Special Topics in CFD

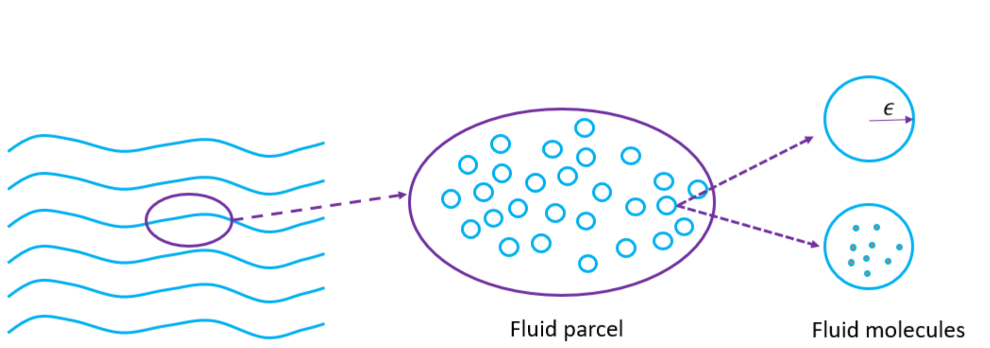
DAY 2

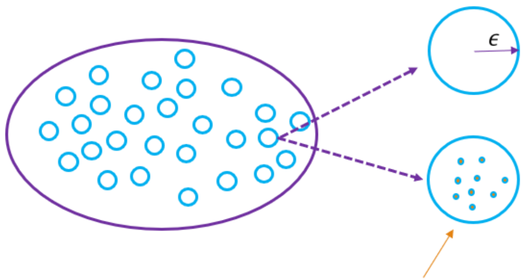
First order derivatives →
forward, backward, and central difference methods

Kumaresh

Quick Recap

A substance whose molecular structure offers no resistance to external forces - Ferziger, Peric



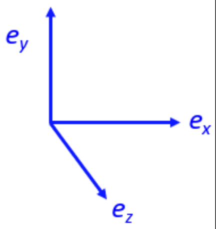


In physics, mean free path is the average distance over which a moving particle

Kn < 0.01	Continuum flow
0.01 < Kn < 0.1	Slip flow
0.1 < Kn < 10	Transitional flow
Kn > 10	Free molecular flow

$$\nabla \rho = \left(\frac{\partial}{\partial x}\boldsymbol{e}_x + \frac{\partial}{\partial y}\boldsymbol{e}_y + \frac{\partial}{\partial z}\boldsymbol{e}_z\right)\rho = \left(\frac{\partial \rho}{\partial x}\boldsymbol{e}_x + \frac{\partial \rho}{\partial y}\boldsymbol{e}_y + \frac{\partial \rho}{\partial z}\boldsymbol{e}_z\right)$$

$$\nabla \boldsymbol{u} = \begin{bmatrix} \partial u/\partial x & \partial v/\partial x & \partial w/\partial x \\ \partial u/\partial y & \partial v/\partial y & \partial w/\partial y \\ \partial u/\partial z & \partial v/\partial z & \partial w/\partial z \end{bmatrix}$$



$$\nabla \cdot \boldsymbol{u} = \left(\frac{\partial}{\partial x}\boldsymbol{e}_x + \frac{\partial}{\partial y}\boldsymbol{e}_y + \frac{\partial}{\partial z}\boldsymbol{e}_z\right)(u\boldsymbol{e}_x + v\boldsymbol{e}_y + w\boldsymbol{e}_z) = \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right)$$

[Exercise-1] Package installations (ANSYS and OpenFOAM) #2

Kumaresh0402 started this conversation in General

Kumaresh0402 44 minutes ago Maintainer

ANSYS Fluent Package: https://www.ansys.com/products/fluids/ansys-fluent/ansys-fluent-trial

Please install OpenFOAM and GNU Octave following the documentation in https://1drv.ms/f/s!AqT2YEB97-1RgP8MtsMPqoOGsq4ddg?e=locXv0

Follow instructions in installation_steps.pdf

Once after you finish installing, try installing GNU Octave on either Windows or Ubuntu.

