first

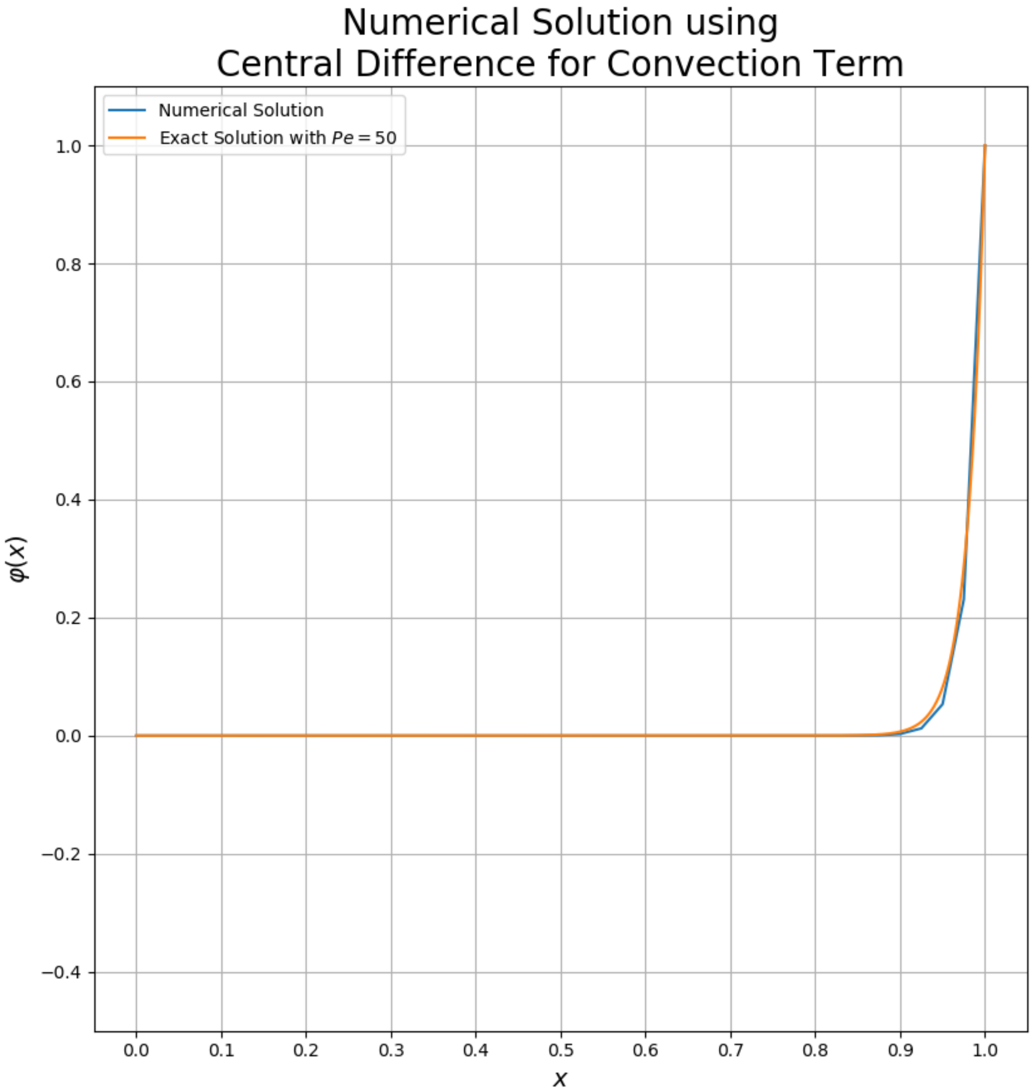


Figure 4

order. Hence, the truncation error decreases much rapidly with decreasing distance between consecutive grid points for central difference scheme.

Overall, both the schemes have visibly reduced global error with increasing grid density. This shows both the methods converge and are stable. However, when we have extremely limited number of grid points, upwind scheme proves to be more useful in visualizing the trend of the solution. While central difference would prove more efficient when we try to increase iterations to approach a more accurate solution.

