Applied Computational Fluid Dynamics with OpenFOAM

Day - 4

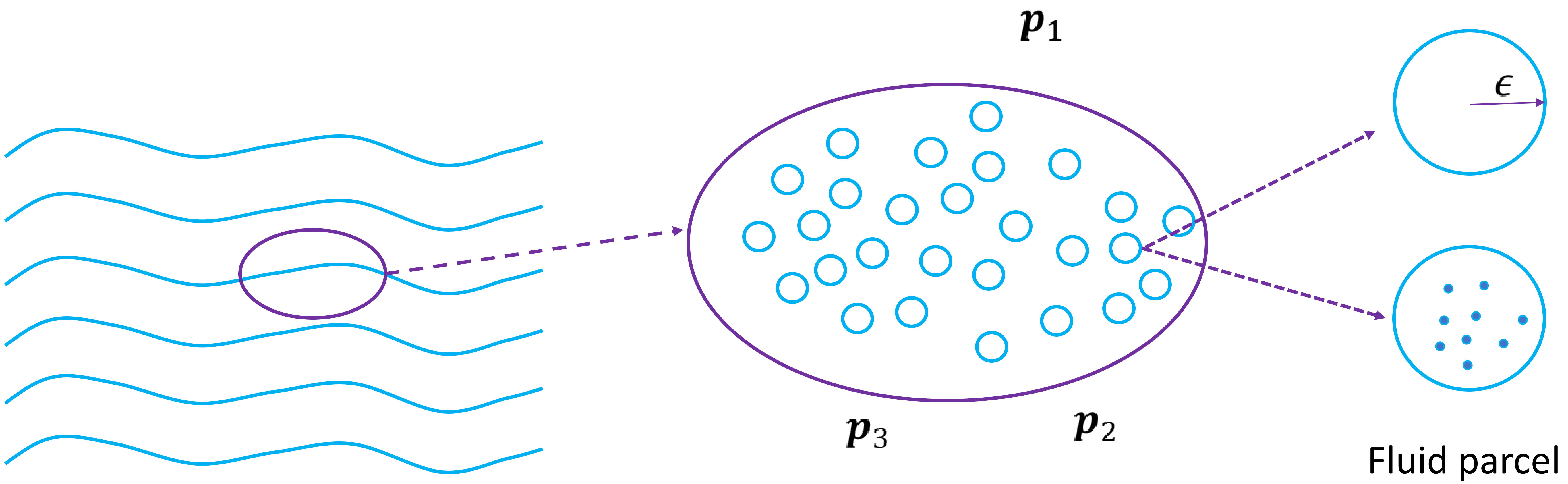
ExaSlate

Develop ≡ Guide ≡ Collab

Contents

Kumaresh Selvakumar
kumaresh@exaslate.com

Lagrangian frame – discrete phase



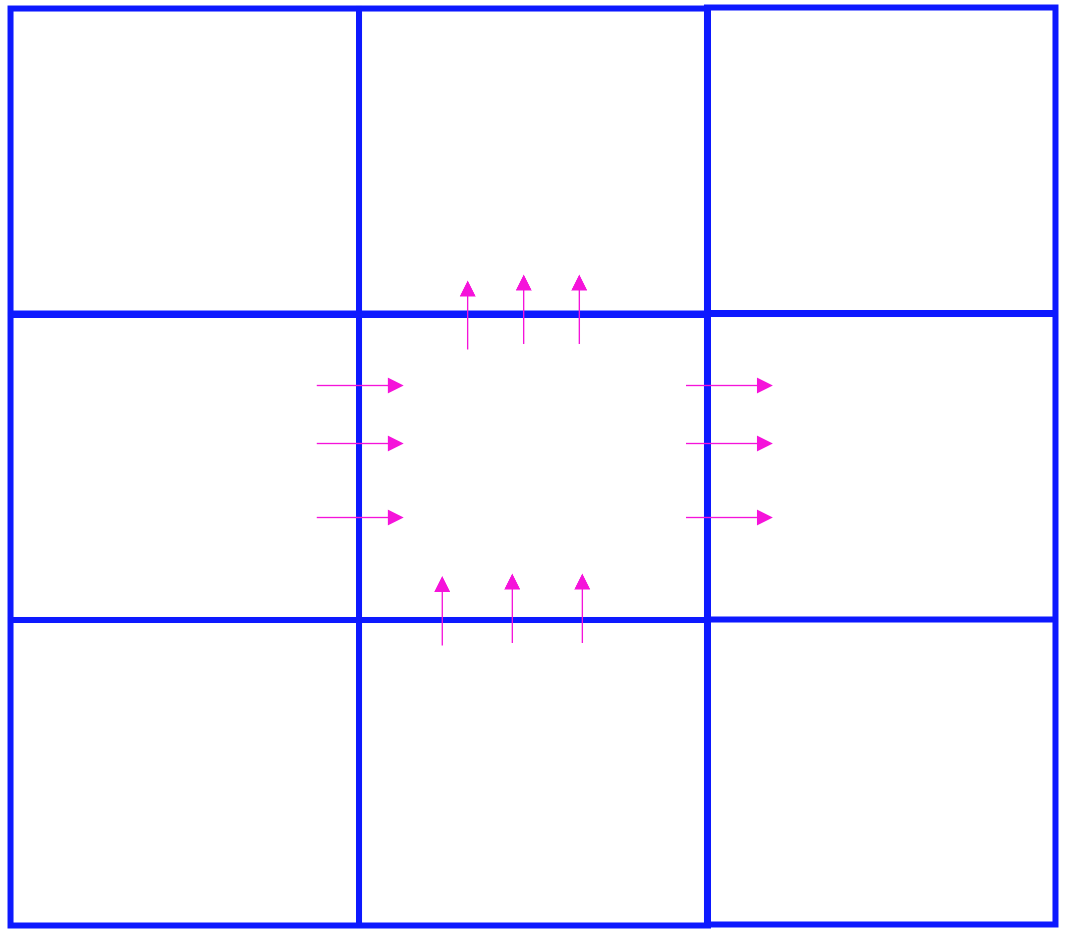
- Follow a fluid parcel $(\boldsymbol{p}_1, \boldsymbol{p}_2, \ldots)$
- Flow property at a location is obtained from the fluid parcel that happens to be at that location at that time
- Useful to derive conservation laws

Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop · Guide · Collab

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:

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

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

$$\underbrace{\frac{\partial}{\partial t}\iiint \rho\phi \mathrm{dV}}_{1} + \underbrace{\iint \rho\phi(u.\mathrm{dA})}_{2} = \underbrace{\iint \Gamma\nabla\phi.\,\mathrm{dA}}_{3} + \underbrace{\iiint S\mathrm{dV}}_{4}$$