Post your queries and make a comment here as part of your Exercise-1.

↑ 1

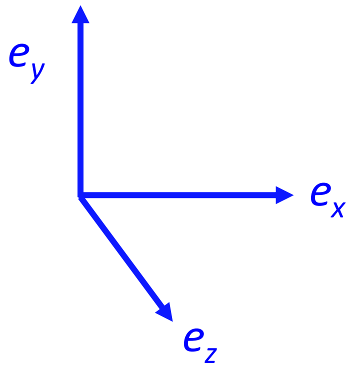
Contents

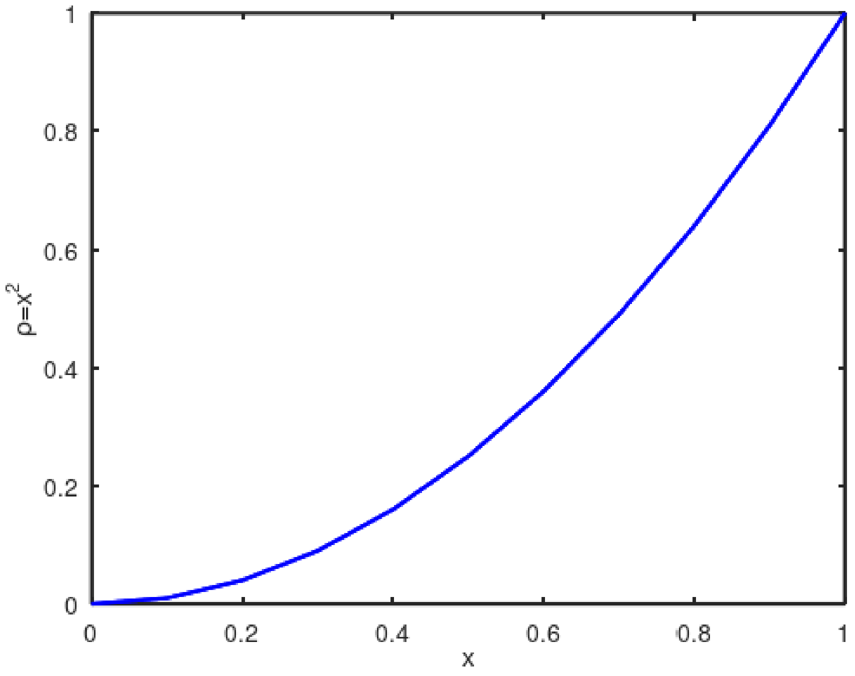
Mathematical operations

Gradient

$$\nabla\rho = \left(\frac{\partial}{\partial x}\boldsymbol{e}_x + \frac{\partial}{\partial y}\boldsymbol{e}_y + \frac{\partial}{\partial z}\boldsymbol{e}_z\right)\rho = \left(\frac{\partial\rho}{\partial x}\boldsymbol{e}_x + \frac{\partial\rho}{\partial y}\boldsymbol{e}_y + \frac{\partial\rho}{\partial z}\boldsymbol{e}_z\right)$$

