# Special Topics in CFD

DAY 3

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

*Kumaresh*

# Quick Recap

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

Kumaresh0402 started this conversation in General

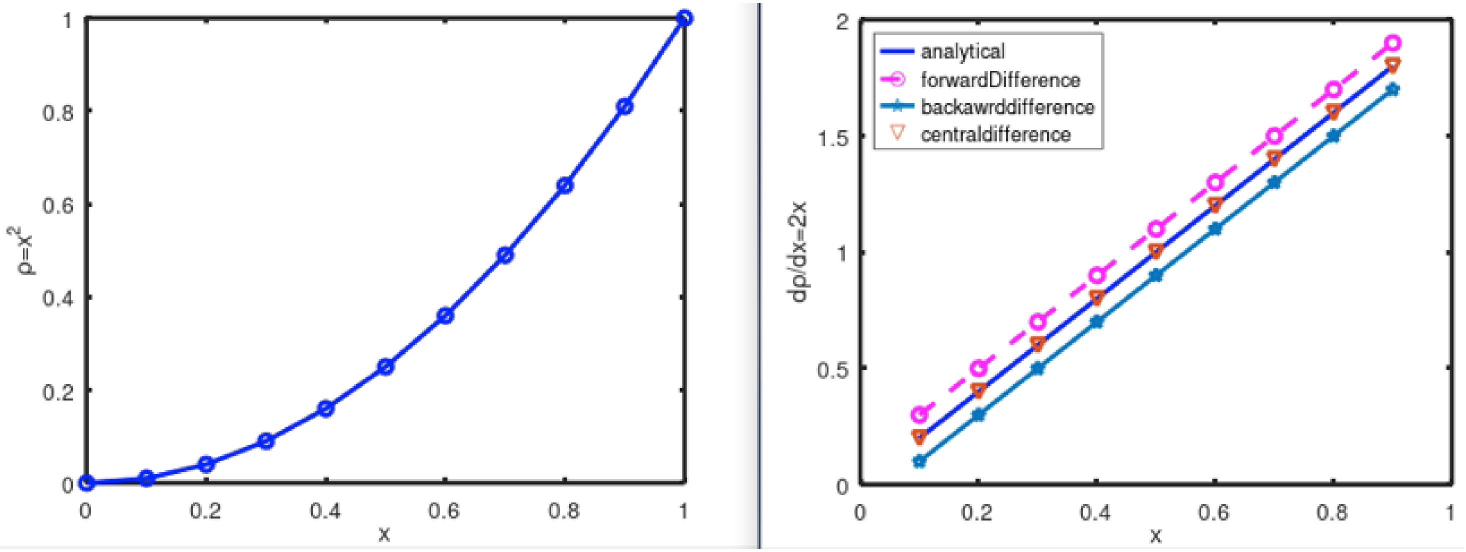
Kumaresh0402 last week Maintainer

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

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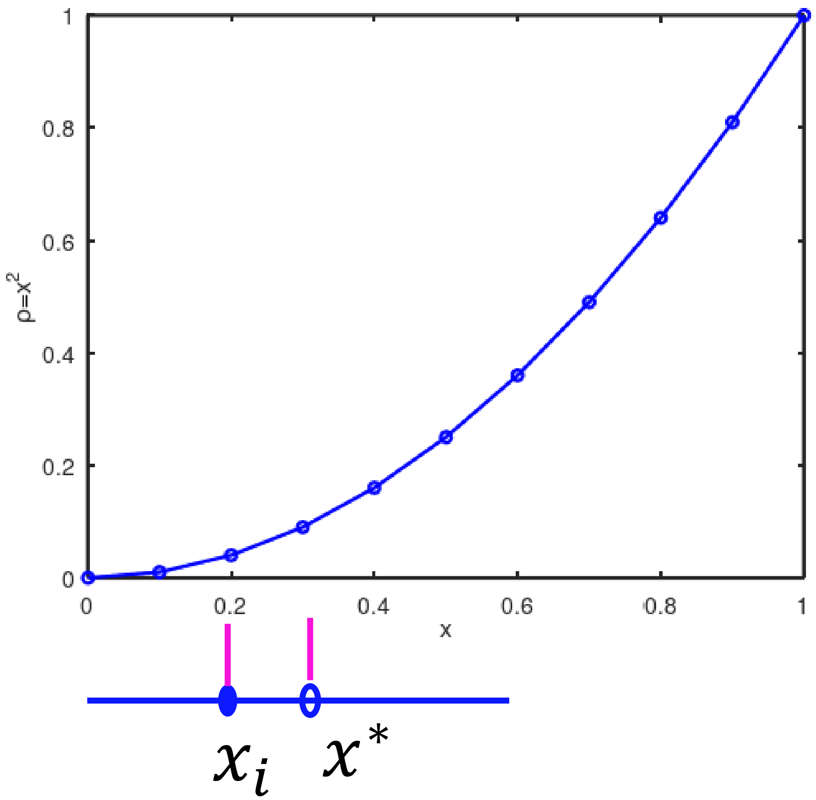
# Contents