1 Unsteady/Transient term

2 Advection/Convection term

3 Diffusion term

4 Source term

Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop = Guide = Collab

Governing Equations

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

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

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

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

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

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

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

Kumaresh Selvakumar
kumaresh@exaslate.com

Integral Form – Differential Form

- Conservation of mass

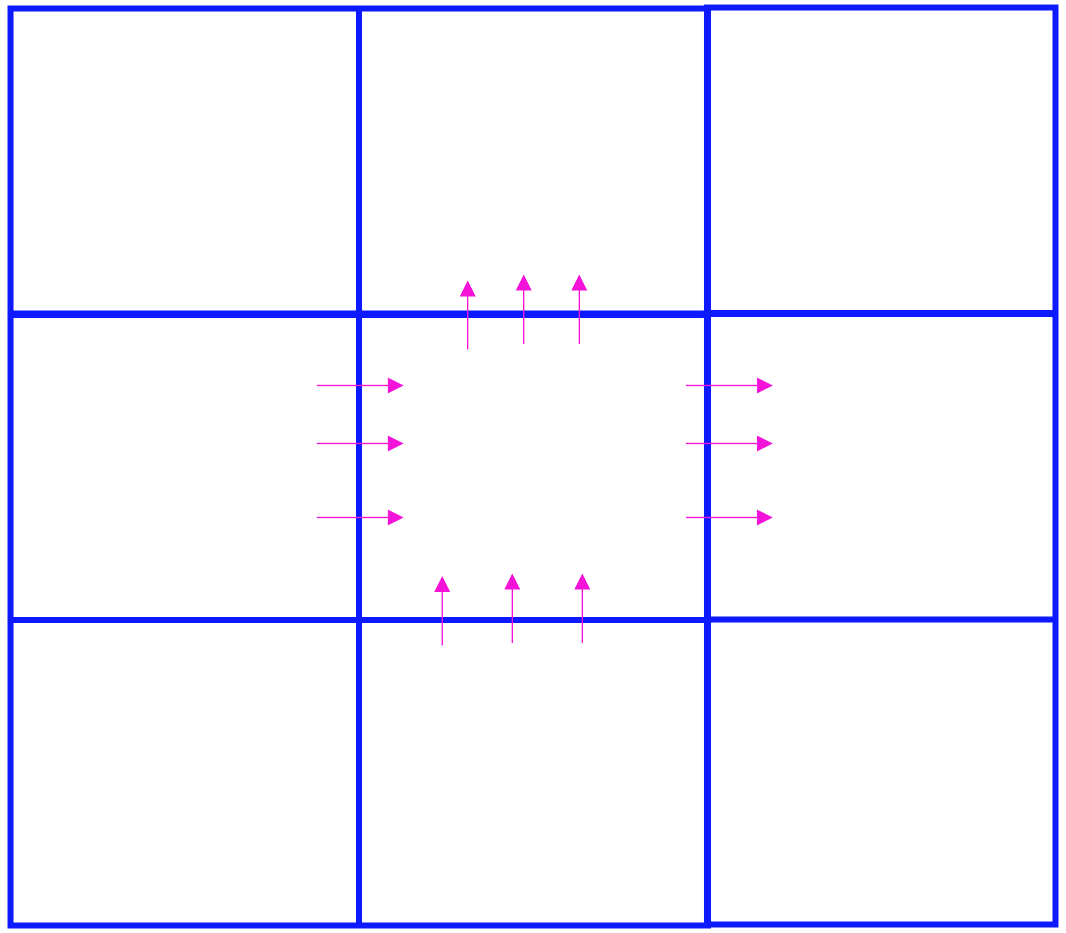
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

- 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

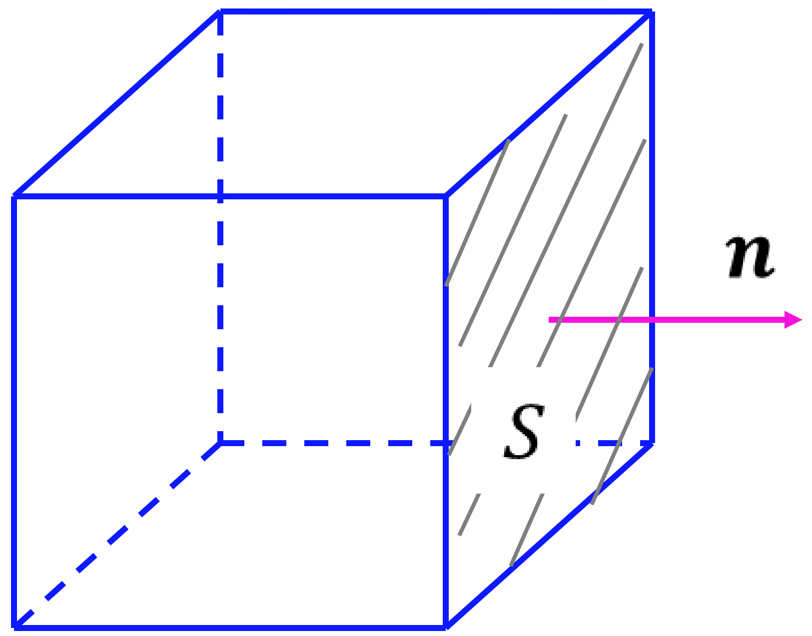
Gauss Divergence Theorem

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

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

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

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



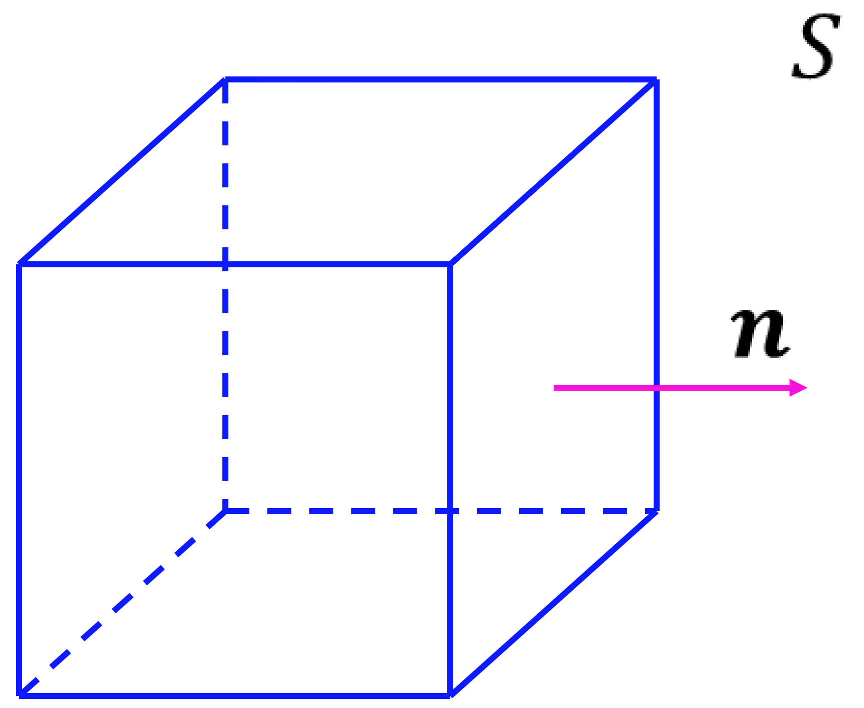
Kumaresh Selvakumar
kumaresh@exaslate.com

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.



Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop = Guide = Collab

Gauss Divergence Theorem

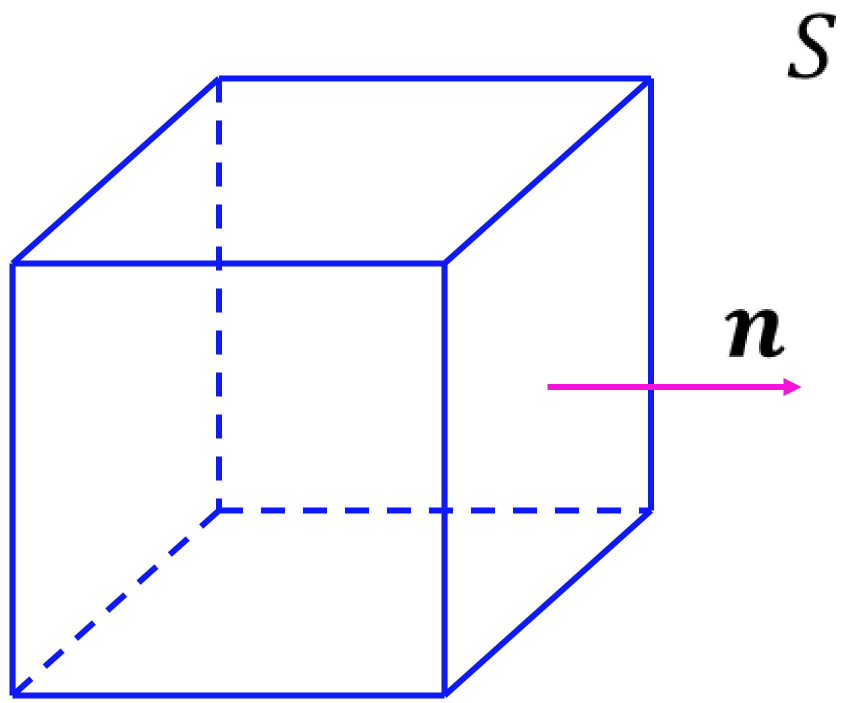
- For a vector: $\boldsymbol{F}$

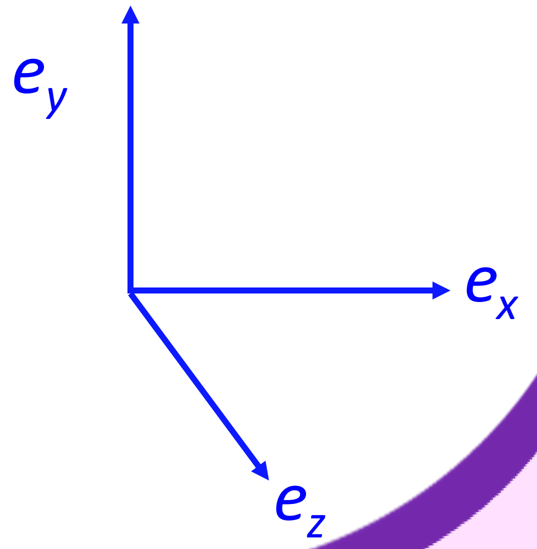
$$\int (\boldsymbol{\nabla} \cdot \boldsymbol{F}) \boldsymbol{dV} \approx \sum \boldsymbol{F} \cdot \boldsymbol{S}$$

