# Contents

- Governing Equations

- Gauss Divergence Theorem

- Reynolds Transport Theorem

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Lagrangian frame – discrete phase

ExaSlate
Develop ≡ Guide ≡ Collab

$$p_1$$

$$\epsilon$$

$$p_3 \qquad p_2$$
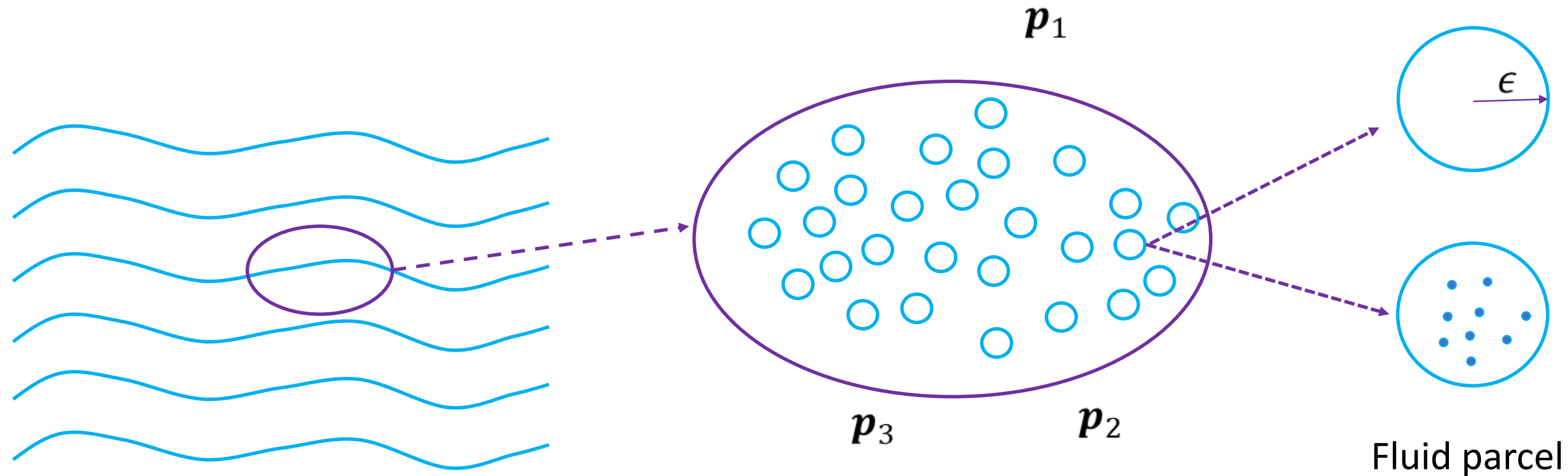
Fluid parcel

- Follow a fluid parcel $(\boldsymbol{p}_1, \boldsymbol{p}_2, \dots)$
- Flow property at a location is obtained from the fluid parcel that happens to be at that location at that time
- Useful to derive conservation laws

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# 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

**Kumaresh Selvakumar**
kumaresh@exaslate.com
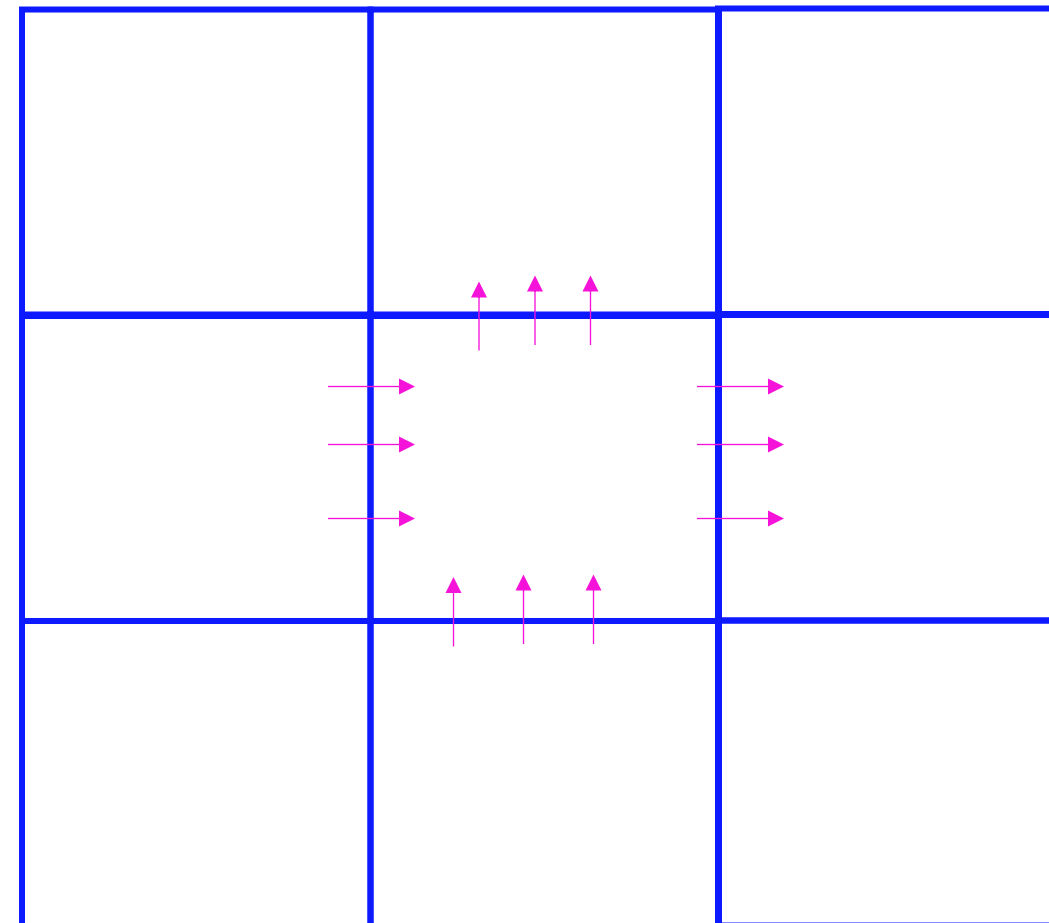
# Governing Equations

- The general equation can be written in the form as:

$$\frac{\partial}{\partial t}\left(\rho\phi\right) + \nabla\bullet\left(\rho u\phi\right) = \nabla\bullet(\Gamma\nabla\phi) + S$$

$$\frac{\partial}{\partial t}\left(\rho\phi\right) + \frac{\partial}{\partial x_j}\left(\rho u_j\phi\right) = \frac{\partial}{\partial x_j}\left(\Gamma\frac{\partial\phi}{\partial x_j}\right) + S$$

$$\frac{\partial}{\partial t}\iiint \rho\phi\,\mathrm{dV} + \iint \rho\phi\left(u.\mathrm{dA}\right) = \iint \Gamma\nabla\phi.\,\mathrm{dA} + \iiint S\mathrm{dV}$$

**1**  **2**  **3**  **4**

**1**  Unsteady/Transient term     **3**  Diffusion term

**2**  Advection/Convection term    **4**  Source term

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Governing Equations

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla\bullet(\rho u\phi) = \nabla\bullet(\Gamma\nabla\phi) + S$$

Continuity equation: $\phi = 1, S = 0$ ➔ $\boxed{\dfrac{\partial}{\partial t}(\rho) + \nabla\bullet(\rho u) = 0}$

Momentum equation: $\phi = u, \Gamma = \mu, S = S_u$ ➔ $\boxed{\dfrac{\partial}{\partial t}(\rho u) + \nabla\bullet(\rho u u) = \nabla\bullet(\mu\,\nabla u) - \nabla p + S_u}$

Energy equation: $\phi = h, \Gamma = k/C_p, S = S_h$ ➔ $\boxed{\dfrac{\partial}{\partial t}(\rho h) + \nabla\bullet(\rho u h) = \nabla\bullet\left(\dfrac{k}{C_p}\,\nabla h\right) + S_h}$

Species equation: $\phi = h, \Gamma = \Gamma_l, S = S_m$ ➔ $\boxed{\dfrac{\partial}{\partial t}(\rho m_l) + \nabla\bullet(\rho u m_l) = \nabla\bullet(\Gamma_l\nabla m_l) + S_m}$

Turbulence equation: $\phi = k(or)\varepsilon, \Gamma = \Gamma_k(or)\Gamma_\varepsilon, S = S_k(or)S_\varepsilon$ ➔ $\boxed{\dfrac{\partial}{\partial t}(\rho k) + \nabla\bullet(\rho u k) = \nabla\bullet(\Gamma_k\nabla k) + S_k}$

Ideal Gas equation: $\boxed{p = \rho R T}$

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Integral Form – Differential Form

- Conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
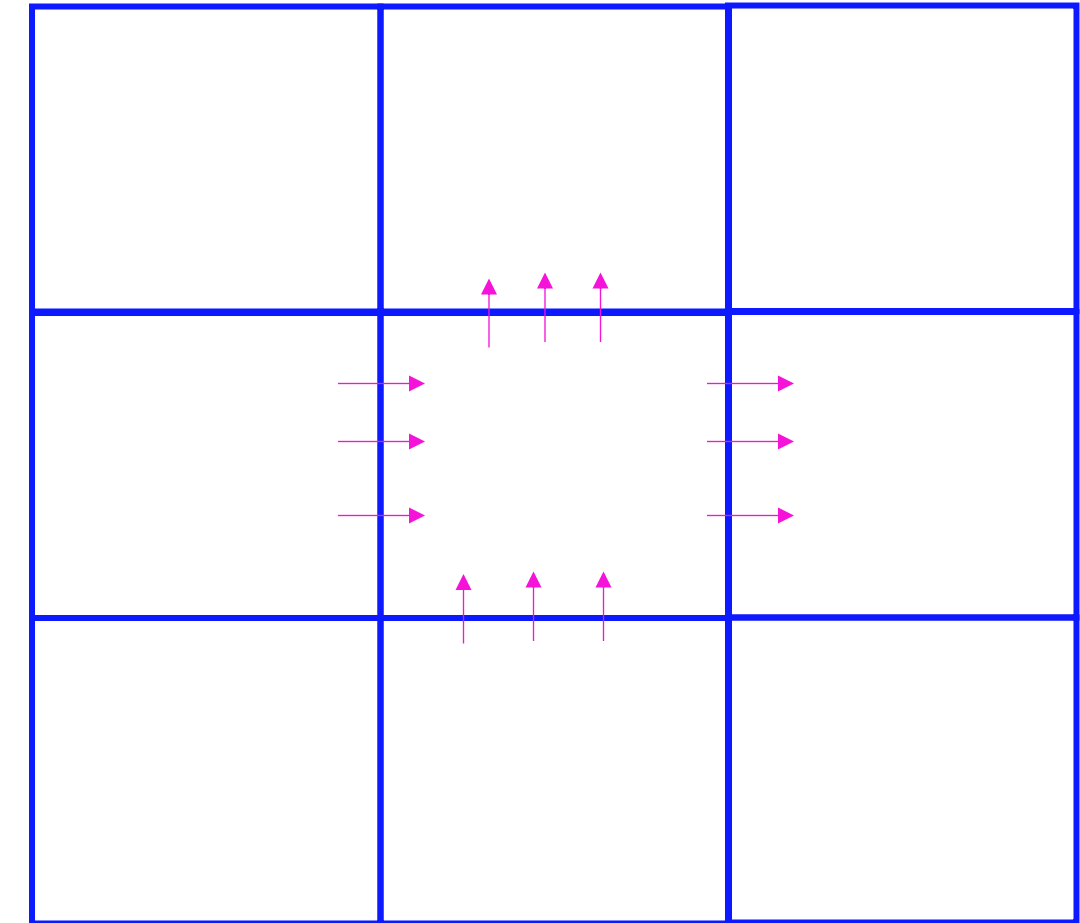
- Integrate over a control volume

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

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

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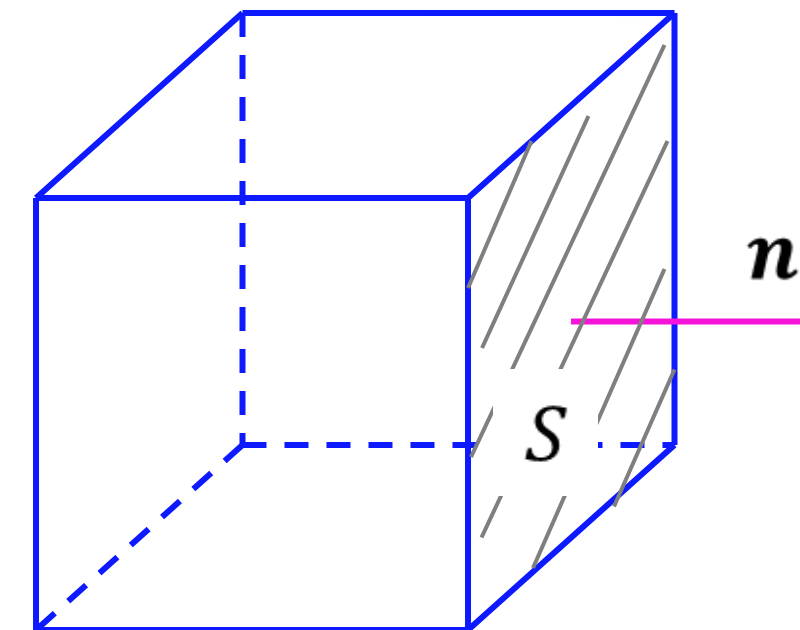
Gauss – divergence theorem

Kumaresh Selvakumar
kumaresh@exaslate.com

# Gauss Divergence Theorem

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

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

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

- 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: $\boldsymbol{F}$

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

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com
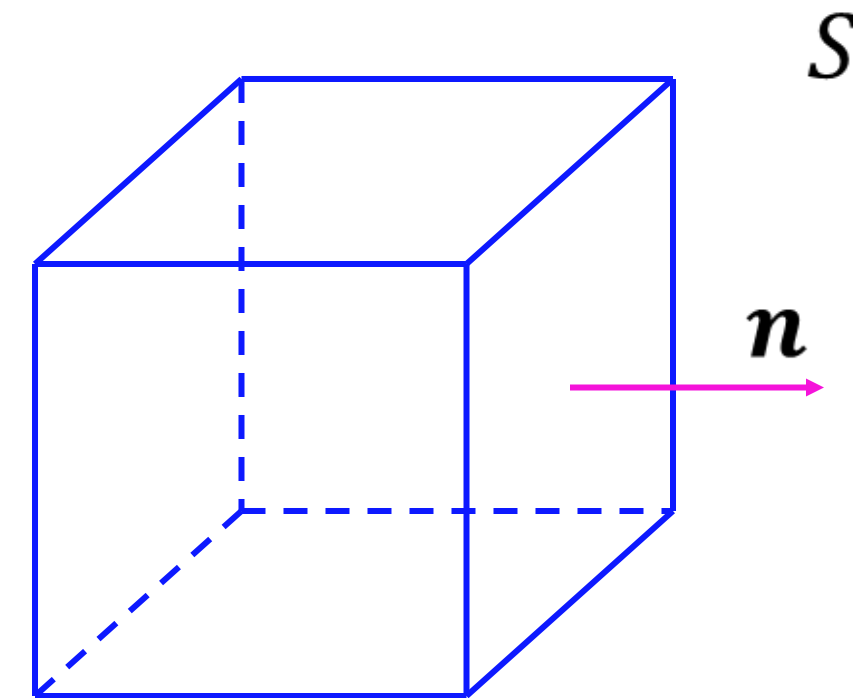
# Gauss Divergence Theorem

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

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

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

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

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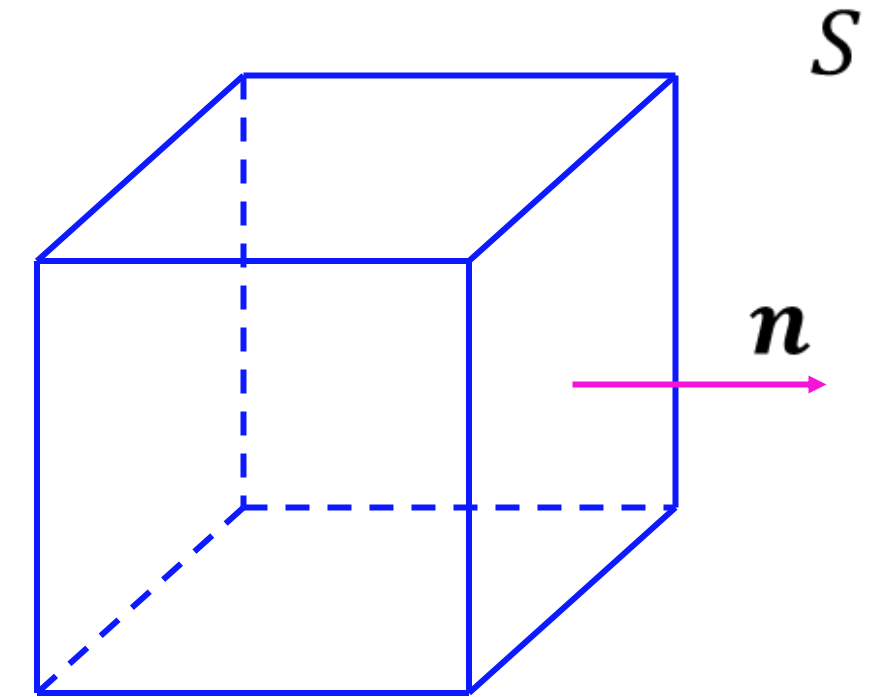
$S$