$$\frac{\partial\rho}{\partial x} = \frac{d\rho}{dx}(in\ 1D)$$

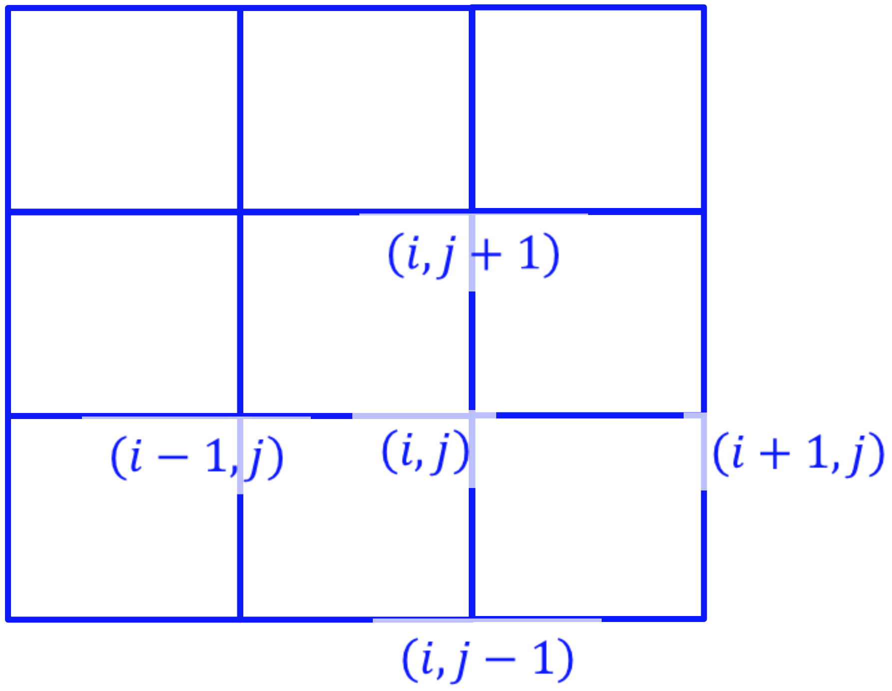




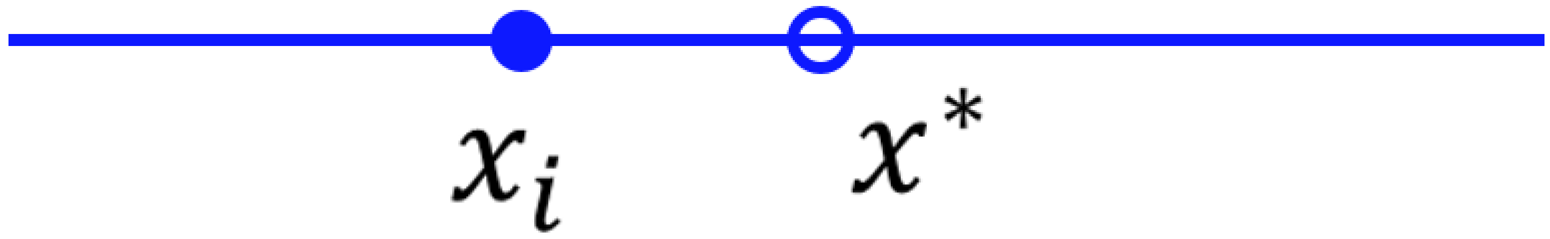
Finite Difference Method (FDM)

$$\nabla\rho = \left(\frac{\partial}{\partial x}\boldsymbol{e}_x + \frac{\partial}{\partial y}\boldsymbol{e}_y + \frac{\partial}{\partial z}\boldsymbol{e}_z\right)\rho = \left(\frac{\partial\rho}{\partial x}\boldsymbol{e}_x + \frac{\partial\rho}{\partial y}\boldsymbol{e}_y + \frac{\partial\rho}{\partial z}\boldsymbol{e}_z\right)$$

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



Taylor series expansion



$$\rho(x^*) = \rho(x_i) + (x^* - x_i)\left(\frac{d\rho}{dx}\right)_i + (x^* - x_i)^2\left(\frac{d^2\rho}{dx^2}\right)_i + (x^* - x_i)^3\left(\frac{d^3\rho}{dx^3}\right)_i + \cdots$$

Taylor series expansion

$$\rho(x_{i+1}) = \rho(x_i) + (x_{i+1} - x_i)\left(\frac{\partial \rho}{\partial x}\right)_i + (x_{i+1} - x_i)^2\left(\frac{\partial^2 \rho}{\partial x^2}\right)_i + (x_{i+1} - x_i)^3\left(\frac{\partial^3 \rho}{\partial x^3}\right)_i + \cdots$$

$$\rho(x_{i+1}) = \rho(x_i) + (x_{i+1} - x_i)\left(\frac{\partial \rho}{\partial x}\right)_i + O\left(\Delta x_i^2\right); \qquad \Delta x_i = (x_{i+1} - x_i)$$

$$\rho(x_{i+1}) = \rho(x_i) + \Delta x_i\left(\frac{\partial \rho}{\partial x}\right)_i + O\left(\Delta x_i^2\right)$$