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

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

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





Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop = Guide = Collab

Gauss Divergence Theorem

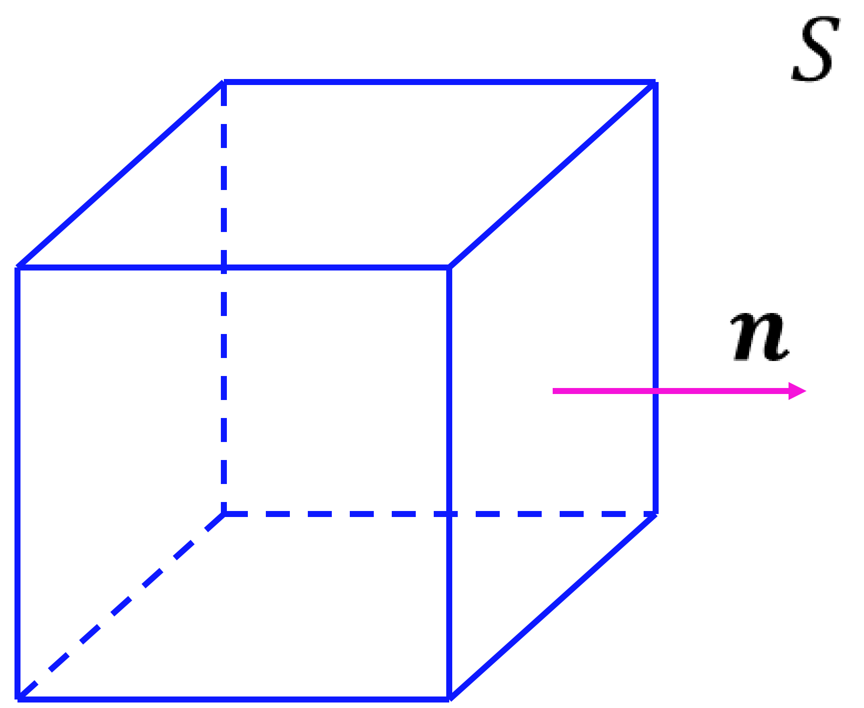
$$\boxed{\int (\nabla \cdot \boldsymbol{F}) d\boldsymbol{V} \approx \sum \boldsymbol{F} \cdot \boldsymbol{S}}$$

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

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

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

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



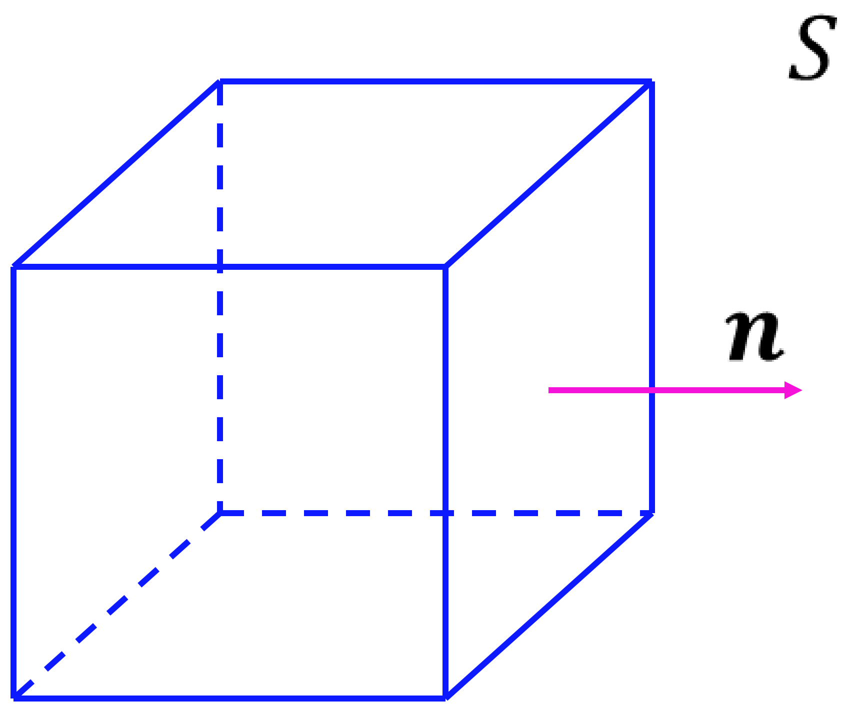
$S = \Delta x \Delta y$

$V = \Delta x \Delta y \Delta z$

Kumaresh Selvakumar
kumaresh@exaslate.com

Reynolds Transport Theorem

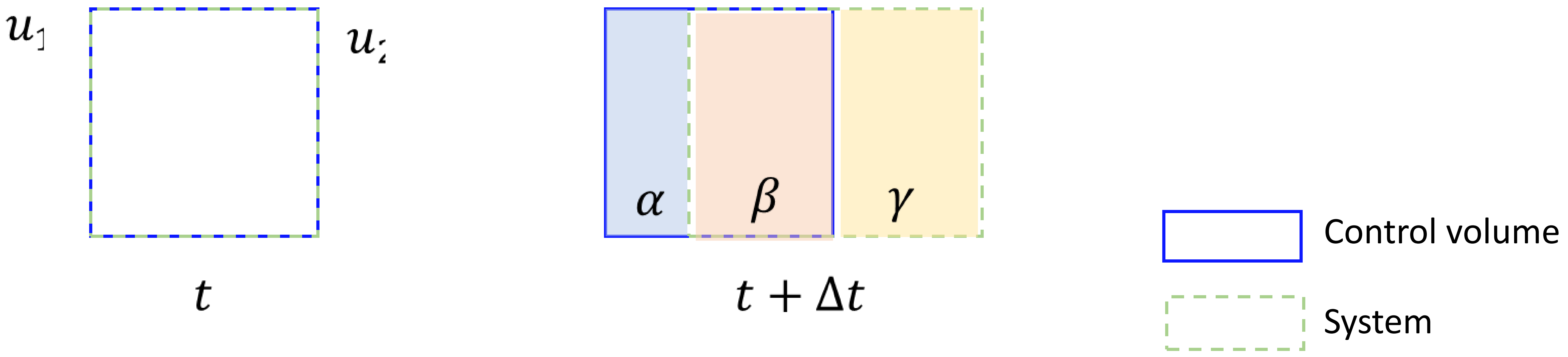
$$\frac{d}{dt}\int_{V_S} \rho\phi dV = \frac{d}{dt}\int_{V_{CV}} \rho\phi dV + \int_{S} \rho\phi \boldsymbol{u}\cdot\boldsymbol{n} dS$$



Kumaresh Selvakumar
kumaresh@exaslate.com

Reynolds Transport Theorem

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



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

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

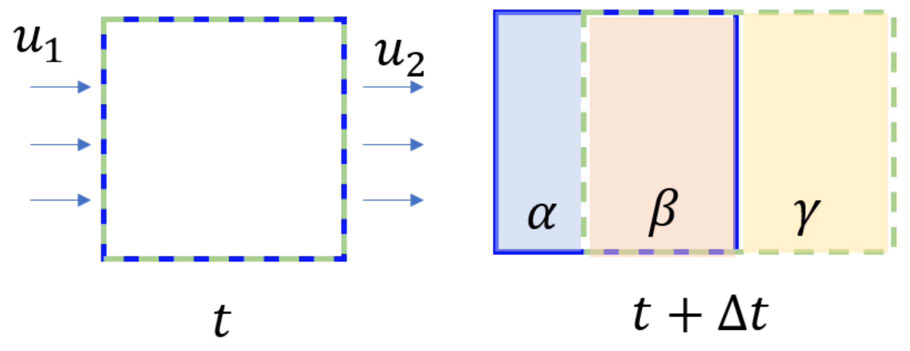
Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop = Guide = Collab