- Taylor series
- Numerical discretization
- Gauss-Divergence theorem
- Reynolds Transport Theorem
- Solve Exercise – 3 in Octave

# Taylor series: Discrete Operations




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

# 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

# Taylor series: Central Difference Scheme (2nd order)


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

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

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

# Taylor series: Central Difference Scheme (2nd order)

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

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

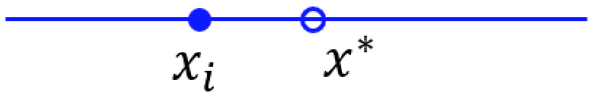

Subtract (2) from (1)

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

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

First order derivative –
Second order central difference scheme

# Taylor series: Summary (first order derivative)




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

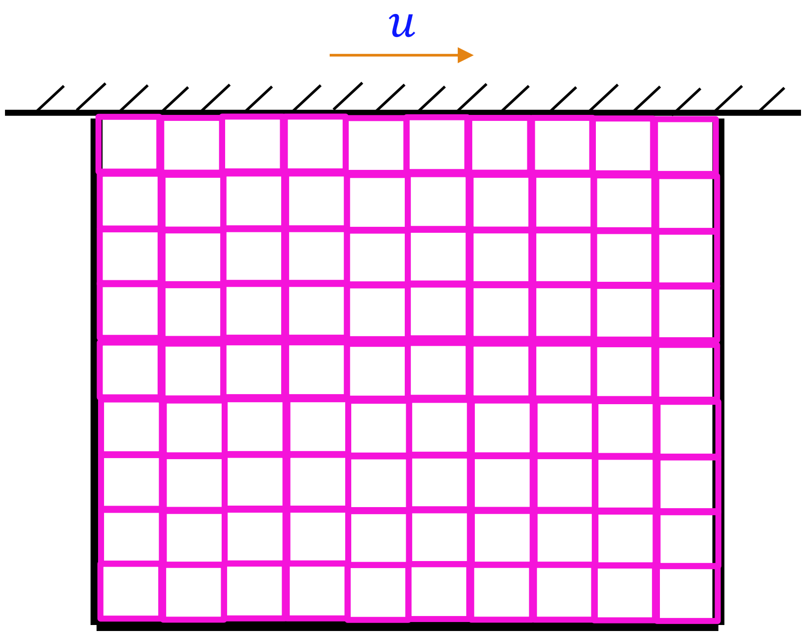

$$\left(\frac{d\rho}{dx}\right)_i \approx \frac{\rho(x_{i+1}) - \rho(x_i)}{\Delta x_i}$$