$\boldsymbol{n}$

$e_y$

$e_x$

$e_z$

**Kumaresh Selvakumar**
kumaresh@exaslate.com
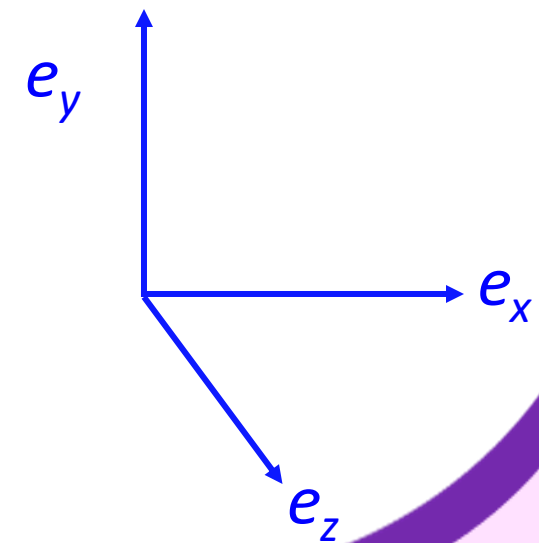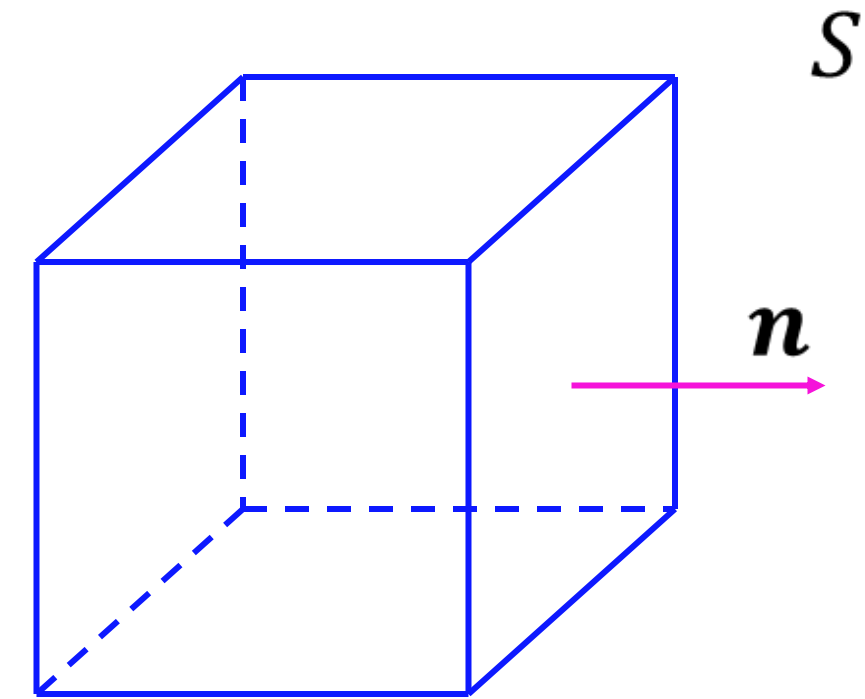
# Gauss Divergence Theorem

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

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

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

$$= \int \left(\frac{\partial x}{\partial x} + \frac{\partial y}{\partial y}\right)dV = 2V$$

$$\sum \boldsymbol{F} \cdot \boldsymbol{S} = \sum (x\boldsymbol{e}_x + y\boldsymbol{e}_y) \cdot \boldsymbol{S}$$

$S$
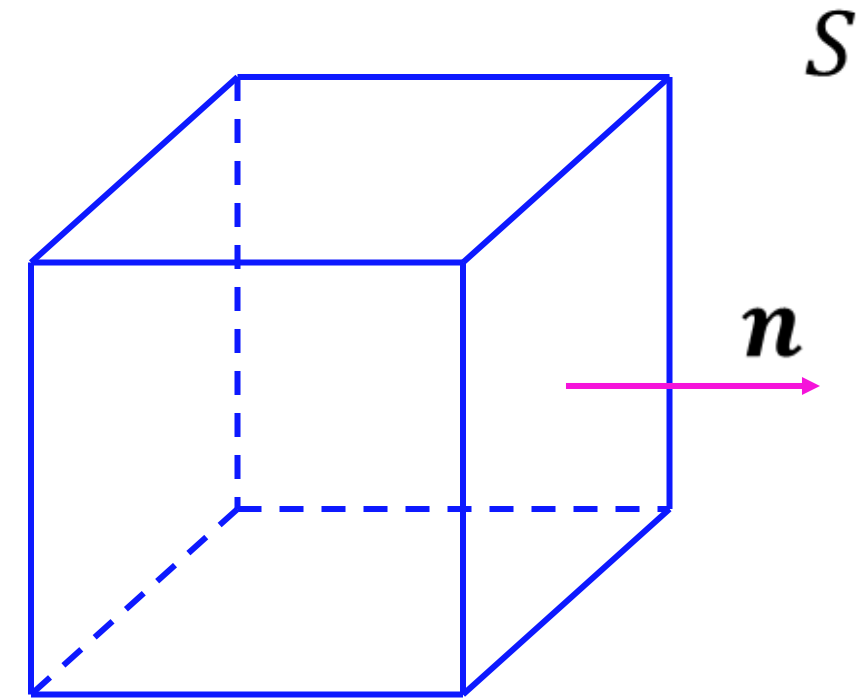
$n$

$S = \Delta x \Delta y$

$V = \Delta x \Delta y \Delta z$
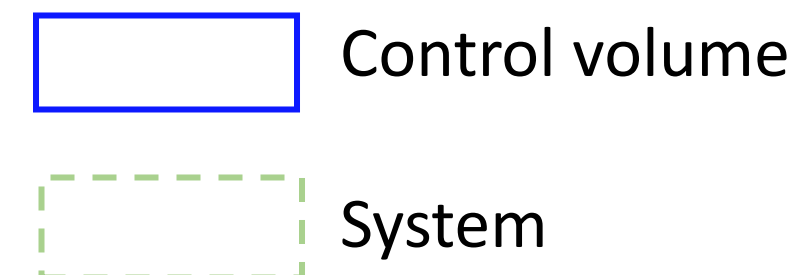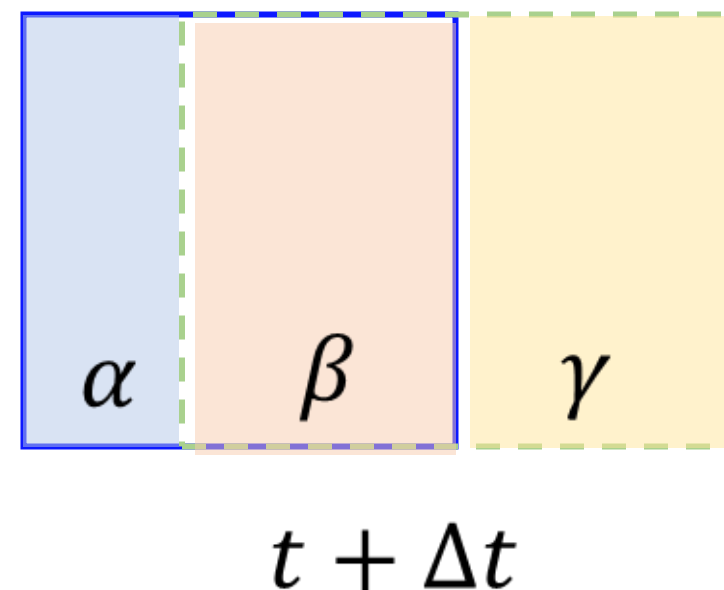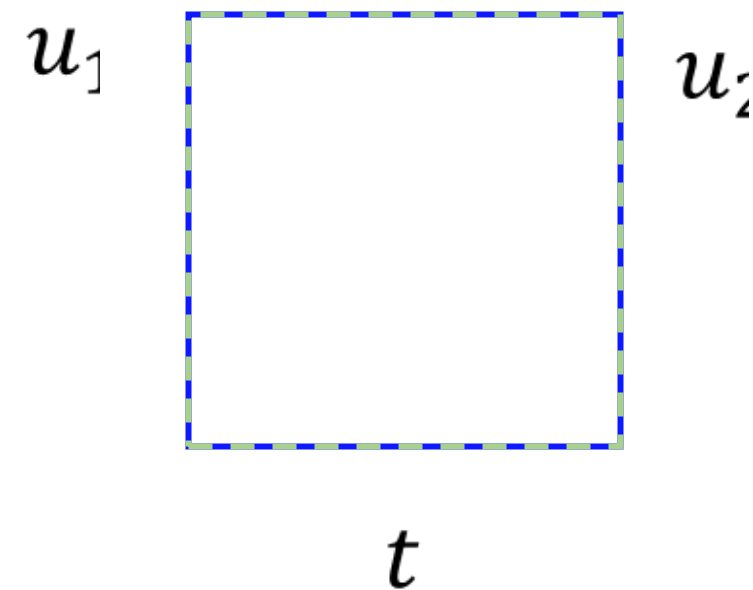
**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Reynolds Transport Theorem