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)

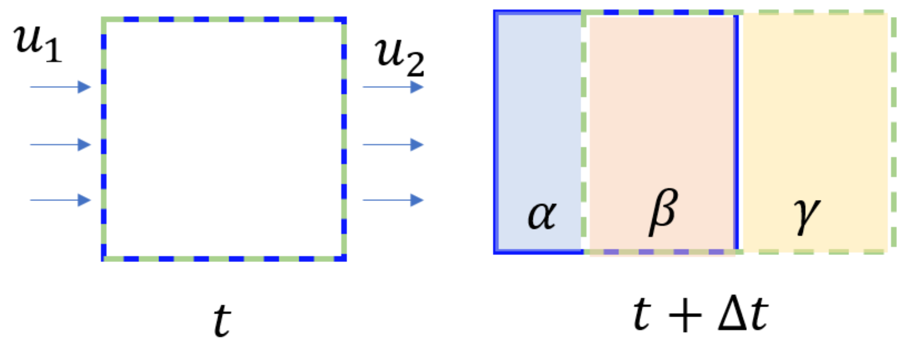
$$\left(\frac{\Phi(t+\Delta t) - \Phi(t)}{\Delta t}\right)_{System} = \left(\frac{\Phi(t+\Delta t) - \Phi(t)}{\Delta t}\right)_{CV} - \dot{\Phi}_\alpha + \dot{\Phi}_\gamma$$

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

Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop = Guide = Collab

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

ExaSlate
Develop = Guide = Collab

Conservation Laws

- Conservation of mass

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

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

- Conservation of momentum

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

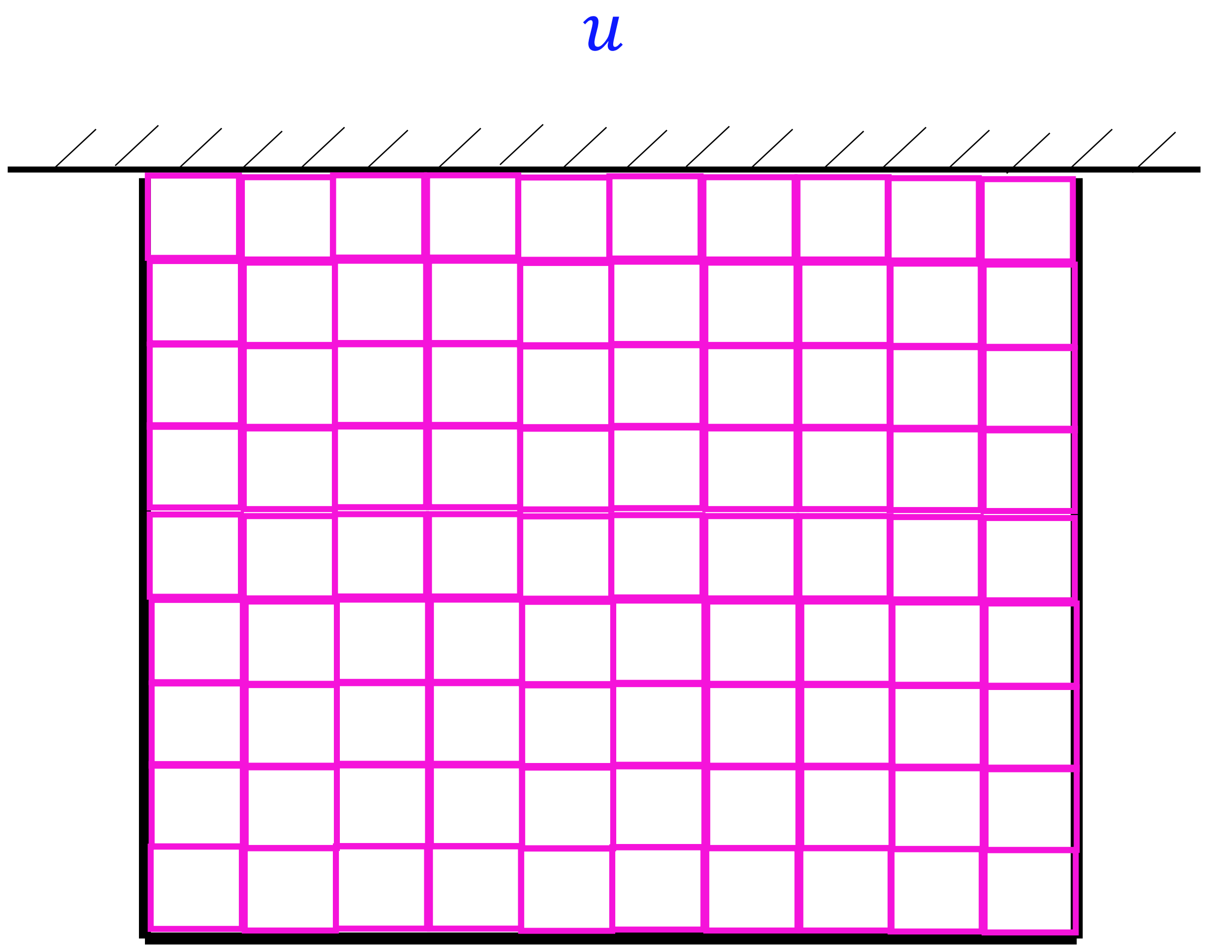
- Scalar conservation law

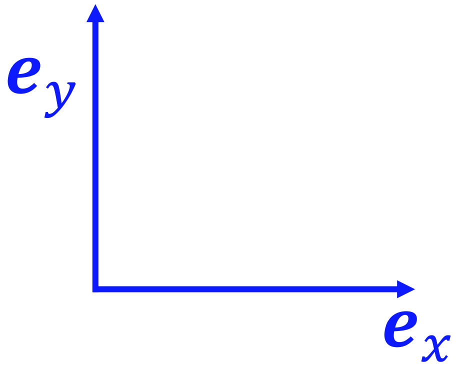
$$\frac{\partial \rho\phi}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi$$

Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop • Guide • Collab

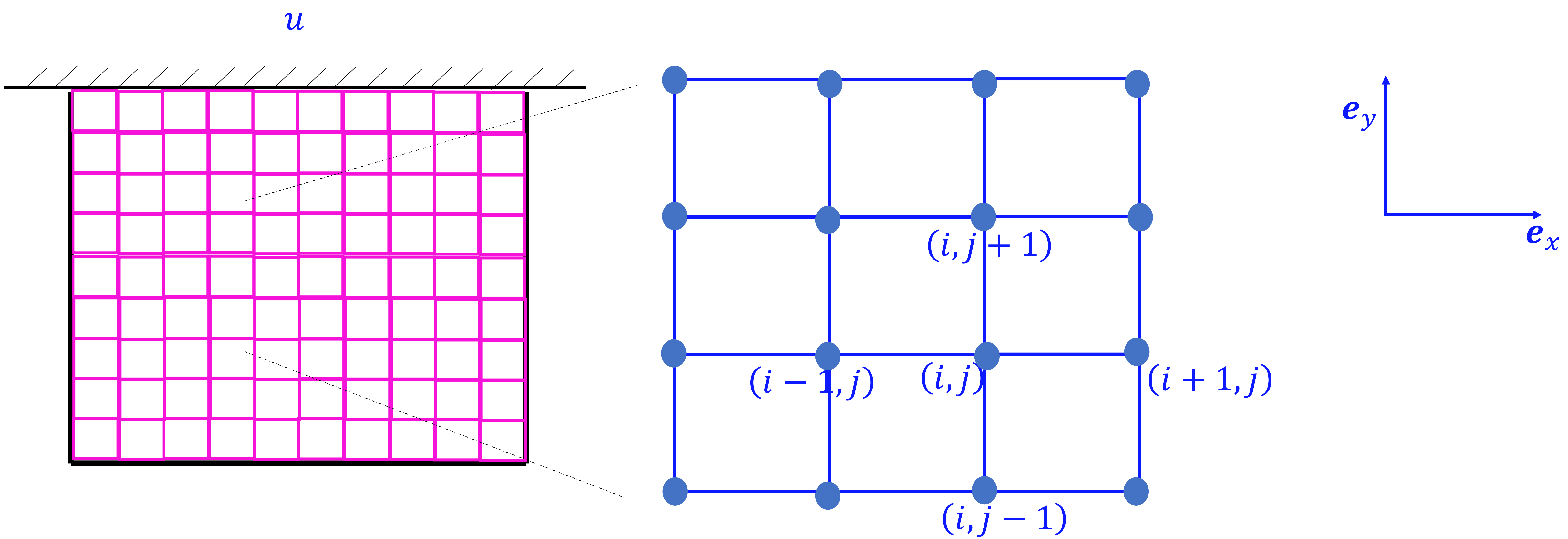
Numerical Discretization (Grid layout)