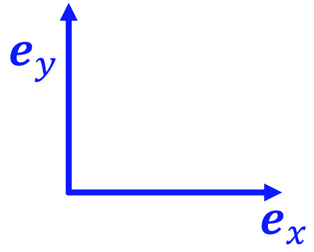
First order forward difference

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

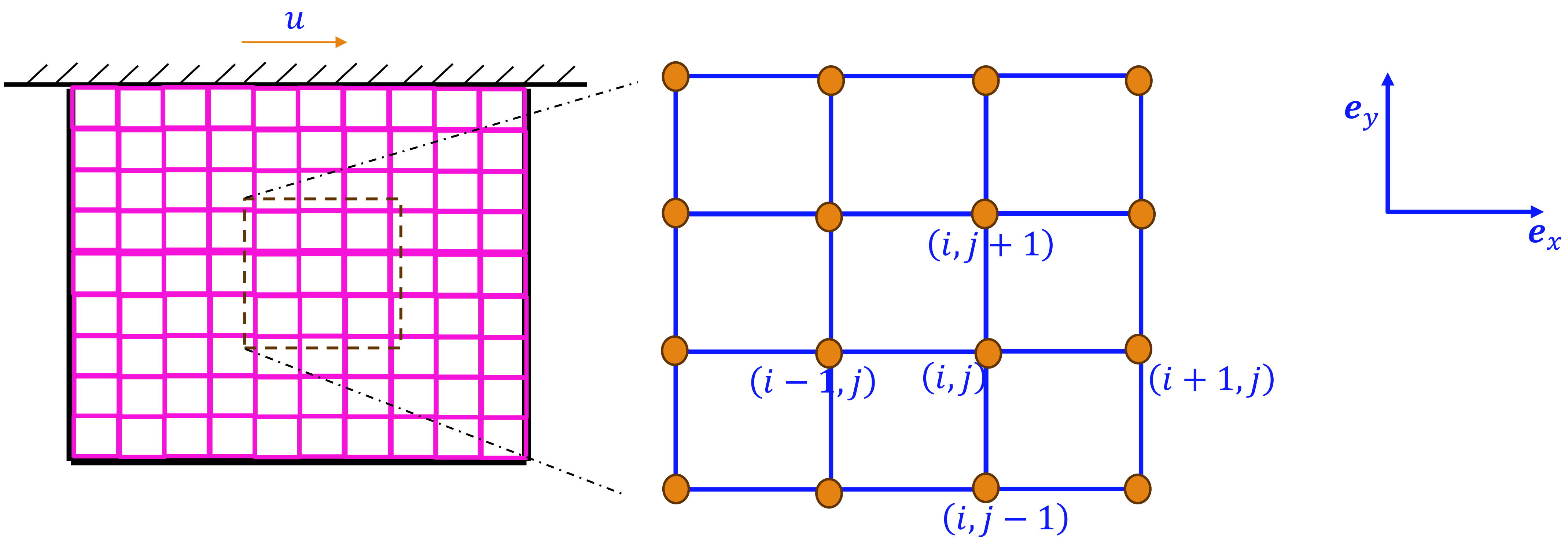
Second order central difference

# Numerical discretization (Grid layout)



# Numerical discretization (Grid layout)

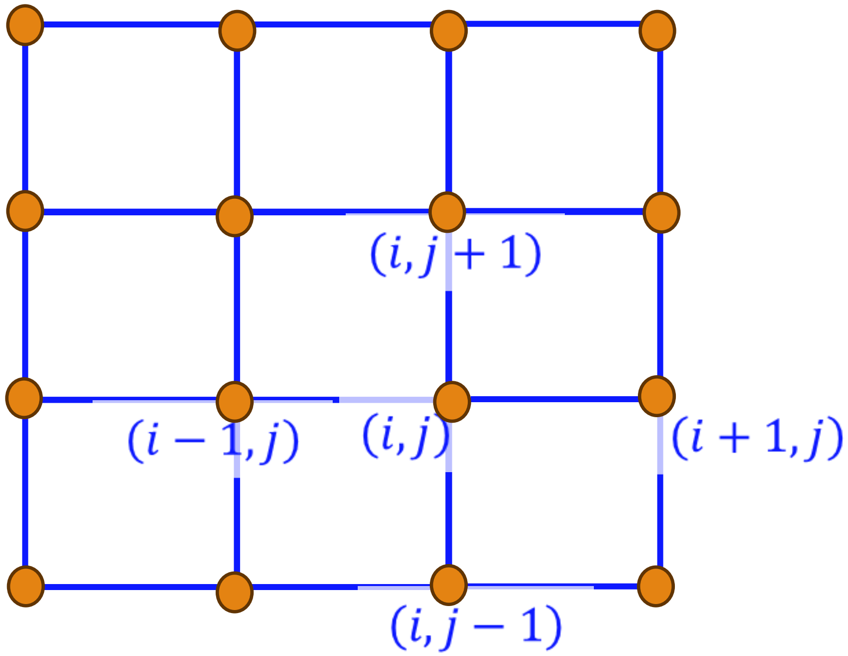



- Flow properties are assigned at each grid locations.

# Finite Difference – Finite Volume

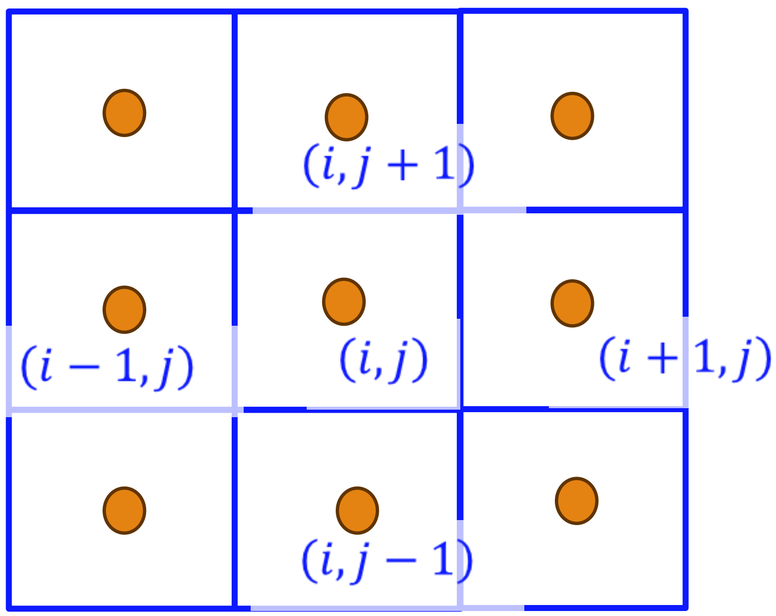
## Differential form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$