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Reynolds Transport Theorem

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

$u_1$ $u_2$

$t$

$\alpha$ $\beta$ $\gamma$

$t + \Delta t$

Control volume

System

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

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

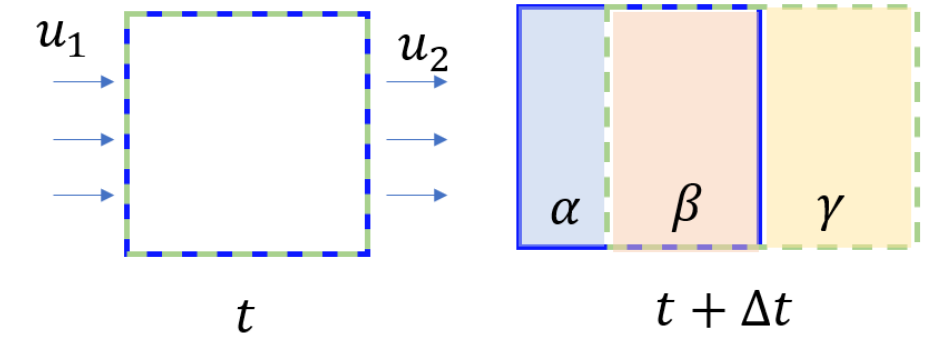# Reynolds Transport Theorem

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

$$(2) \quad \Phi_S(t + \Delta t) = \Phi_{CV}(t + \Delta t) - \Phi_\alpha + \Phi_\gamma$$
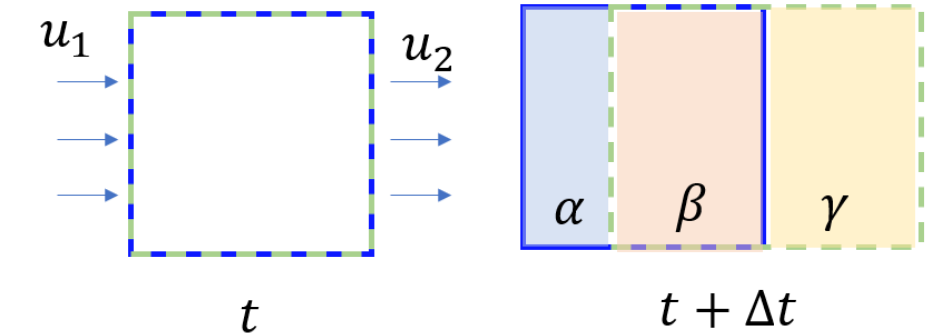
Subtract (1) from (2)

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

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Reynolds Transport Theorem

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



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

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

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Conservation Laws

- Conservation of mass

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

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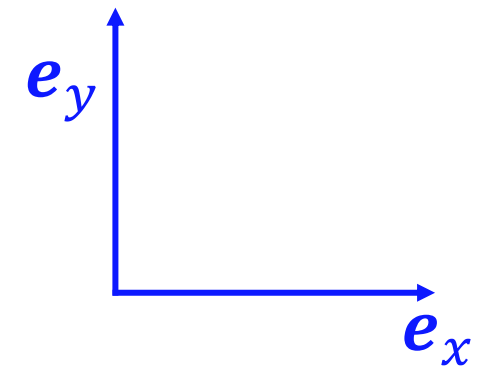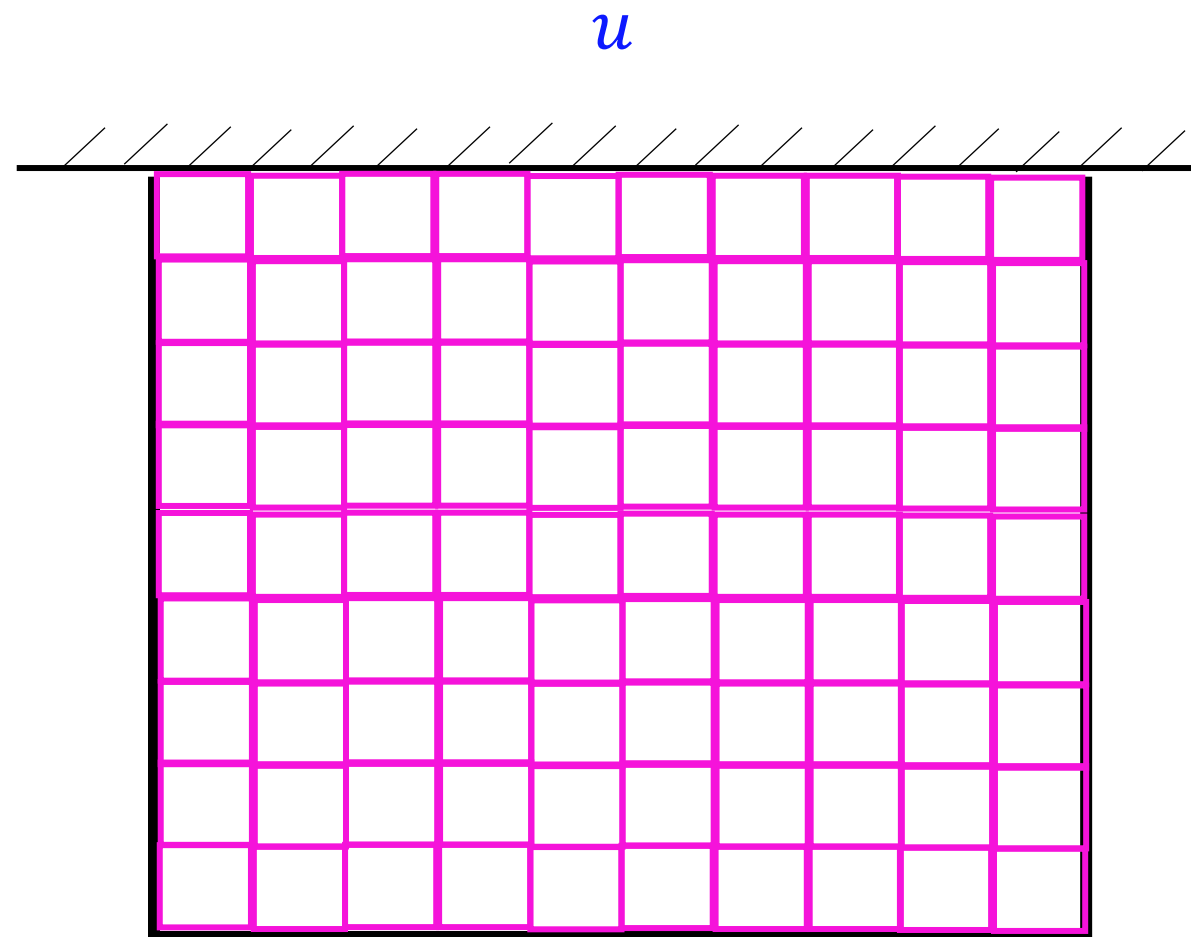
- Conservation of momentum

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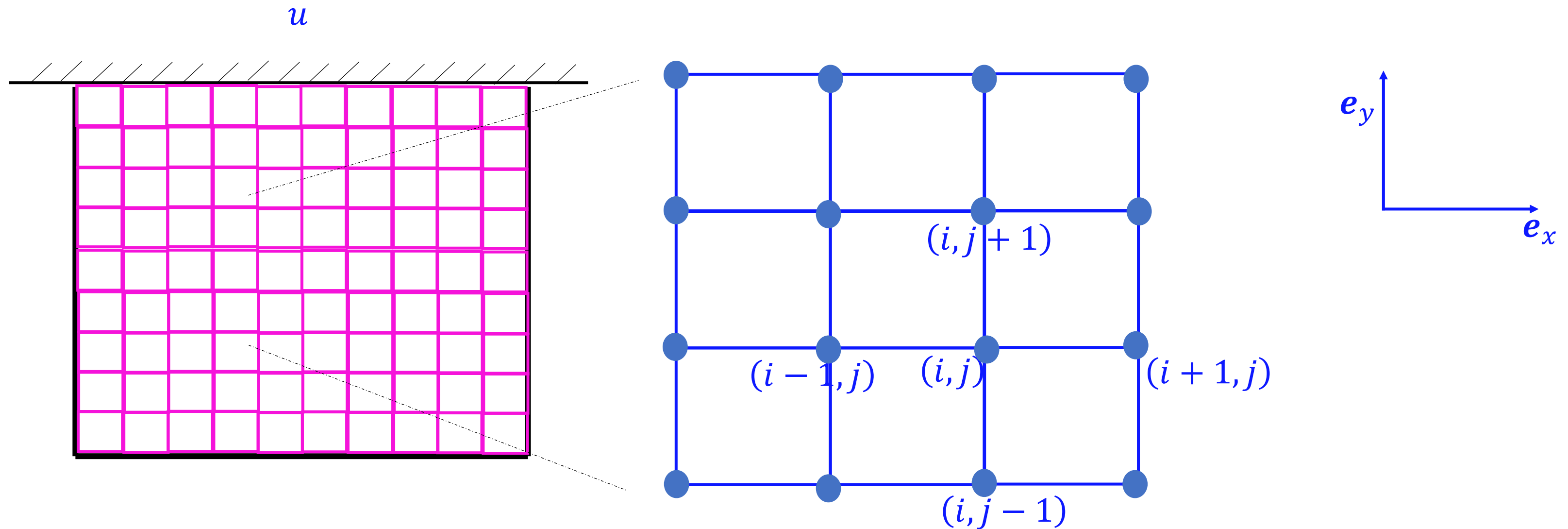
- Scalar conservation law

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Numerical Discretization (Grid layout)

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Numerical Discretization (Grid layout)



- Flow properties are assigned at each grid locations.