5. Non-Uniform Grids and Higher Order Approximations

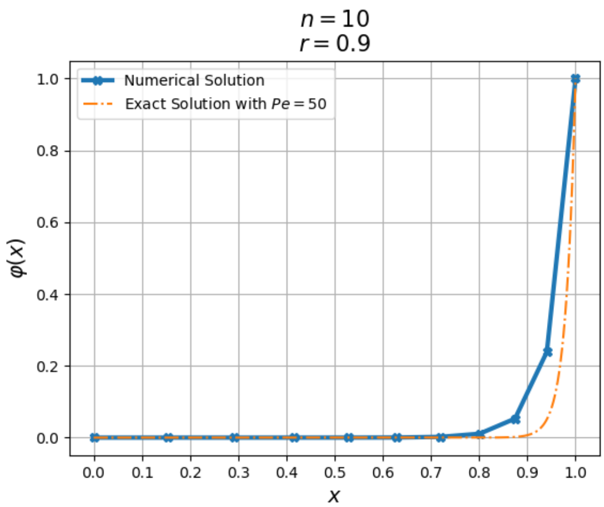
a. Non – Uniform Grid

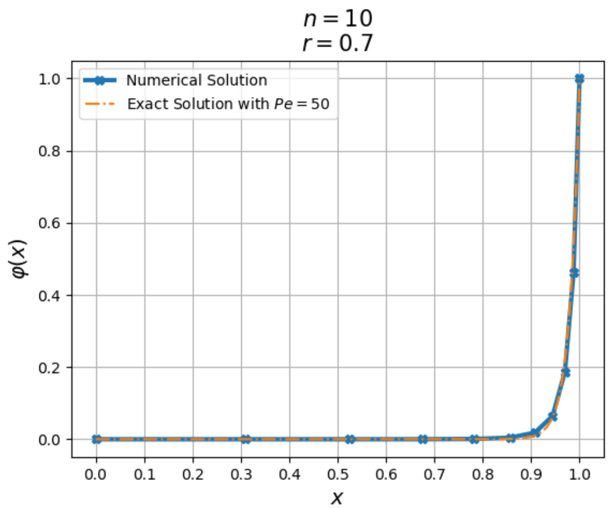
We have implemented a non-uniform grid with the consecutive distance between grid points to be in a geometric progression. We observe from previous solutions that slope of the solution curve progressively increases. Hence, decreasing grid point distances will result in a more stable numerical solution.

Let $\Delta x_1 = a$, and $\frac{\Delta x_{i+1}}{\Delta x_i} = r$. If we choose r, then a is constrained by the fact that sum of all grid differences must equal $x_{max} - x_{min} = 1$

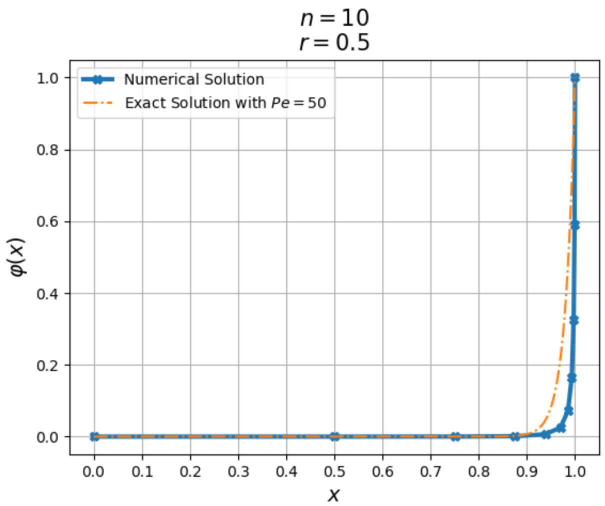
$$\sum_{i=1}^{n} a \cdot r^{i-1} = 1 \Rightarrow a \cdot \frac{r^n - 1}{r - 1} = 1 \Rightarrow a = \frac{1 - r}{1 - r^n}$$

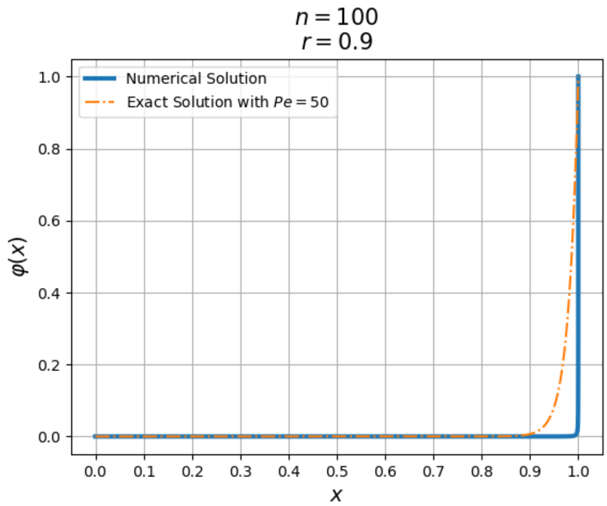
Following are the plots of numerical solutions using upwind scheme for different pairs of (n, r) –