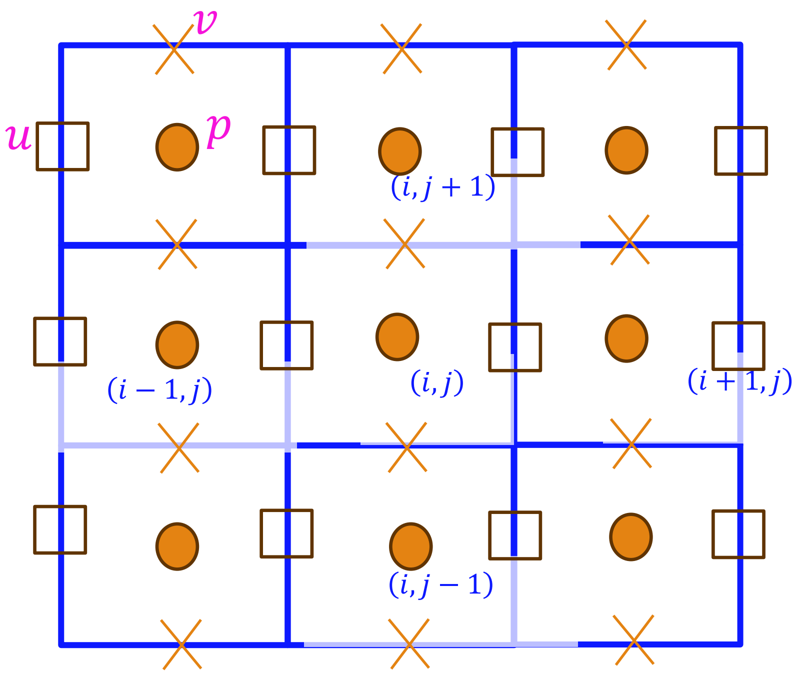

## Integral form

$$\frac{\partial}{\partial t}\int_V \rho dV + \oint_S \rho \boldsymbol{u} \cdot d\boldsymbol{S} = 0$$

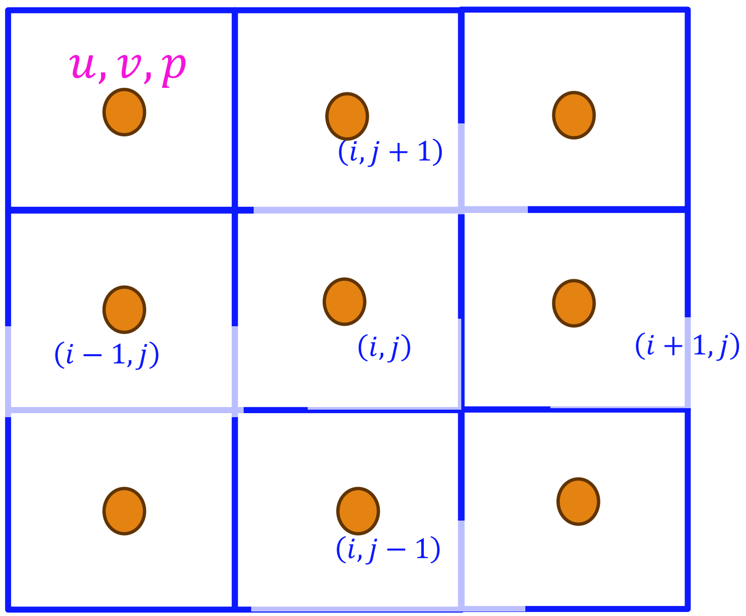


# Numerical discretization (Grid layout)

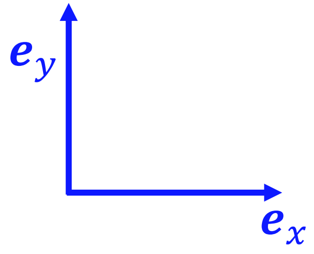
- Cell centered representation




Staggered grid

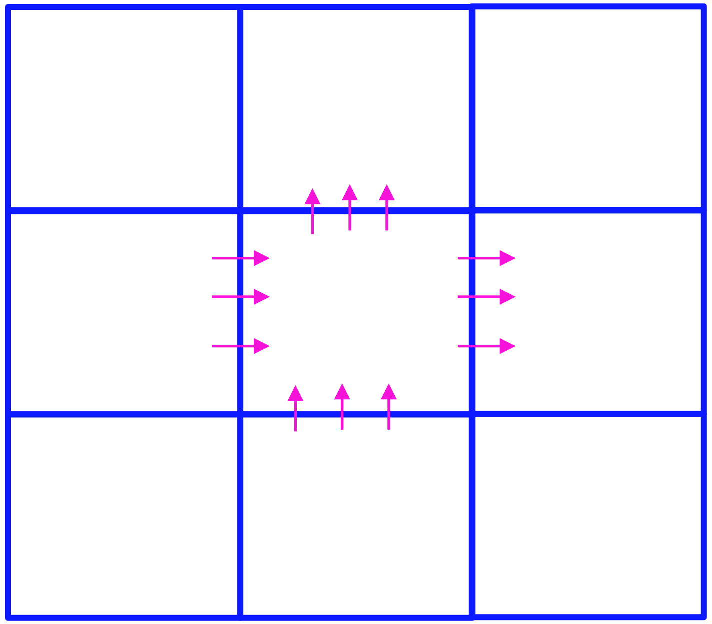



Collocated grid



# Eulerian frame

- Conservation laws are applied around a fixed "control volume" in space
- Flux of quantities through the boundary is used to estimate the flow variables
- Useful to take observations at fixed locations