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Numerical Discretization (Grid layout)

$u$

$e_y$

$e_x$

$(i, j + 1)$

$(i - 1, j)$  $(i, j)$  $(i + 1, j)$

$(i, j - 1)$

$(i, j + 1)$

$(i - 1, j)$  $(i, j)$  $(i + 1, j)$

$(i, j - 1)$

Cell centered representation

**Kumaresh Selvakumar**
kumaresh@exaslate.com
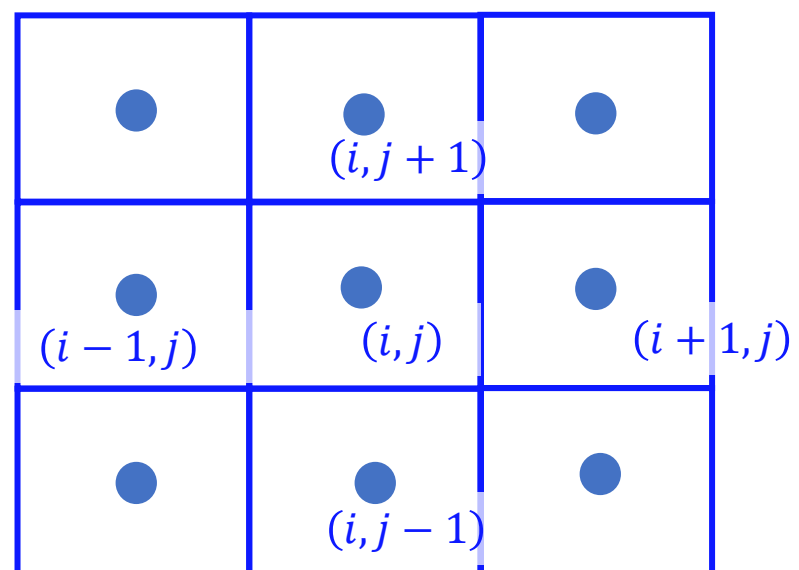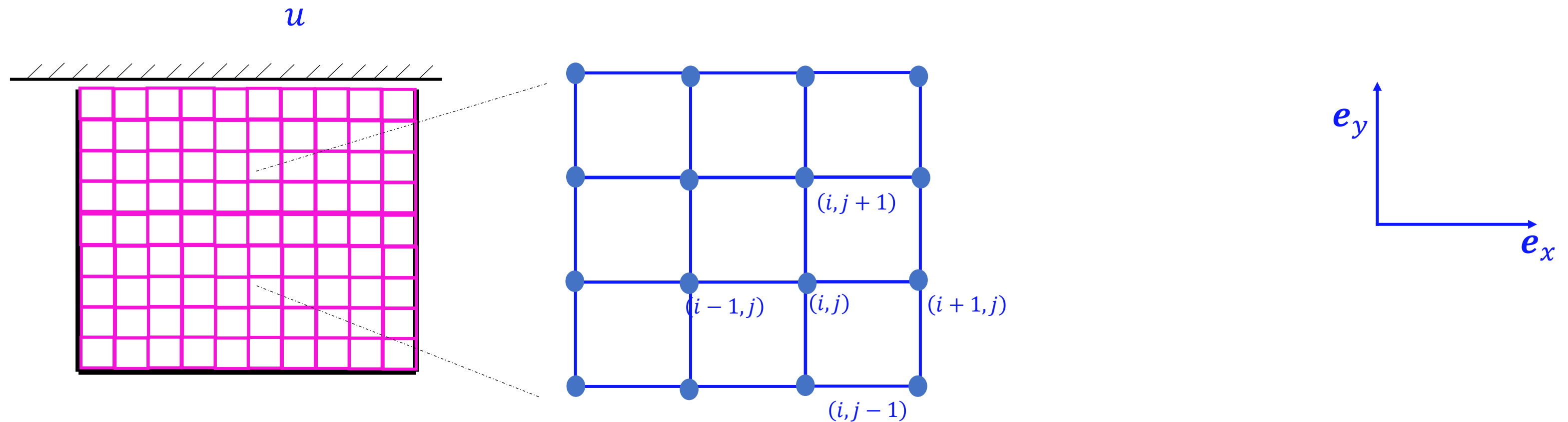
# Numerical Discretization (Grid layout)