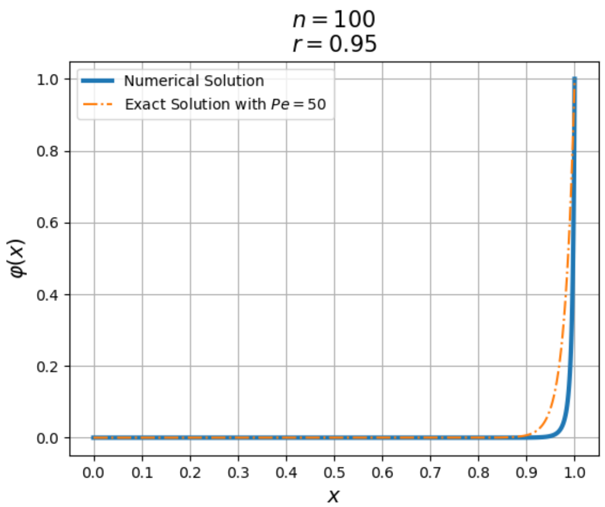


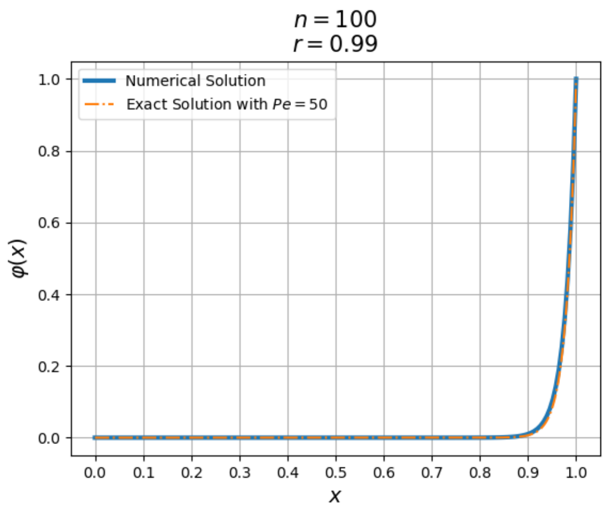


We can observe in the cases with $n = 10$, the as r approaches 1, the plot assumes the curve we found using upwind scheme for uniform grid, which was closer to the exact solution with $Pe = 18$ than that with $Pe = 50$. Peculiarly, at $r = 0.7$, we find the numerical solution with 11 grid points that is closest to the exact solution for $Pe = 50$. For other values of r, the solution plot retains the shape but seems to match the exact solution for some other Pe. As we increase n, we can see the optimal value of r, that gives the solution closest to the exact solution for $Pe = 50$, very quickly approaches 1.