Taylor series and FDM

Taylor series:

$$\rho(x_{i+1}) = \rho(x_i) + \Delta x_i \left(\frac{\partial \rho}{\partial x}\right)_i + O(\Delta x_i^2)$$

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

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

$$\left(\frac{\partial \rho}{\partial x}\right)_i \approx \frac{\rho(x_{i+1}) - \rho(x_i)}{\Delta x_i}$$

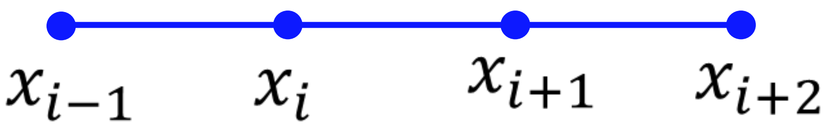
Finite difference

$$\nabla \rho = \left(\frac{\partial}{\partial x}\boldsymbol{e}_x + \frac{\partial}{\partial y}\boldsymbol{e}_y + \frac{\partial}{\partial z}\boldsymbol{e}_z\right)\rho = \left(\frac{\partial \rho}{\partial x}\boldsymbol{e}_x + \frac{\partial \rho}{\partial y}\boldsymbol{e}_y + \frac{\partial \rho}{\partial z}\boldsymbol{e}_z\right)$$

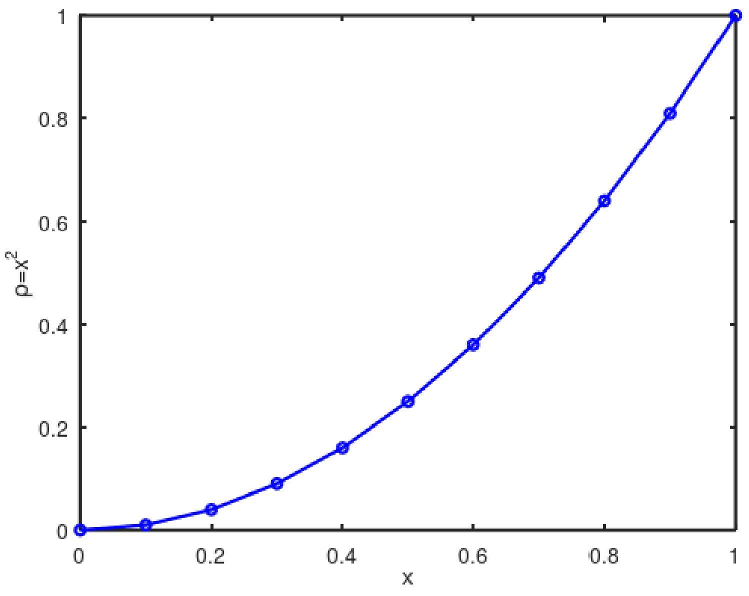
$$\boxed{\left(\frac{\partial \rho}{\partial x}\right)_i = \frac{\rho(x_{i+1}) - \rho(x_i)}{\Delta x_i} + O(\Delta x_i)}$$

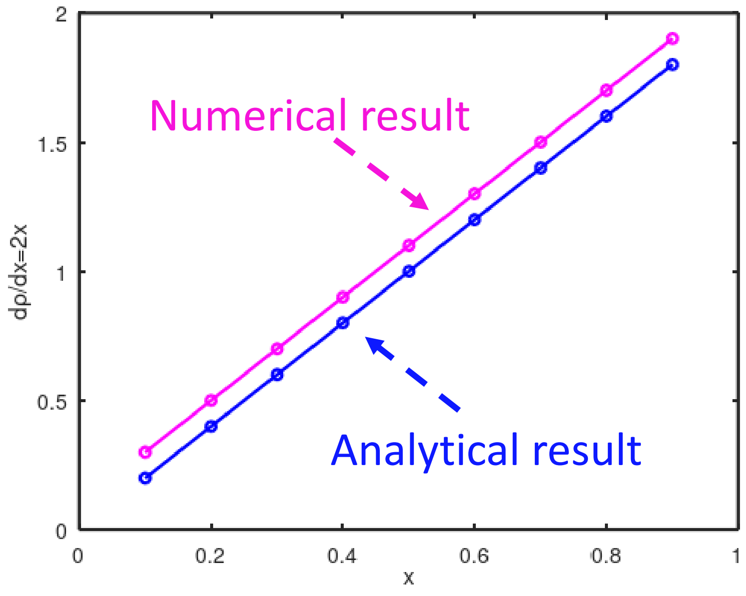
First order derivative – forward difference method