Kumaresh Selvakumar
kumaresh@exaslate.com

Numerical Discretization (Grid layout)

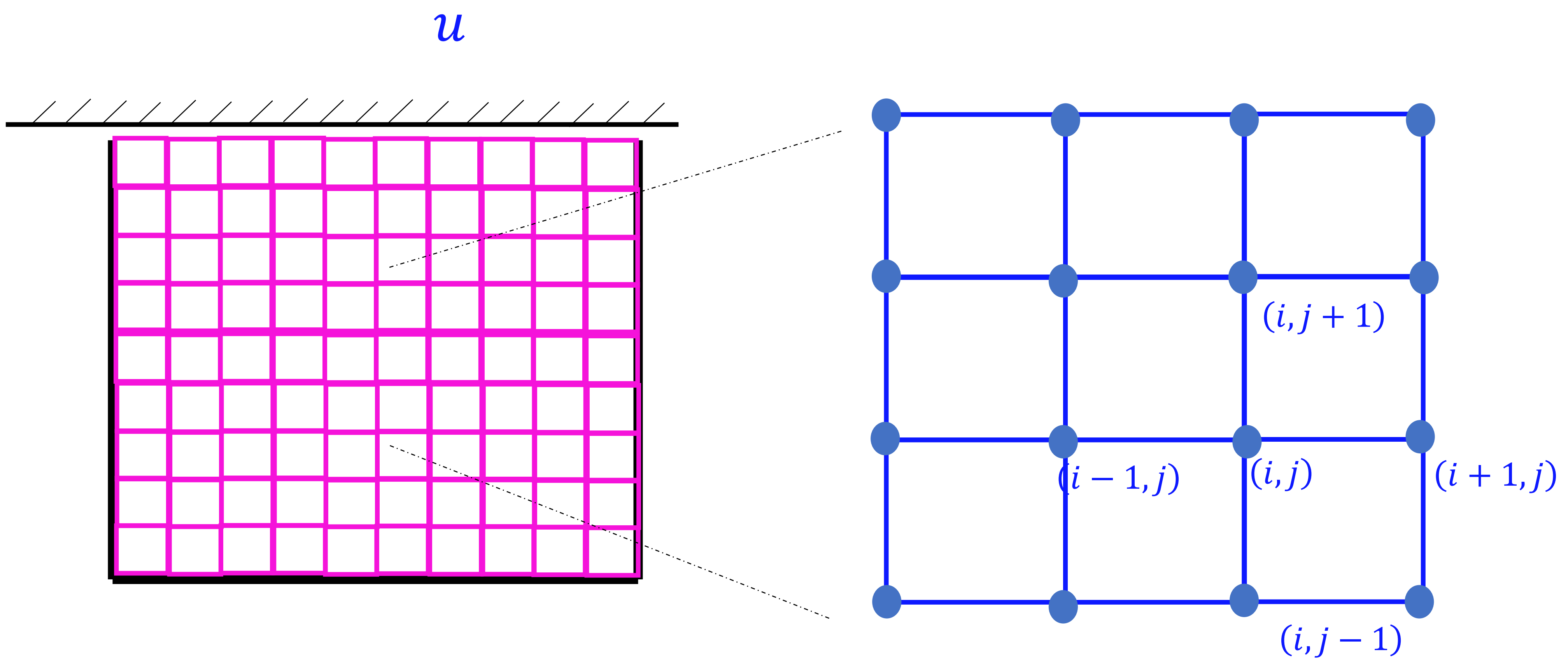


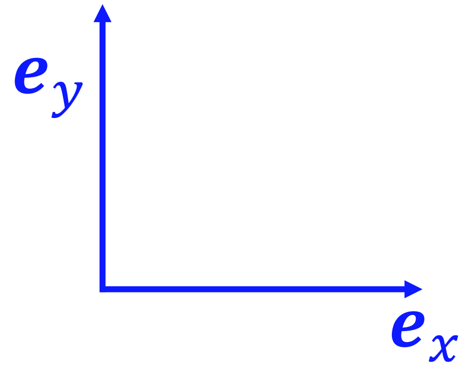
- Flow properties are assigned at each grid locations.

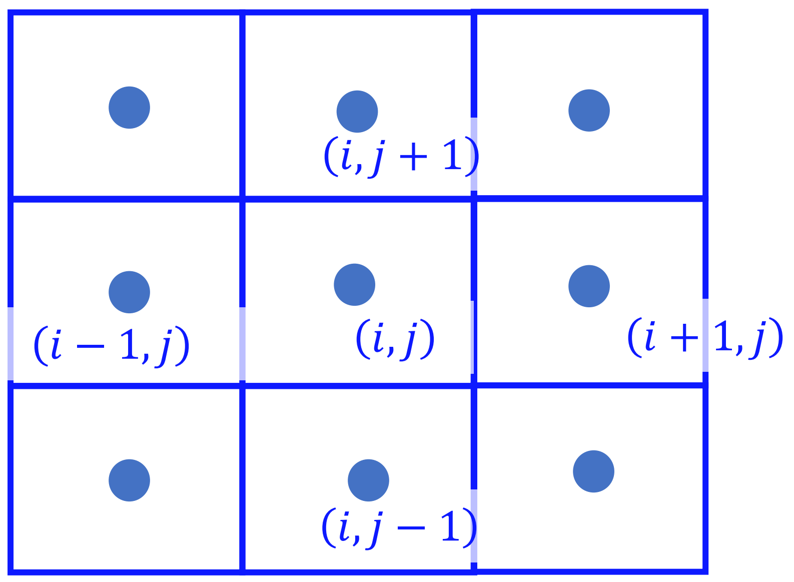
Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop = Guide = Collab

Numerical Discretization (Grid layout)