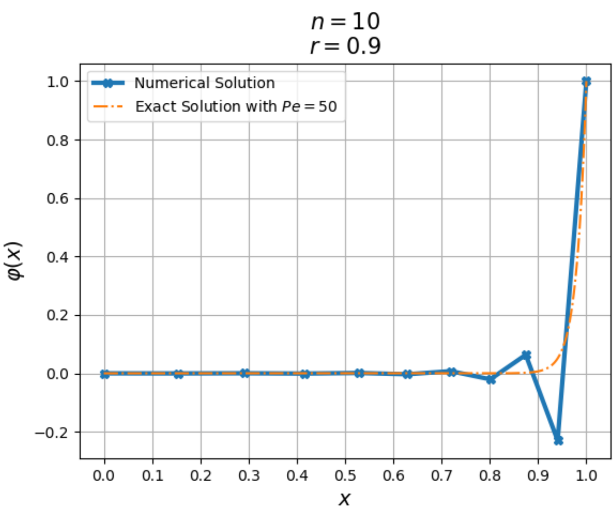


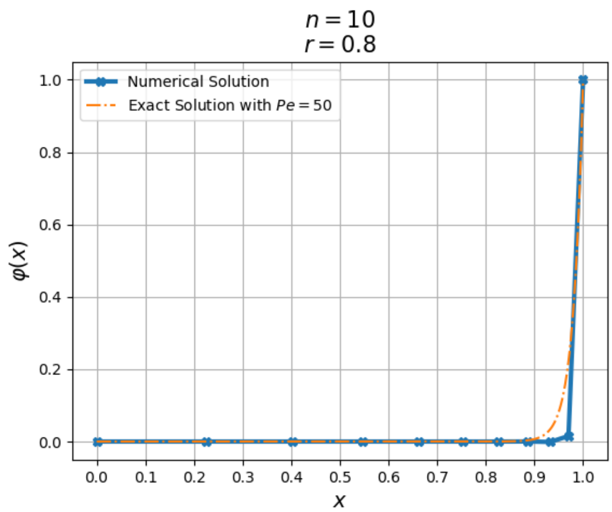


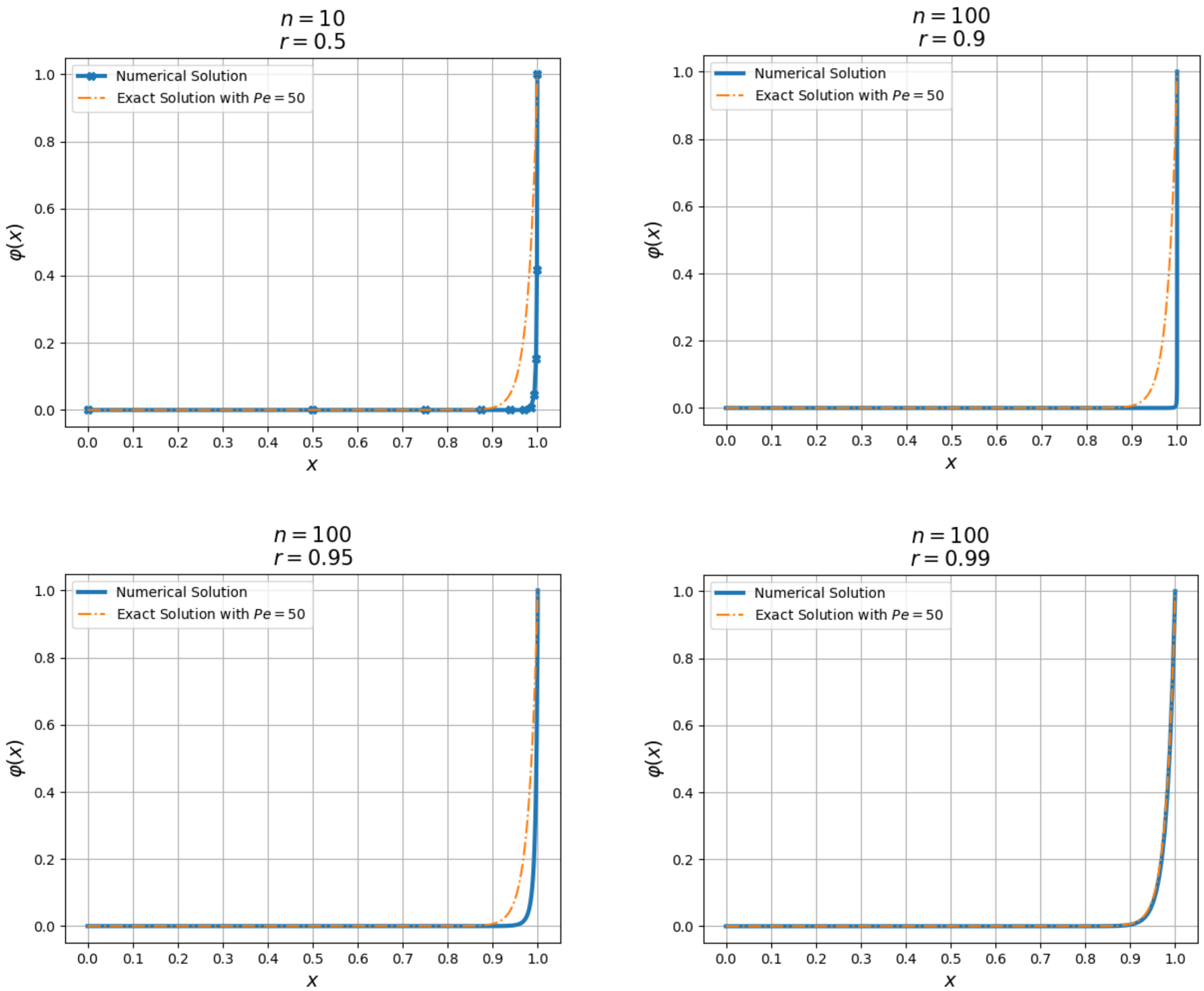




Following are the plots of numerical solutions using central difference scheme for different pairs of (n, r) –







In these plots too, we observe the oscillating behavior similar to the case with uniform grid as r approaches 1, for $n = 10$. Here, we find a critical r for given n, less than which, the oscillations disappear. For $n = 10$, that value is close to $r = 8.2$. Though the oscillations disappear but the error is not reduced. Error is only reduced for large n and $r \rightarrow 1$. Also, error is reduced more rapidly compared to upwind difference scheme.

b. Higher Order Discretization Schemes

Let us use a uniform grid with $n+1$ grid points and $\Delta x = \frac{1}{n}$.

At the ith grid point, we can approximate $\varphi(x)$ as a polynomial of $(x - x_i)$ to find higher order discretization

- Using 3rd order scheme for convective term

  Let $\varphi_i(x) = a_i + b_i \cdot (x - x_i) + c_i \cdot (x - x_i)^2 + d_i \cdot (x - x_i)^3$. We need to find α_1, α_2, α_3 and α_4 such that

$$\frac{d\varphi}{dx}\Big|_{x=x_i} = \alpha_1\varphi_{i+1} + \alpha_2\varphi_i + \alpha_3\varphi_{i-1} + \alpha_4\varphi_{i-2}$$