# Integral Form – Differential Form

- Conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

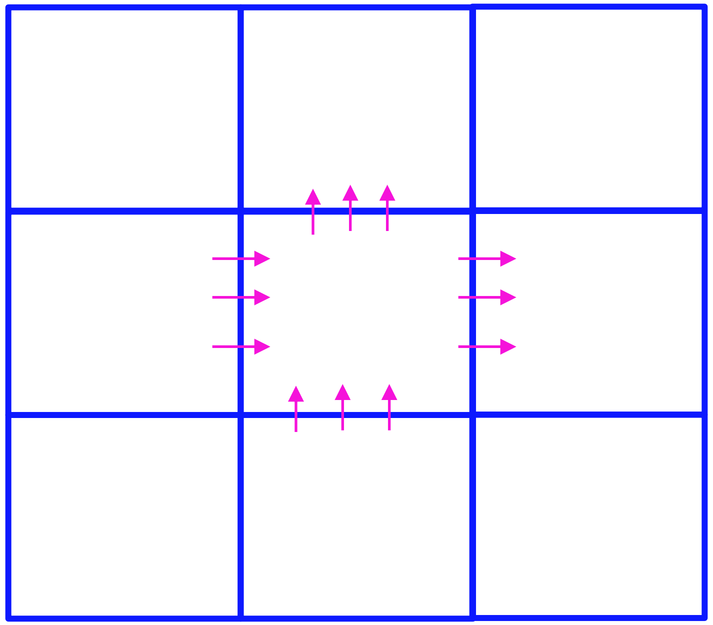
- Integrate over a control volume

$$\int_V \left( \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) \right) dV = 0$$

$$\int_V \frac{\partial \rho}{\partial t} dV + \int_V \nabla \cdot (\rho \boldsymbol{u}) dV = 0$$

$$\frac{\partial}{\partial t} \int_V \rho dV + \oint_S \rho \boldsymbol{u} \cdot d\boldsymbol{S} = 0$$

Gauss – divergence theorem



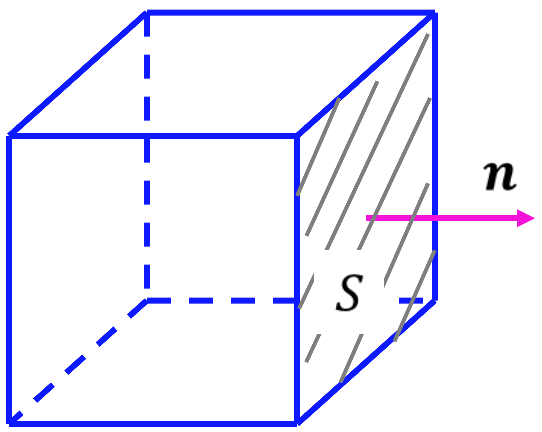
# Gauss Divergence Theorem

- Surface Area Vector: $\boldsymbol{S}$

$$\boldsymbol{S} = |\boldsymbol{S}|\boldsymbol{n}$$

$$\boldsymbol{S} = S\boldsymbol{n}$$

- Extensive property: $\boldsymbol{\Phi}$
- Intensive property: $\phi$
  - Conserved property calculated by mass
- Mass: $\rho V = \int_V \rho dV$

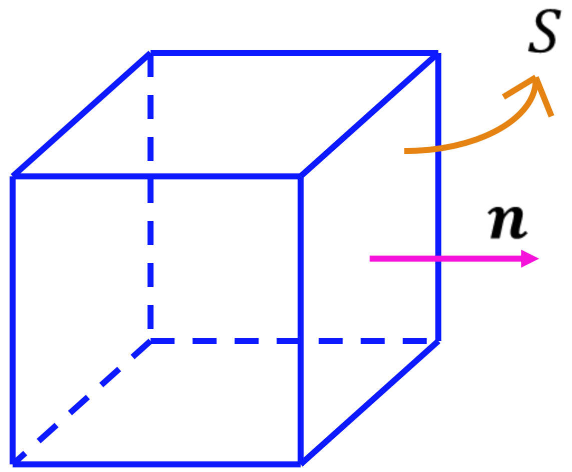


# Gauss Divergence Theorem

- For a vector: $\boldsymbol{F}$

$$\int (\nabla \cdot \boldsymbol{F}) d\boldsymbol{V} \approx \sum \boldsymbol{F} \cdot \boldsymbol{S}$$

- Rate of change of a quantity over a control volume = Rate of flow through control surface.



# Gauss Divergence Theorem

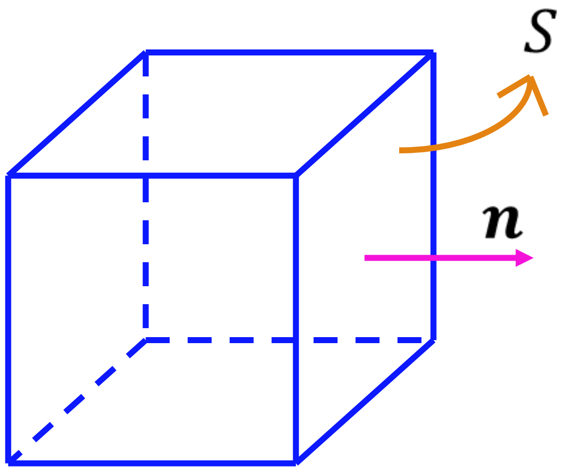
- For a vector: $\boldsymbol{F}$

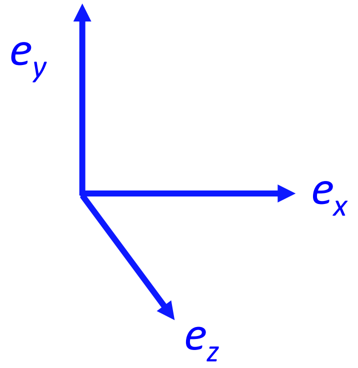
$$\int (\boldsymbol{\nabla} \cdot \boldsymbol{F}) \boldsymbol{dV} \approx \sum \boldsymbol{F} \cdot \boldsymbol{S}$$