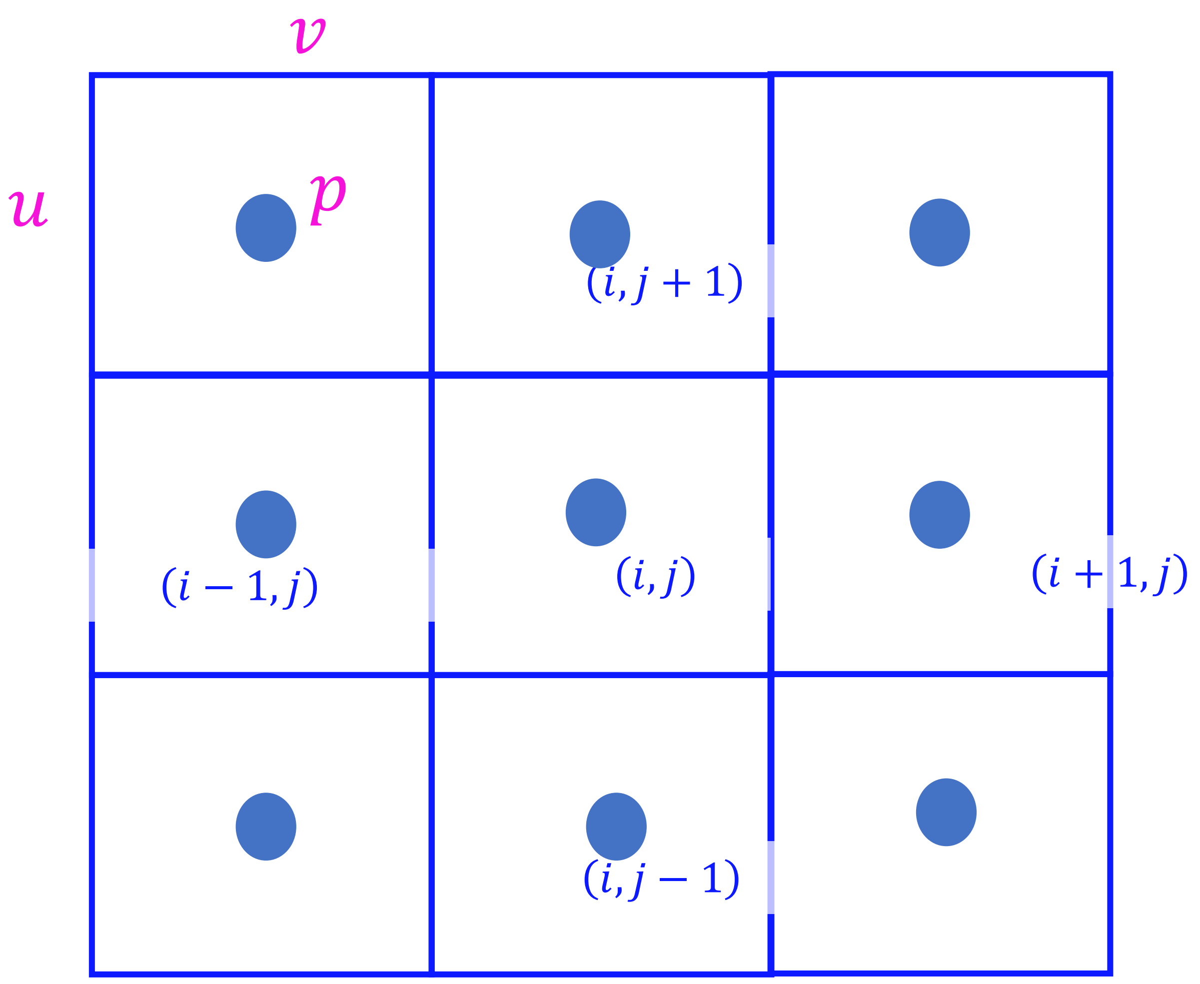


Cell centered representation

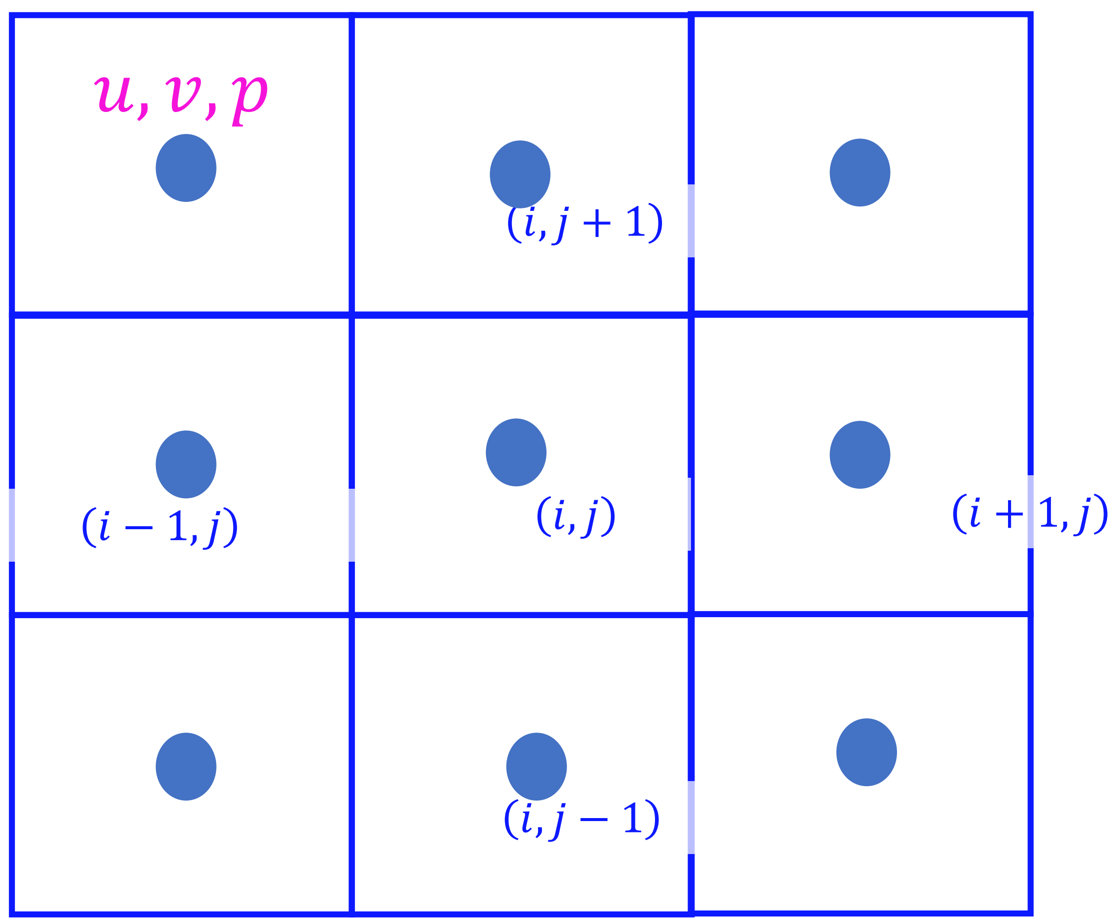
Kumaresh Selvakumar
kumaresh@exaslate.com

Numerical Discretization (Grid layout)