  Observe that

$$\frac{d\varphi_i}{dx} = b_i + 2 \cdot c_i \cdot (x - x_i) + 3 \cdot d_i \cdot (x - x_i)^2$$

$$\Rightarrow \frac{d\varphi_i}{dx}\Big|_{x=x_i} = b_i$$

  Solving for b_i such that

$$\varphi_i = a_i$$

$$\varphi_{i+1} = a_i + b_i \cdot \Delta x + c_i \cdot (\Delta x)^2 + d_i \cdot (\Delta x)^3$$

$$\varphi_{i-1} = a_i - b_i \cdot \Delta x + c_i \cdot (\Delta x)^2 - d_i \cdot (\Delta x)^3$$

$$\varphi_{i-2} = a_i - 2 \cdot b_i \cdot \Delta x + 4 \cdot c_i \cdot (\Delta x)^2 - 8 \cdot d_i \cdot (\Delta x)^3$$

  We get,

$$b_i = \frac{1}{\Delta x} \cdot \left(\frac{\varphi_i}{2} - \varphi_{i-1} + \frac{\varphi_{i-2}}{6} + \frac{\varphi_{i+1}}{3}\right)$$

$$\Rightarrow \frac{d\varphi}{dx}\Big|_{x=x_i} = \frac{2\varphi_{i+1} + 3\varphi_i - 6\varphi_{i-1} + \varphi_{i-2}}{6\Delta x}$$

- Using 4th order scheme for diffusion term

  Let

  $\varphi_i(x) = a_i + b_i \cdot (x - x_i) + c_i \cdot (x - x_i)^2 + d_i \cdot (x - x_i)^3 + e_i \cdot (x - x_i)^4$

  We need to find α_1, α_2, α_3, α_4 and α_5 such that

$$\frac{d^2\varphi}{dx^2}\Big|_{x=x_i} = \alpha_1\varphi_{i+2} + \alpha_2\varphi_{i+1} + \alpha_3\varphi_i + \alpha_4\varphi_{i-1} + \alpha_5\varphi_{i-2}$$