Let: $\boldsymbol{F} = x\boldsymbol{e}_x + y\boldsymbol{e}_y$

$$\int (\boldsymbol{\nabla} \cdot \boldsymbol{F}) \boldsymbol{dV} = \int \left( \frac{\partial}{\partial x} \boldsymbol{e}_x + \frac{\partial}{\partial y} \boldsymbol{e}_y \right) \cdot \left( x\boldsymbol{e}_x + y\boldsymbol{e}_y \right) \boldsymbol{dV}$$

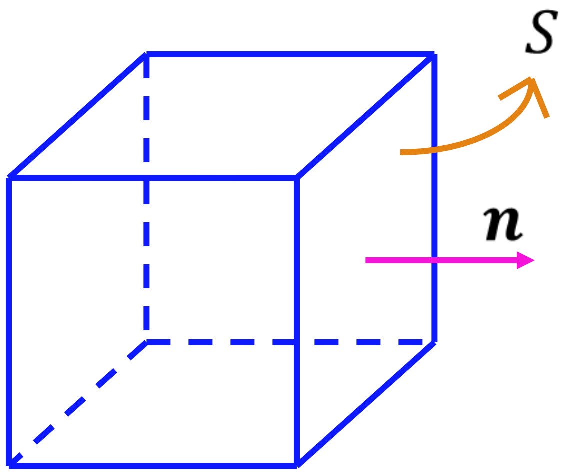
$$\nabla \cdot \boldsymbol{u} = \left( \frac{\partial}{\partial x} \boldsymbol{e}_x + \frac{\partial}{\partial y} \boldsymbol{e}_y + \frac{\partial}{\partial z} \boldsymbol{e}_z \right) \left( u\boldsymbol{e}_x + v\boldsymbol{e}_y + w\boldsymbol{e}_z \right) = \left( \frac{\partial u}{\partial x} + \frac{\partial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



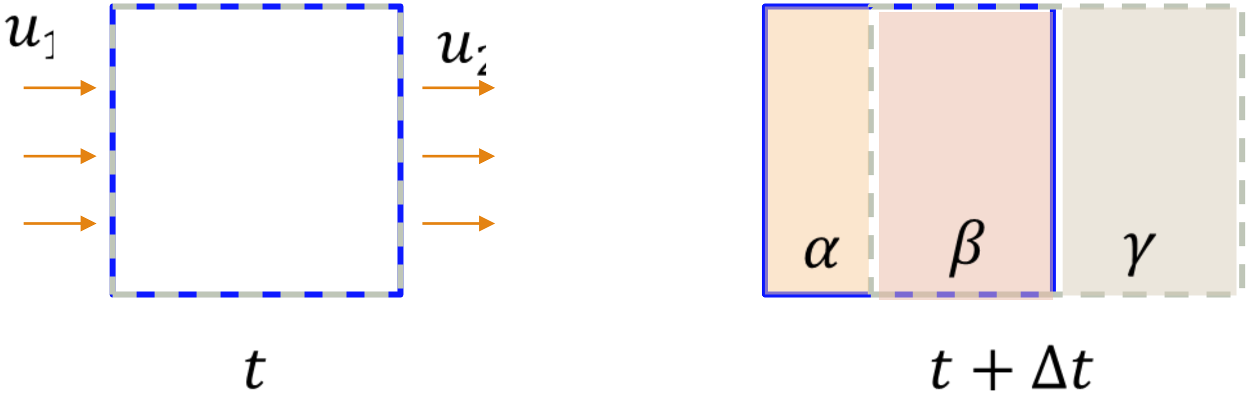
# Reynolds Transport Theorem

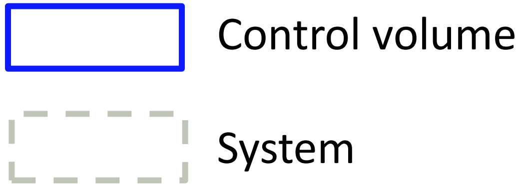
$$\boxed{\frac{d}{dt}\int_{V_S} \rho\phi dV = \frac{d}{dt}\int_{V_{CV}} \rho\phi dV + \int_S \rho\phi \boldsymbol{u}\cdot\boldsymbol{n} dS}$$



# Reynolds Transport Theorem

$$\frac{d}{dt}\int_{V_S} \rho\phi dV = \frac{d}{dt}\int_{V_{CV}} \rho\phi dV + \int_{S} \rho\phi \boldsymbol{u}\cdot\boldsymbol{n} dS$$