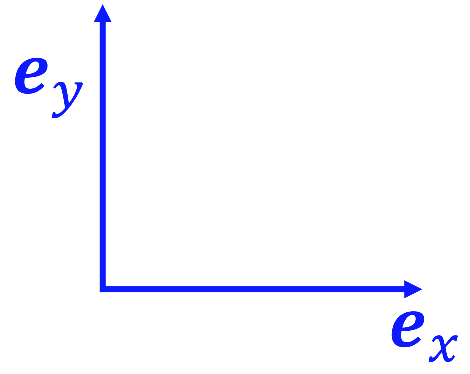
- Cell centered representation



Staggered grid



Collocated grid



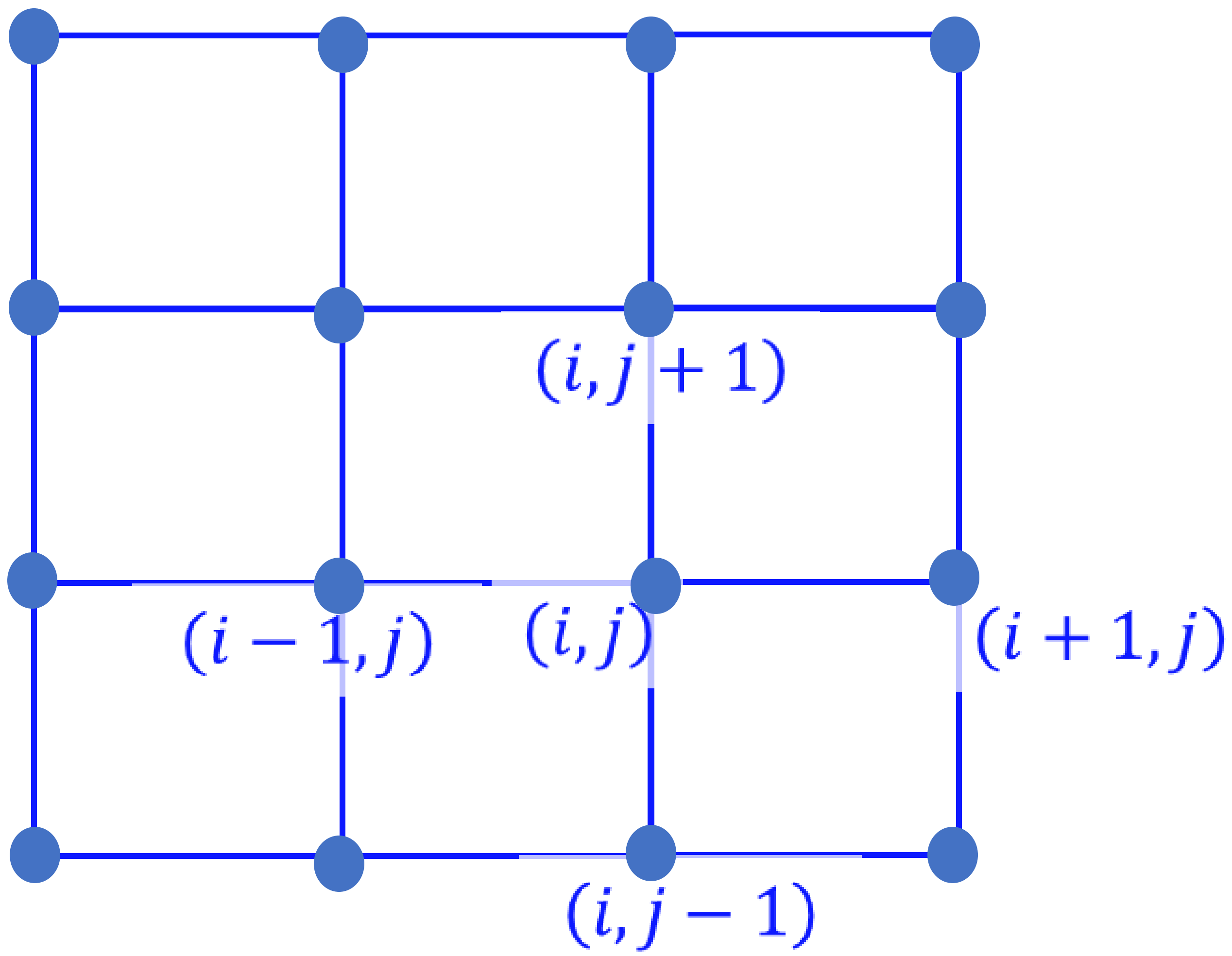
Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop · Guide · Collab

Finite Difference – Finite Volume

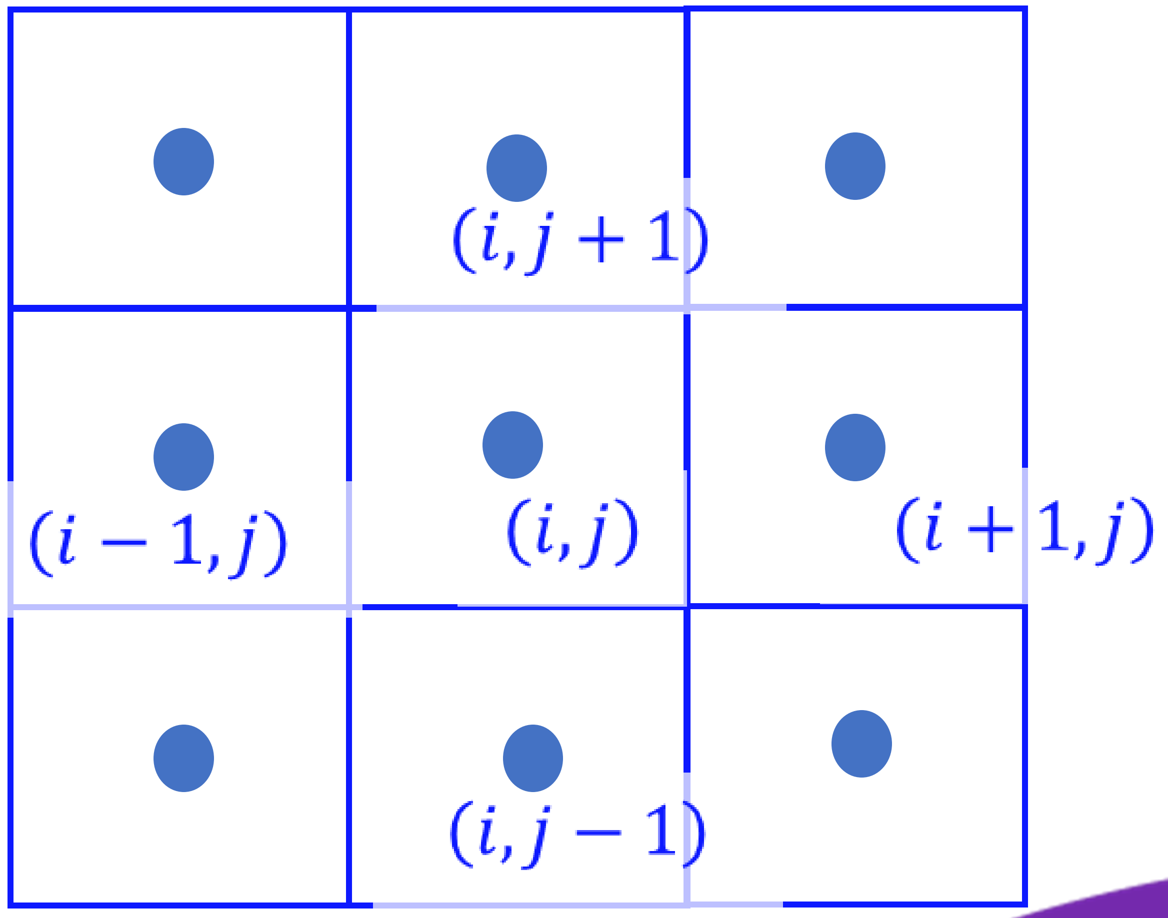
Differential form

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



Integral form

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



Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate

Develop = Guide = Collab

ExaSlate
Develop = Guide = Collab

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

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

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

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

Kumaresh Selvakumar
kumaresh@exaslate.com

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)

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

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

Second order central difference scheme

Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate
Develop = Guide = Collab

Taylor series: Backward Difference Scheme (1st order)

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

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

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

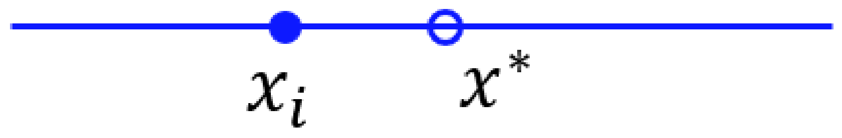
$$\left(\frac{d\rho}{dx}\right)_i = \frac{\rho(x_i) - \rho(x_{i-1})}{\Delta x_i} + O\,(\Delta x_i)$$

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

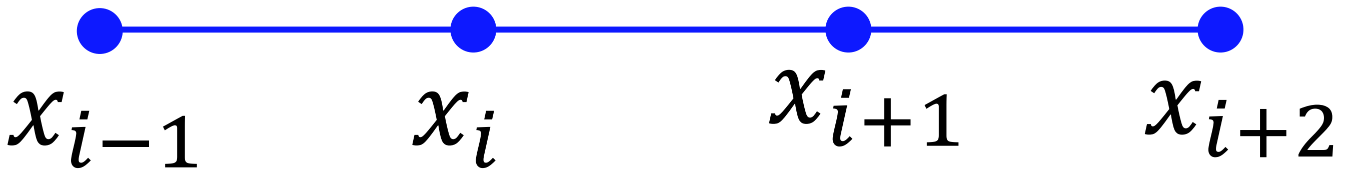
First order backward difference scheme

Kumaresh Selvakumar
kumaresh@exaslate.com

Taylor series: Summary



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



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 $\left(\frac{d^2\rho}{dx^2}\right)_i$

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

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

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

Kumaresh Selvakumar
kumaresh@exaslate.com

ExaSlate

Develop = Guide = Collab

Approximating Second Order Derivative

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

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

Add (1) and (2)