  Observe that

$$\frac{d\varphi_i}{dx} = b_i + 2 \cdot c_i \cdot (x - x_i) + 3 \cdot d_i \cdot (x - x_i)^2 + 4 \cdot e_i \cdot (x - x_i)^3$$

$$\Rightarrow \frac{d^2\varphi_i}{dx^2} = 2 \cdot c_i + 6 \cdot d_i \cdot (x - x_i) + 12 \cdot e_i \cdot (x - x_i)^2$$

$$\Rightarrow \frac{d^2\varphi_i}{dx^2} \Big|_{x=x_i} = 2 \cdot c_i$$

Solving for c_i such that

$$\varphi_i = a_i$$

$$\varphi_{i+1} = a_i + b_i \cdot \Delta x + c_i \cdot (\Delta x)^2 + d_i \cdot (\Delta x)^3 + e_i \cdot (\Delta x)^4$$

$$\varphi_{i-1} = a_i - b_i \cdot \Delta x + c_i \cdot (\Delta x)^2 - d_i \cdot (\Delta x)^3 + e_i \cdot (\Delta x)^4$$

$$\varphi_{i-2} = a_i + 2 \cdot b_i \cdot \Delta x + 4 \cdot c_i \cdot (\Delta x)^2 + 8 \cdot d_i \cdot (\Delta x)^3 + 16 \cdot e_i \cdot (\Delta x)^4$$

$$\varphi_{i-2} = a_i - 2 \cdot b_i \cdot \Delta x + 4 \cdot c_i \cdot (\Delta x)^2 - 8 \cdot d_i \cdot (\Delta x)^3 + 16 \cdot e_i \cdot (\Delta x)^4$$

We get,

$$c_i = \frac{-30\varphi_i + 16\varphi_{i-1} - \varphi_{i-2} + 16\varphi_{i+1} - \varphi_{i+2}}{12(\Delta x)^2}$$

$$\Rightarrow \frac{d^2\varphi}{dx^2} \Big|_{x=x_i} = \frac{-\varphi_{i+2} + 16\varphi_{i+1} - 30\varphi_i + 16\varphi_{i-1} - \varphi_{i-2}}{12(\Delta x)^2}$$

Thus, we get the discretized form of the convection diffusion equation

$$Pe \cdot \frac{d\varphi}{dx} = \frac{d^2\varphi}{dx^2}$$

$$\Rightarrow Pe \cdot \frac{2\varphi_{i+1} + 3\varphi_i - 6\varphi_{i-1} + \varphi_{i-2}}{6\Delta x} = \frac{-\varphi_{i+2} + 16\varphi_{i+1} - 30\varphi_i + 16\varphi_{i-1} - \varphi_{i-2}}{12(\Delta x)^2}$$

$$\Rightarrow 2 \cdot \Delta x \cdot Pe \cdot (2\varphi_{i+1} + 3\varphi_i - 6\varphi_{i-1} + \varphi_{i-2}) + \varphi_{i+2} - 16\varphi_{i+1} + 30\varphi_i - 16\varphi_{i-1} + \varphi_{i-2} = 0$$

$$\Rightarrow \varphi_{i+2} + (4 \cdot Pe \cdot \Delta x - 16) \cdot \varphi_{i+1} + (6 \cdot Pe \cdot \Delta x + 30) \cdot \varphi_i - (12 \cdot Pe \cdot \Delta x + 16) \cdot \varphi_{i-1} + (2 \cdot Pe \cdot \Delta x + 1) \cdot \varphi_{i-2} = 0$$

The arithmetic for deriving these equations was done using P1_Q5_B_Discretization.py

Define

$$\delta = 4 \cdot Pe \cdot \Delta x - 16$$

$$\gamma = 6 \cdot Pe \cdot \Delta x + 30$$

$$\lambda = -(12 \cdot Pe \cdot \Delta x + 16)$$

$$\mu = 2 \cdot Pe \cdot \Delta x + 1$$

Hence, we have,

$$\varphi_{i+2} + \delta \cdot \varphi_{i+1} + \gamma \cdot \varphi_i + \lambda \cdot \varphi_{i-1} + \mu \cdot \varphi_{i-2} = 0$$

$$\forall\, i \in \{2, 3, \dots, n-2\}$$

From boundary conditions we have, $\varphi_0 = 0$ and $\varphi_n = 1$. We need to find $\varphi_i\ \forall\, i \in \{1, 2, \dots, n-1\}$, i.e., $n-1$ unknowns. But we have only $n-3$ equations so far. So, we use lower order schemes at $i = 1$ and $i = n-1$ to get two more equations. From previously derived lower order discretized equations –