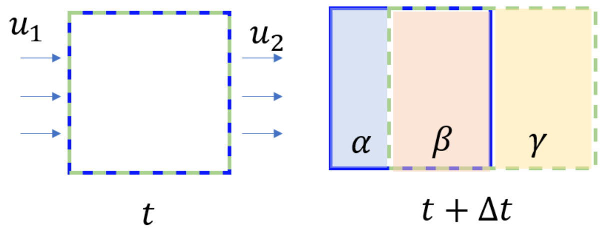

$$(1) \quad \Phi_S(t) = \Phi_{CV}(t)$$

$$(2) \quad \Phi_S(t+\Delta t) = \Phi_{CV}(t+\Delta t) - \Phi_\alpha + \Phi_\gamma$$

# Reynolds Transport Theorem

$$(1)\quad \Phi_S(t) = \Phi_{CV}(t)$$

$$(2)\quad \Phi_S(t+\Delta t) = \Phi_{CV}(t+\Delta t) - \Phi_\alpha + \Phi_\gamma$$

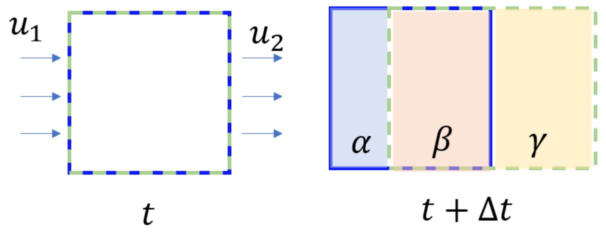



Subtract (1) from (2)

$$\left(\frac{\Phi(t+\Delta t) - \Phi(t)}{\Delta t}\right)_{System} = \left(\frac{\Phi(t+\Delta t) - \Phi(t)}{\Delta t}\right)_{CV} - \dot{\Phi}_\alpha + \dot{\Phi}_\gamma$$

$$\frac{d\Phi}{dt}_{System} = \frac{d\Phi}{dt}_{CV} - \dot{\Phi}_\alpha + \dot{\Phi}_\gamma$$

# Reynolds Transport Theorem




$$\left.\frac{d\Phi}{dt}\right|_{System} = \left.\frac{d\Phi}{dt}\right|_{CV} - \dot{\Phi}_\alpha + \dot{\Phi}_\gamma$$

$$\Phi_\alpha = \phi_\alpha m_\alpha = \phi_\alpha \rho_\alpha V_\alpha = \phi_\alpha \rho_\alpha (u_1 \Delta t) S$$

Using $\Phi = \int \rho\phi dV$ and net flux as $\int \rho\phi \boldsymbol{u} \cdot \boldsymbol{n} dS$

$$\frac{d}{dt}\int_{V_S} \rho\phi dV = \frac{d}{dt}\int_{V_{CV}} \rho\phi dV + \int_S \rho\phi \boldsymbol{u} \cdot \boldsymbol{n} dS$$

# Conservation Laws

$$\frac{d}{dt}\int_{V_S} \rho\phi dV = \frac{d}{dt}\int_{V_{CV}} \rho\phi dV + \int_{S} \rho\phi \boldsymbol{u}\cdot\boldsymbol{n} dS$$

- Conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}) = 0; \quad \nabla\cdot(\rho\boldsymbol{u}) = \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z}$$

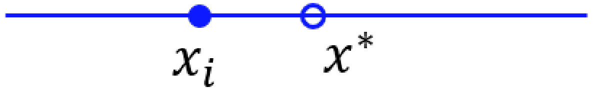
- Conservation of momentum

$$\frac{\partial \rho\boldsymbol{u}}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla\cdot\boldsymbol{\sigma} + \rho\boldsymbol{g};$$

- Scalar conservation law

$$\frac{\partial \rho\phi}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}\phi) = \nabla\cdot(\Gamma\nabla\phi) + S_\phi$$

# Taylor series




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


$$\boxed{\left(\frac{d\rho}{dx}\right)_i \approx \frac{\rho(x_{i+1}) - \rho(x_i)}{\Delta x_i}}$$

$$\boxed{\left(\frac{d\rho}{dx}\right)_i \approx \frac{\rho(x_{i+1}) - \rho(x_{i-1})}{2\Delta x_i}}$$

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

First Order Derivative
forward difference

First Order Derivative
Second order central difference

Second Order Derivative
Second order central difference

# Exercise – 3 ➔ Octave

(1) Derive second order derivative for central difference scheme. (Use Pen and paper)


$$\rho(x_{i+1}) = \rho(x_i) + (x_{i+1} - x_i)\left(\frac{d\rho}{dx}\right)_i + \frac{(x_{i+1} - x_i)^2}{2}\left(\frac{d^2\rho}{dx^2}\right)_i + \frac{(x_{i+1} - x_i)^3}{6}\left(\frac{d^3\rho}{dx^3}\right)_i + \frac{(x_{i+1} - x_i)^4}{24}\left(\frac{d^4\rho}{dx^4}\right)_i + \cdots$$