Analytical and Numerical solutions



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



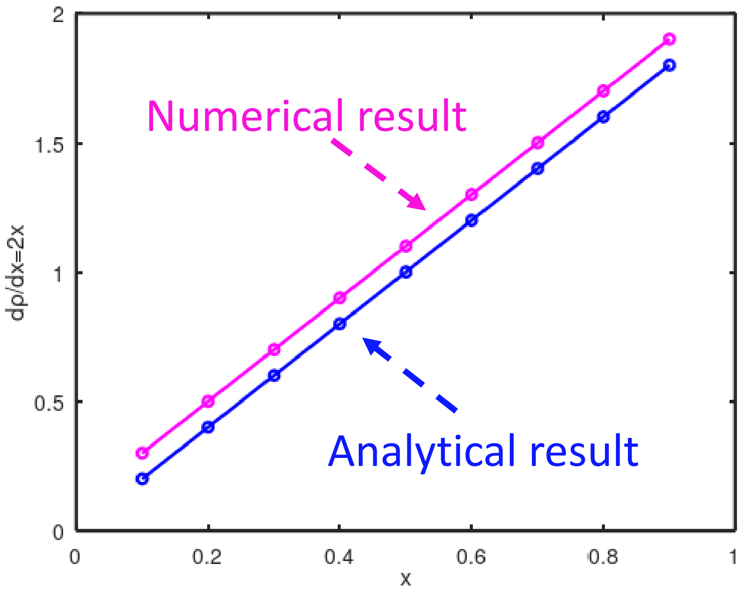


Resolved in OCTAVE

Result of first order derivative of first order forward difference method

Analytical and Numerical solutions

Analytical	Numerical
An analytical solution involves framing the problem in a well-understood form and calculating the exact solution.	A numerical solution means making guesses at the solution and testing whether the problem is solved well enough to stop.



Exercise – 2
OCTAVE

```
%% Approximating derivative using first order numerical scheme.

clear all;
close all;

x = [0:0.1:1]';
y = x.^2;

n = length(x);

figure(1);
%plot(x, y, '-b', 'linewidth', 2);
plot(x, y, '-ob', 'linewidth', 2);
hold on;
xlabel('x');
ylabel('\rho=x^2');
set(gca, "linewidth", 2, "fontsize", 14)

% gradient
yp = 2*x; % Analytical expression

yp_n1 = zeros(size(y));

yp_n1(1, 1) = (y(2, 1) - y(1, 1)) / (x(2, 1) - x(1, 1));
yp_n1(n, 1) = (y(n, 1) - y(n-1, 1)) / (x(n, 1) - x(n-1, 1));

for i = 2 : length(y)-1
  yp_n1(i, 1) = (y(i+1, 1) - y(i, 1)) / (x(i+1, 1) - x(i, 1));
end

figure(2);
hold on;
plot(x(2:n-1), yp(2:n-1), '-ob', 'linewidth', 2);
plot(x(2:n-1), yp_n1(2:n-1), '-om', 'linewidth', 2);
hold on;
xlabel('x');
ylabel('d\rho/dx=2x');
box on;
set(gca, "linewidth", 2, "fontsize", 14)
hold off;
```

Exercise – 2 ➔ Octave

(1) Derive first order derivative for: forward, backward, and central difference schemes. (Use Pen and paper)

<u>Hint: derivation of first order forward difference</u>

$$\rho(x_{i+1}) = \rho(x_i) + (x_{i+1} - x_i)\left(\frac{\partial \rho}{\partial x}\right)_i + (x_{i+1} - x_i)^2\left(\frac{\partial^2 \rho}{\partial x^2}\right)_i + (x_{i+1} - x_i)^3\left(\frac{\partial^3 \rho}{\partial x^3}\right)_i + \cdots$$

$$\rho(x_{i+1}) = \rho(x_i) + (x_{i+1} - x_i)\left(\frac{\partial \rho}{\partial x}\right)_i + O(\Delta x_i^2); \qquad \Delta x_i = (x_{i+1} - x_i)$$

$$\rho(x_{i+1}) = \rho(x_i) + \Delta x_i\left(\frac{\partial \rho}{\partial x}\right)_i + O(\Delta x_i^2)$$