For $i = 1$

$$\varphi_2 - (2 + Pe \cdot \Delta x) \cdot \varphi_1 = -(1 + Pe \cdot \Delta x) \cdot \varphi_0$$

And, for $i = n-1$

$$-(2 + Pe \cdot \Delta x) \cdot \varphi_{n-1} + (1 + Pe \cdot \Delta x) \cdot \varphi_{n-2} = -\varphi_n$$

The above system of equations can be expressed as a penta-diagonal matrix equation and can ideally be solved in order of n time. However, we used simple LU decomposition method to solve the matrix equation in the script P1_Q5_B_18110166.py

Following are the plots –

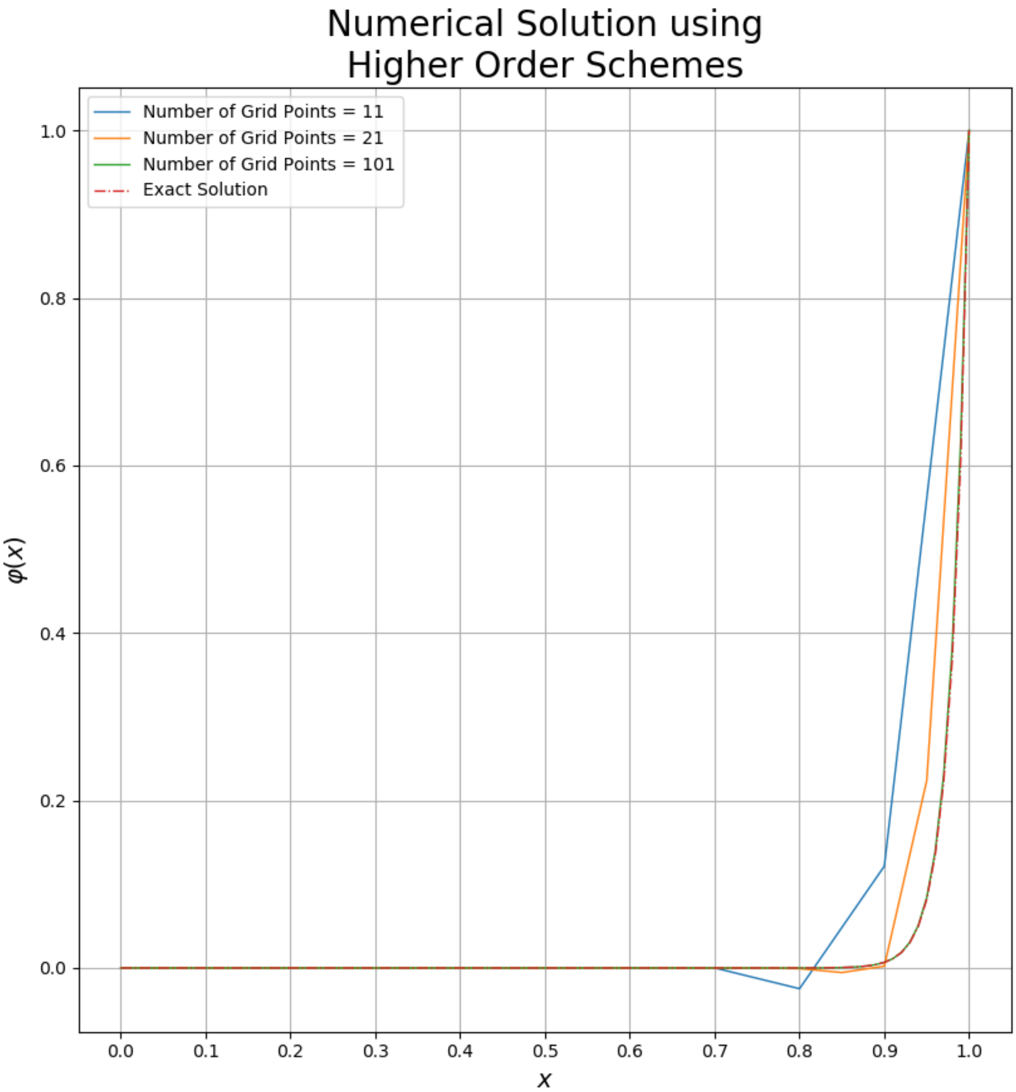


Figure 5

In figure 5, even though the plot of the solution using 11 grid points has significant error, the error reduces rapidly with increasing number of grid points. With 101 grid points, the error is almost insignificant and not detectable from the graph. But for the same number of grid points, in figure 6, where lower order schemes are used, we can see there is still some error. Thus, difficulties of using higher order schemes trade off in terms of rapid convergence to the exact solution with the same number of iterations