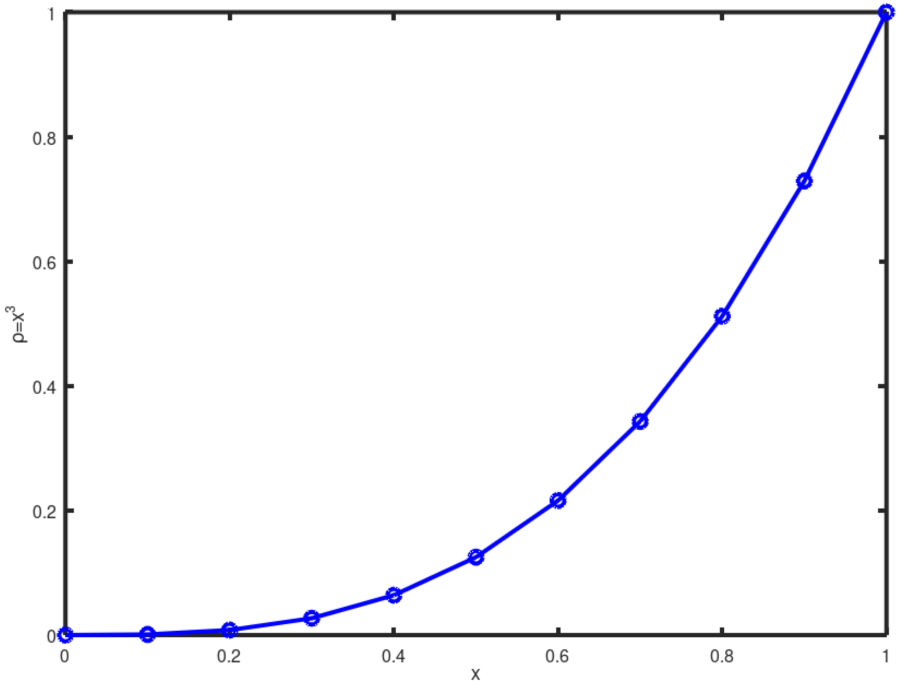
$$(1)\quad \rho(x_{i+1}) = \rho(x_i) + \Delta x_i\left(\frac{d\rho}{dx}\right)_i + \frac{\Delta x_i^2}{2}\left(\frac{d^2\rho}{dx^2}\right)_i + \frac{\Delta x_i^3}{6}\left(\frac{d^3\rho}{dx^3}\right)_i + \frac{\Delta x_i^4}{24}\left(\frac{d^4\rho}{dx^4}\right)_i + O(\Delta x_i^5)$$

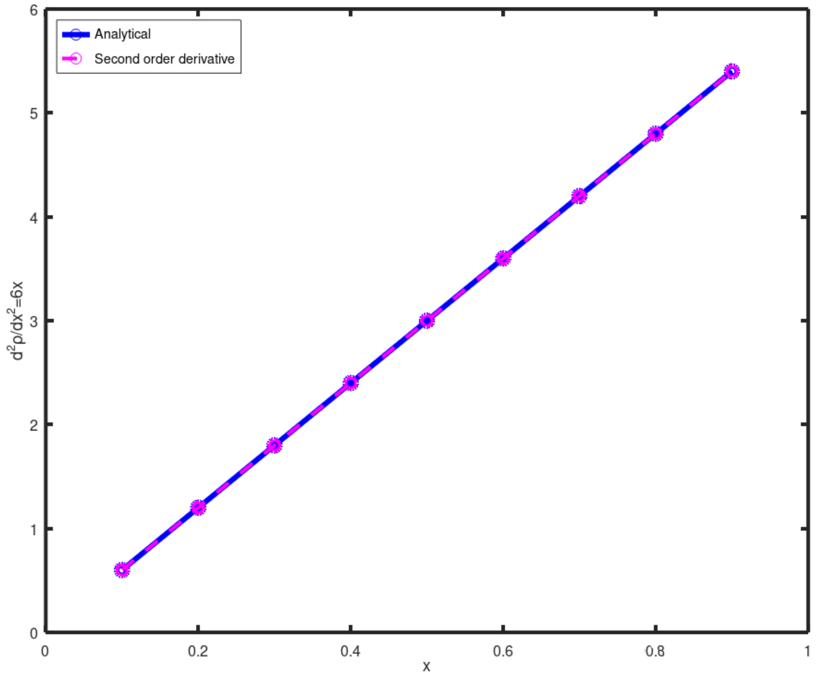
$$(2)\quad \rho(x_{i-1}) = \rho(x_i) - \Delta x_i\left(\frac{d\rho}{dx}\right)_i + \frac{\Delta x_i^2}{2}\left(\frac{d^2\rho}{dx^2}\right)_i - \frac{\Delta x_i^3}{6}\left(\frac{d^3\rho}{dx^3}\right)_i + \frac{\Delta x_i^4}{24}\left(\frac{d^4\rho}{dx^4}\right)_i + O(\Delta x_i^5)$$

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

# Approximating Second Order Derivative

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



https://github.com/Kumaresh0402/SpecialTopicsinComputationalFluidDynamics/discussions/4

# Exercise – 3


1. Use pen and paper to derive $\left(\frac{d^2\rho}{dx^2}\right)_i$
2. This is called second order central difference method. Write the code in Octave.
3. What is the accuracy of the resultant expression ?
4. Paste the respective images in the GitHub and state your comments.