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

<u>Hint: derivation of first order backward difference</u>

$$\rho(x_{i-1}) = \rho(x_i) - \Delta x_i\left(\frac{d\rho}{dx}\right)_i + \Delta x_i^2\left(\frac{d^2\rho}{dx^2}\right)_i + O(\Delta x_i^3)$$

<u>Hint: derivation of first order central difference</u>

$$(i) \quad \rho(x_{i+1}) = \rho(x_i) + \Delta x_i\left(\frac{d\rho}{dx}\right)_i + \Delta x_i^2\left(\frac{d^2\rho}{dx^2}\right)_i + O(\Delta x_i^3)$$

$$(ii) \quad \rho(x_{i-1}) = \rho(x_i) - \Delta x_i\left(\frac{d\rho}{dx}\right)_i + \Delta x_i^2\left(\frac{d^2\rho}{dx^2}\right)_i + O(\Delta x_i^3)$$

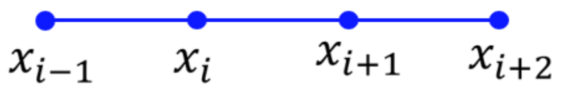
Subtract (2) from (1) and derive $\left(\frac{d\rho}{dx}\right)_i$

Exercise – 2 ➔ Octave

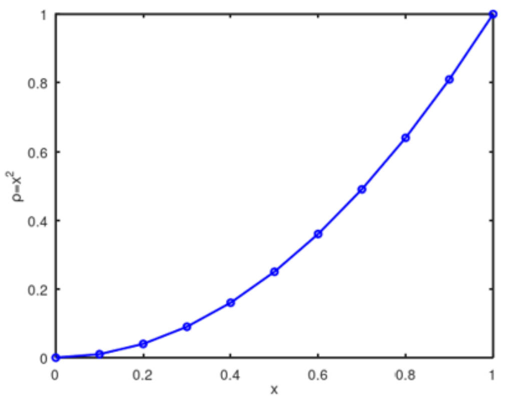
(2) Make use of Octave code and plot for (first order derivative): forward, backward, and central difference schemes, when $\rho = x^2$ and x^3

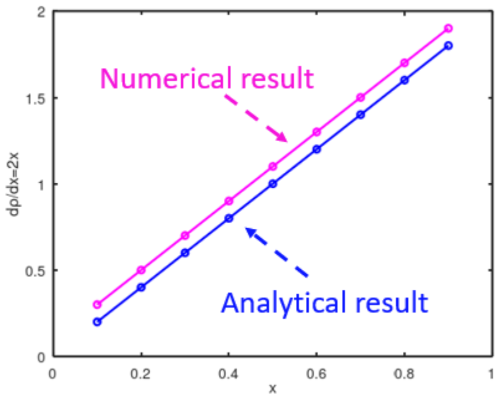
(3) Justify that why central difference scheme is accurate than other first and backward schemes.

Analytical and Numerical solutions



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





Resolved in OCTAVE

Result of first order derivative of first order forward difference method

[Exercise-2] Estimation of first order derivative schemes #3

Kumaresh0402 started this conversation in **General**

Kumaresh0402 5 hours ago Maintainer

edited

1. Derive first order derivative for: forward, backward, and central difference schemes. (Use Pen and paper)
2. Make use of Octave code and plot for (first order derivative): forward, backward, and central difference schemes, when $\rho = x$^2 and x^3
3. Justify that why central difference scheme is accurate than other first and backward schemes.

Make use of OCTAVE code: https://github.com/Kumaresh0402/SpecialTopicsinComputationalFluidDynamics/tree/main/DAY2-First_order_derivative_schemes

Comparing forward, backward, and central difference schemes with analytical method for x^2