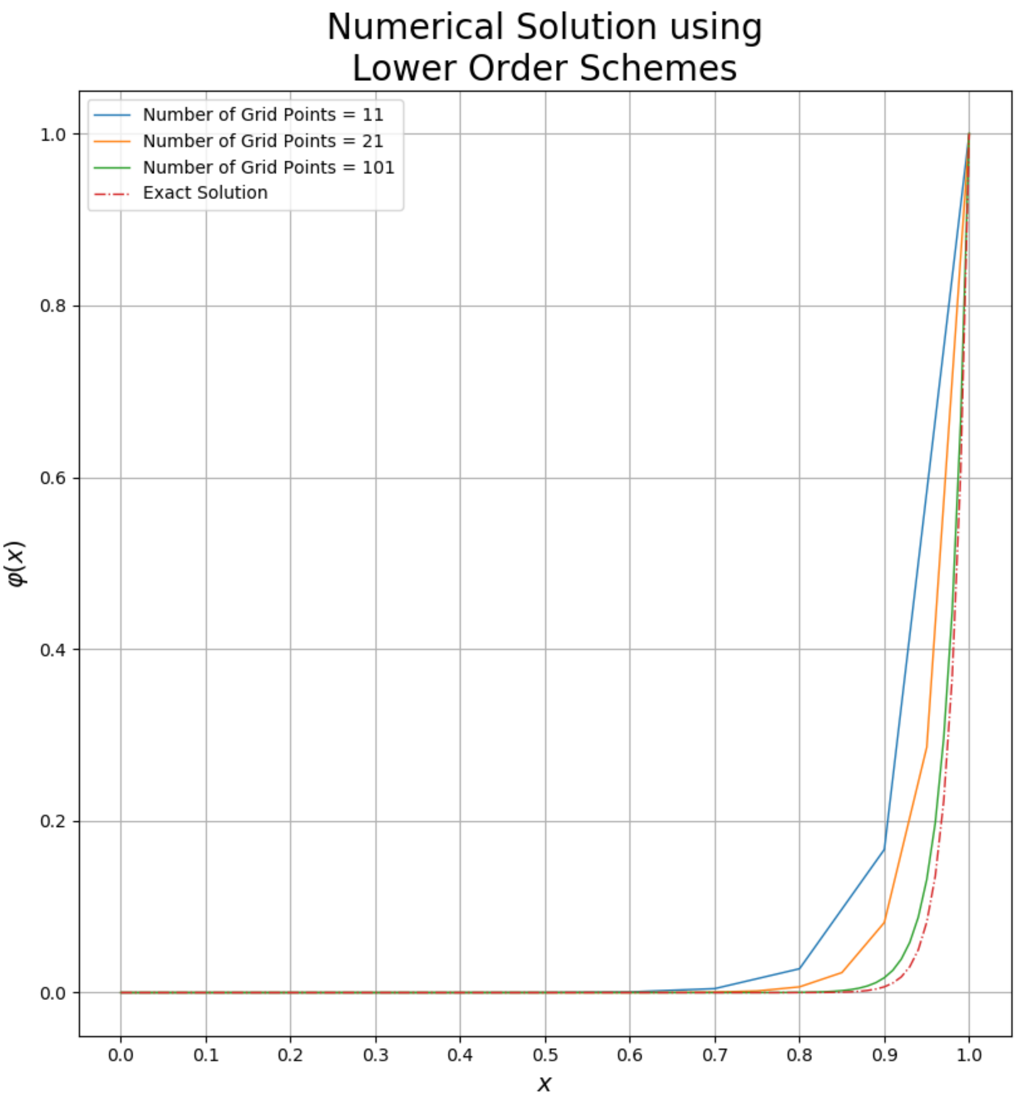

Numerical Solution using
Lower Order Schemes
Number of Grid Points = 11
Number of Grid Points = 21
Number of Grid Points = 101
Exact Solution
1.0
0.8
0.6
0.4
0.2
0.0
φ(x)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x

Figure 6