- Cell centered representation
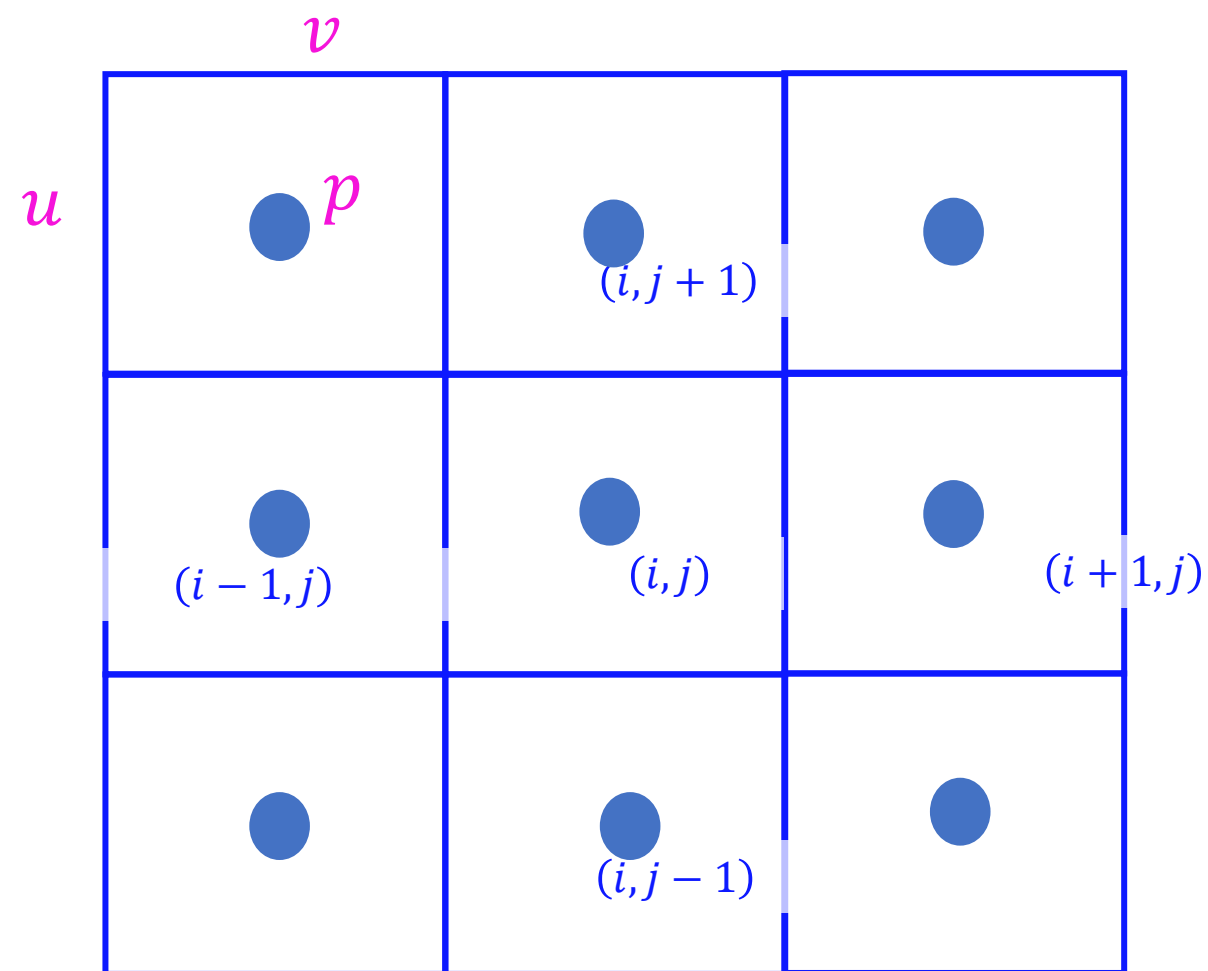


Staggered grid

Collocated grid

**Kumaresh Selvakumar**
kumaresh@exaslate.com
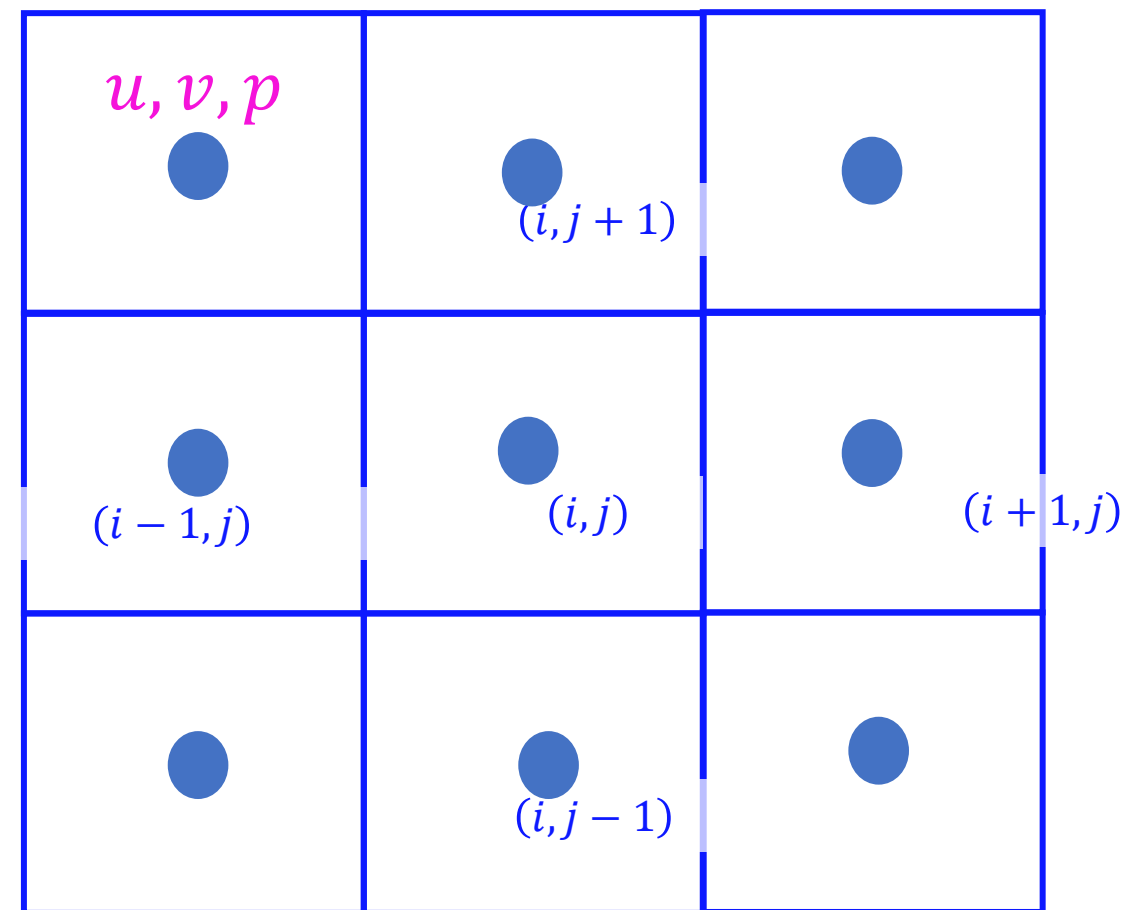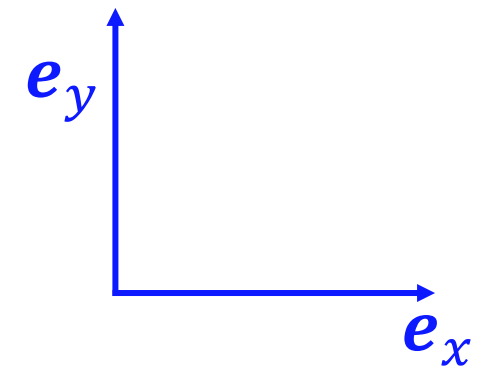
# Finite Difference – Finite Volume