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

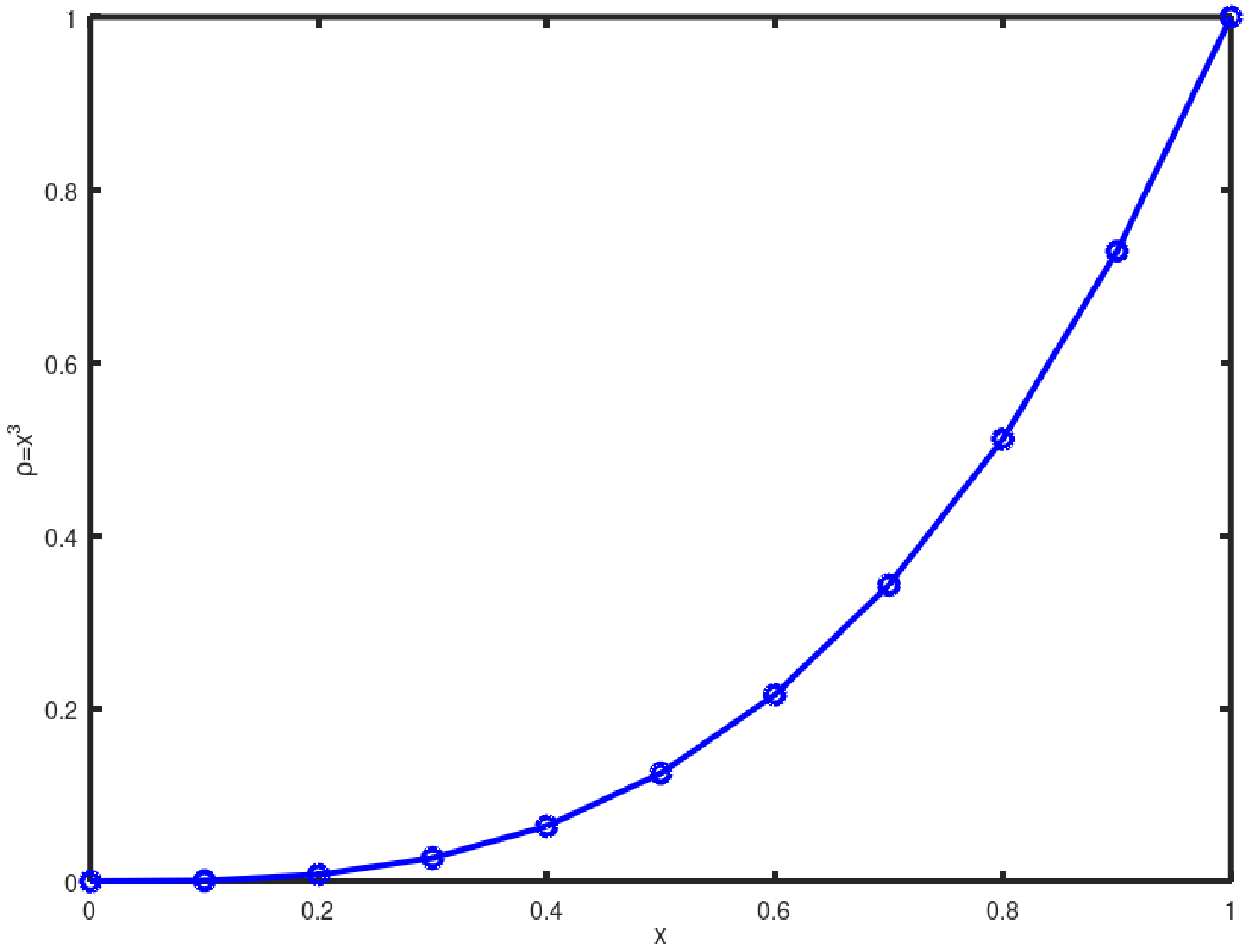
$$\left(\frac{d^2\rho}{dx^2}\right)_i = \frac{\rho(x_{i+1}) - 2\rho(x_i) + \rho(x_{i-1})}{\Delta x_i^2} + \frac{\Delta x_i^4}{12\Delta x_i^2}\left(\frac{d^4\rho}{dx^4}\right)_i + \cdots$$

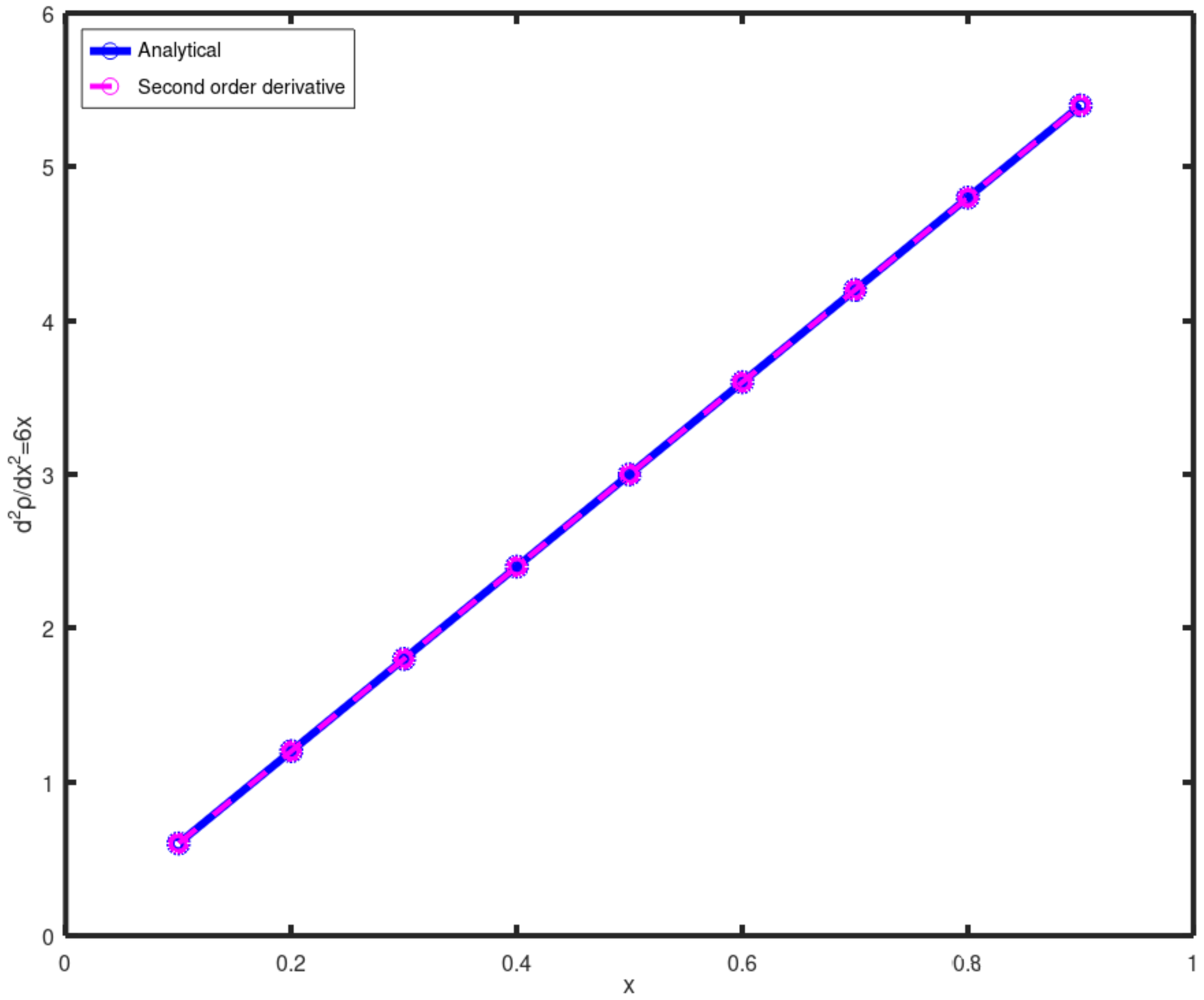
$$\boxed{\left(\frac{d^2\rho}{dx^2}\right)_i = \frac{\rho(x_{i+1}) - 2\rho(x_i) + \rho(x_{i-1})}{\Delta x_i^2} + O\left(\Delta x_i^2\right)}$$

Kumaresh Selvakumar
kumaresh@exaslate.com

Approximating Second Order Derivative

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





Kumaresh Selvakumar
kumaresh@exaslate.com

THANK YOU