## Differential form

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

$(i, j+1)$

$(i-1, j)$ $(i, j)$ $(i+1, j)$

$(i, j-1)$
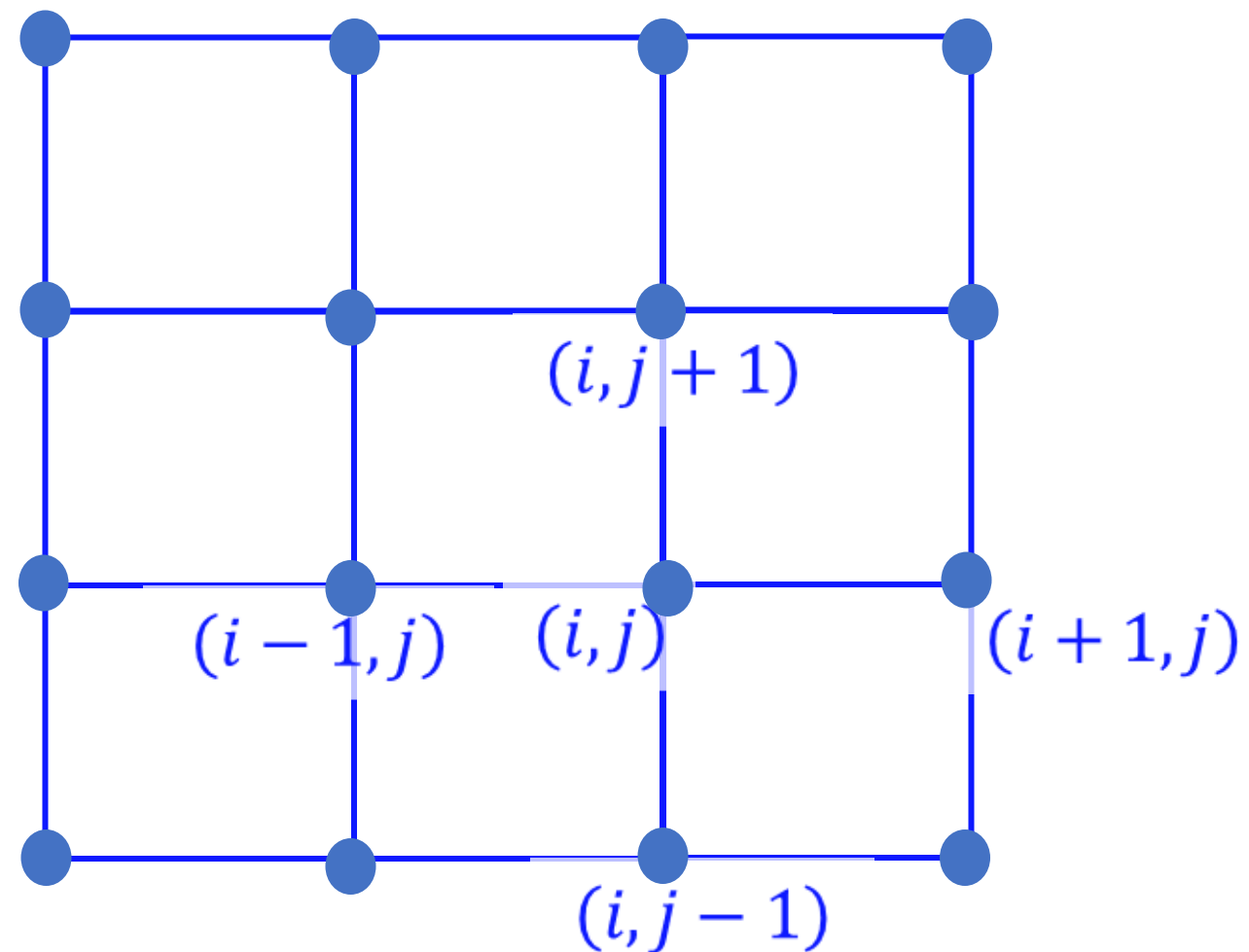
## Integral form

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

$(i, j+1)$

$(i-1, j)$ $(i, j)$ $(i+1, j)$

$(i, j-1)$

**Kumaresh Selvakumar**
kumaresh@exaslate.com
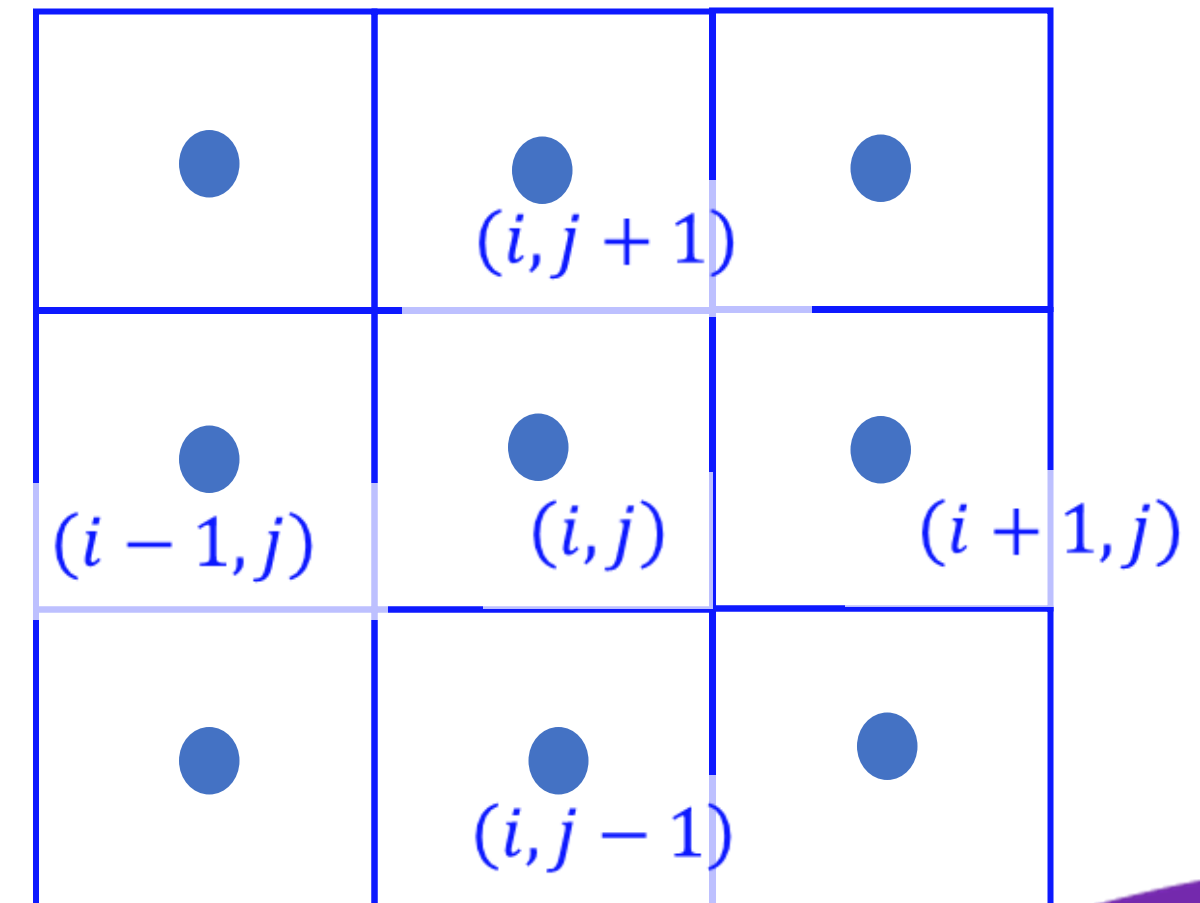
# Taylor series and FDM

## Taylor series:

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

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

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

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

First order forward difference scheme

## Finite difference

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

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Taylor series expansion



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

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

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

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



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

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

Subtract (2) from (1)

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

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

Second order central difference scheme

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Taylor series: Backward Difference Scheme (1st order)

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

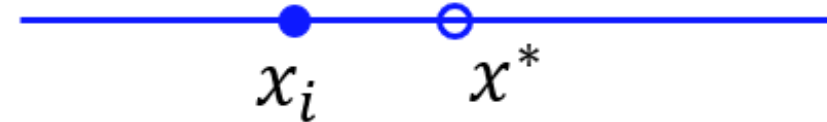$$\rho(x_{i-1}) = \rho(x_i) - \Delta x_i \left(\frac{d\rho}{dx}\right)_i + O(\Delta x_i^2)$$

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

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

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

First order backward difference scheme

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Taylor series: Summary

$$x_i \qquad x^*$$

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

$$x_{i-1} \qquad x_i \qquad x_{i+1} \qquad x_{i+2}$$

First order forward difference

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

Second order central difference

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

First order backward difference

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Approximating Second Order Derivative $\left(\dfrac{d^2\rho}{dx^2}\right)_i$

$$x_{i-1} \quad x_i \quad x_{i+1} \quad x_{i+2}$$

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

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

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Approximating Second Order Derivative

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

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



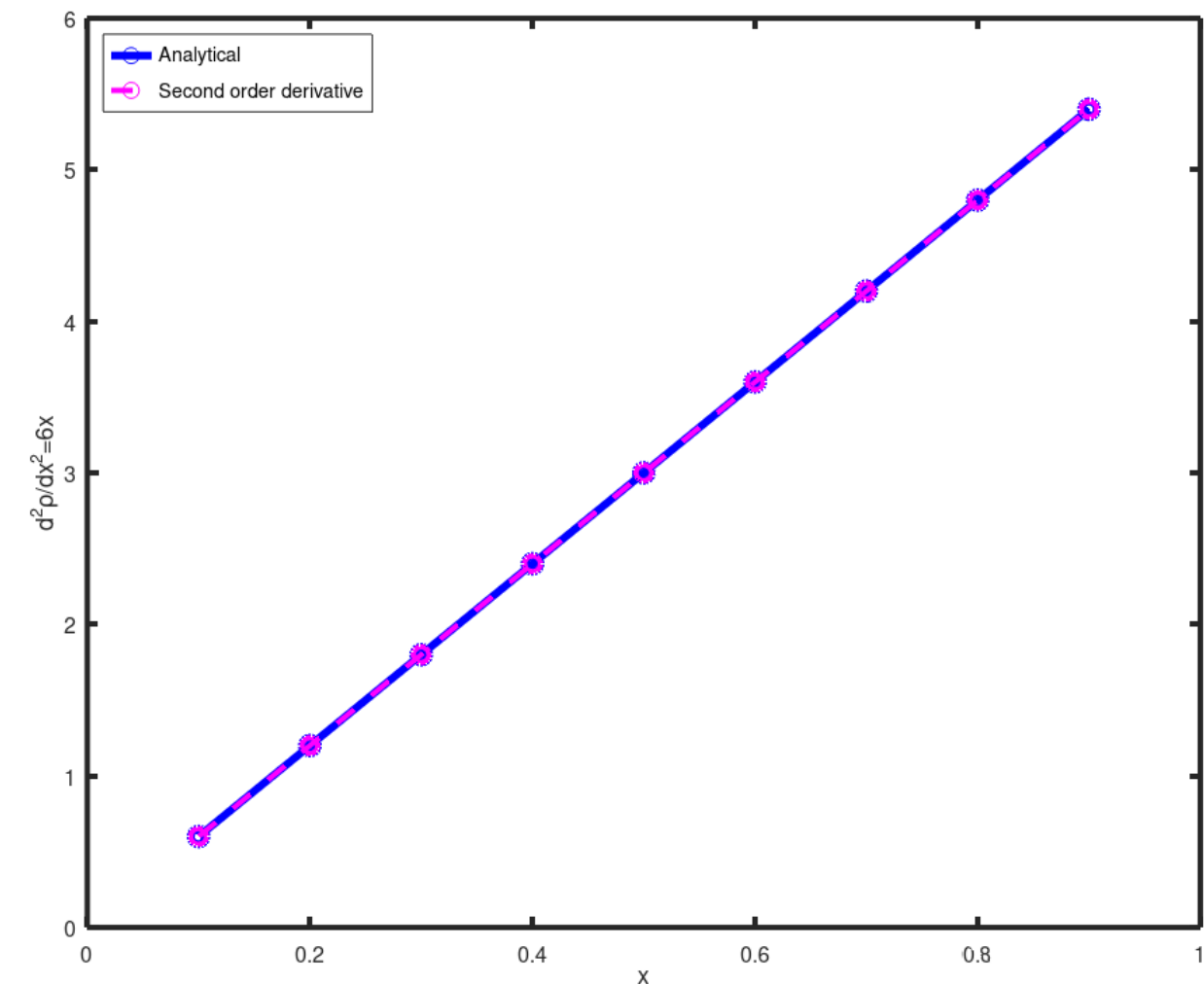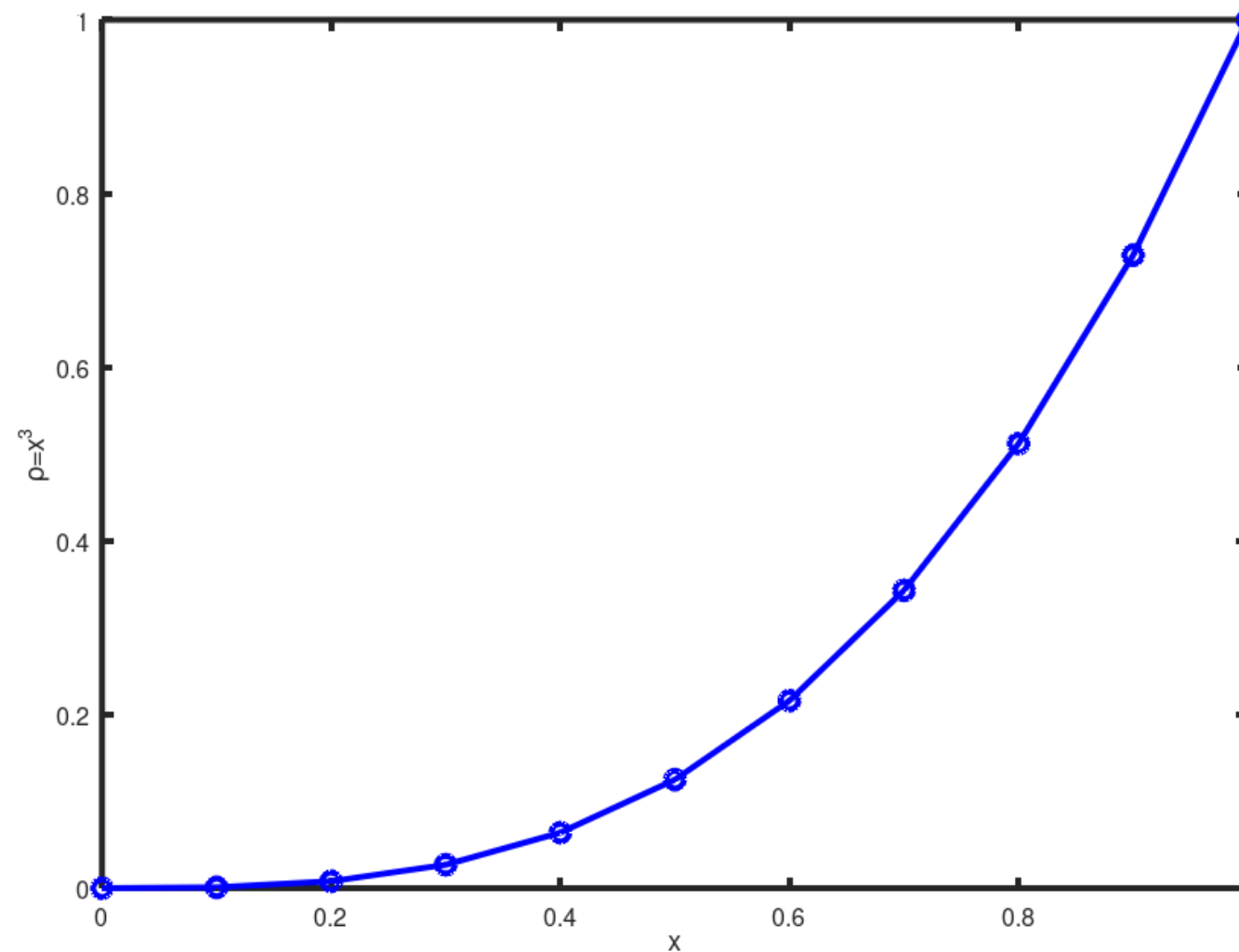$x_{i-1} \quad x_i \quad x_{i+1} \quad x_{i+2}$

Add (1) and (2)

$$\rho(x_{i+1}) + \rho(x_{i-1}) = 2\rho(x_i) + \Delta x_i^2 \left(\frac{d^2\rho}{dx^2}\right)_i + \frac{\Delta x_i^4}{12}\left(\frac{d^4\rho}{dx^4}\right)_i + \cdots$$

$$\left(\frac{d^2\rho}{dx^2}\right)_i = \frac{\rho(x_{i+1}) - 2\rho(x_i) + \rho(x_{i-1})}{\Delta x_i^2} + \frac{\Delta x_i^4}{12\Delta x_i^2}\left(\frac{d^4\rho}{dx^4}\right)_i + \cdots$$

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

**Kumaresh Selvakumar**
kumaresh@exaslate.com

# Approximating Second Order Derivative

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



**Kumaresh Selvakumar**
kumaresh@exaslate.com

**ExaSlate**
Develop ≡ Guide ≡ Collab

[Exercise-6] Estimate second order derivative using second order central difference scheme #7

kummi0402 started this conversation in **General**
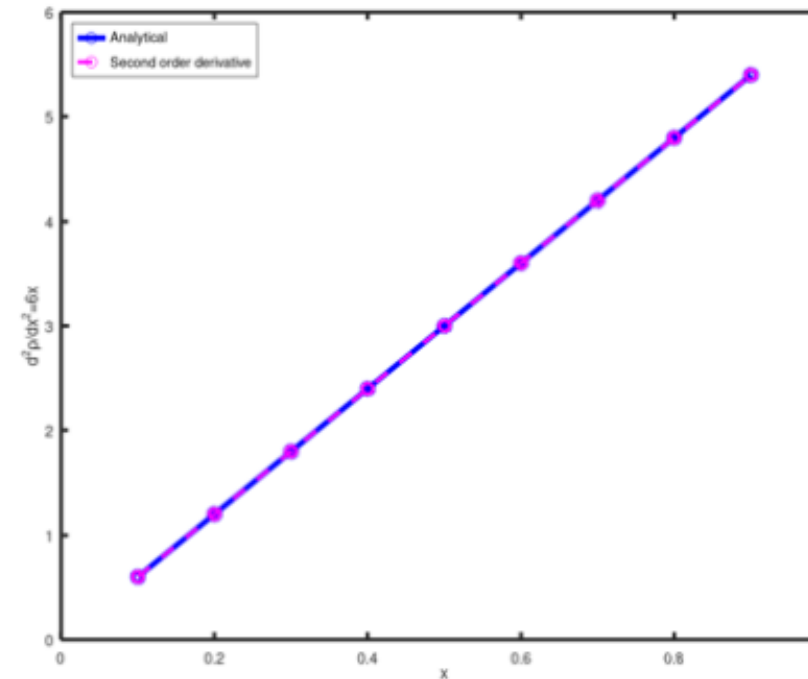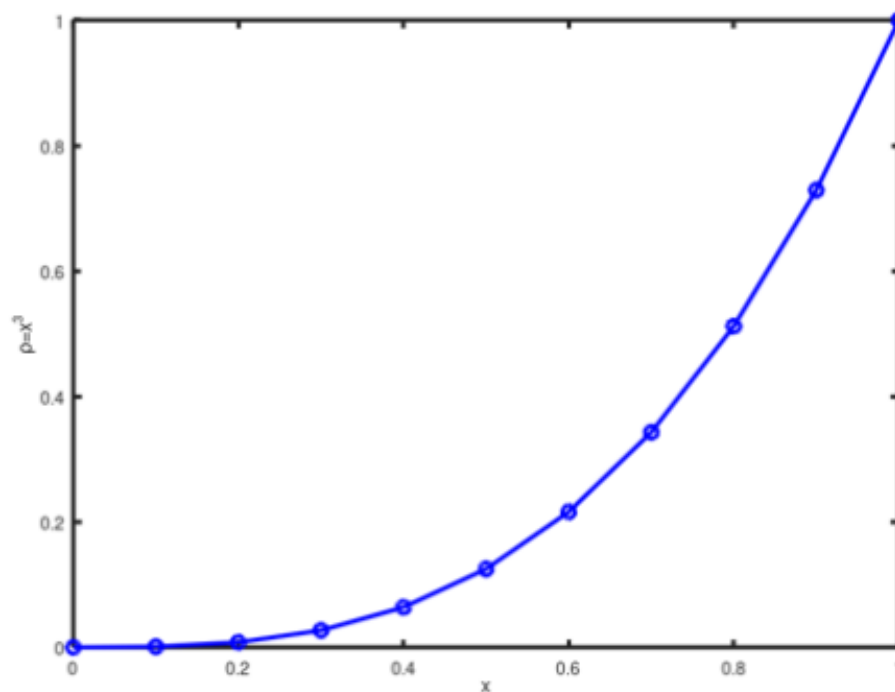


Category
General

Labels
None yet

1 participant

Notifications

🔕 Unsubscribe

You're receiving notifications because you authored the thread.

🔒 Lock conversation
→ Transfer this discussion
📌 Pin discussion
📌 Pin discussion to General
⊙ Create issue from discussion
🗑 Delete discussion

**Kumaresh Selvakumar**
kumaresh@exaslate.com

THANK YOU