Computational Thermal Engineering

Introduction – DAY 1

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Contents

Introduction – About this course

- Course duration per session: 3hrs
- Requirements:
  - Virtual box and installing OS & softwares.
  - Interest to learn CFD using OpenFOAM & Octave
  - Interest to ask questions in discussion forum (github)
  - Work as a team
- Exercises: 20% (equal weightage)
- Projects: 10%, 10%, 20%, 40%
- Final project presentations & aim to use those at conferences

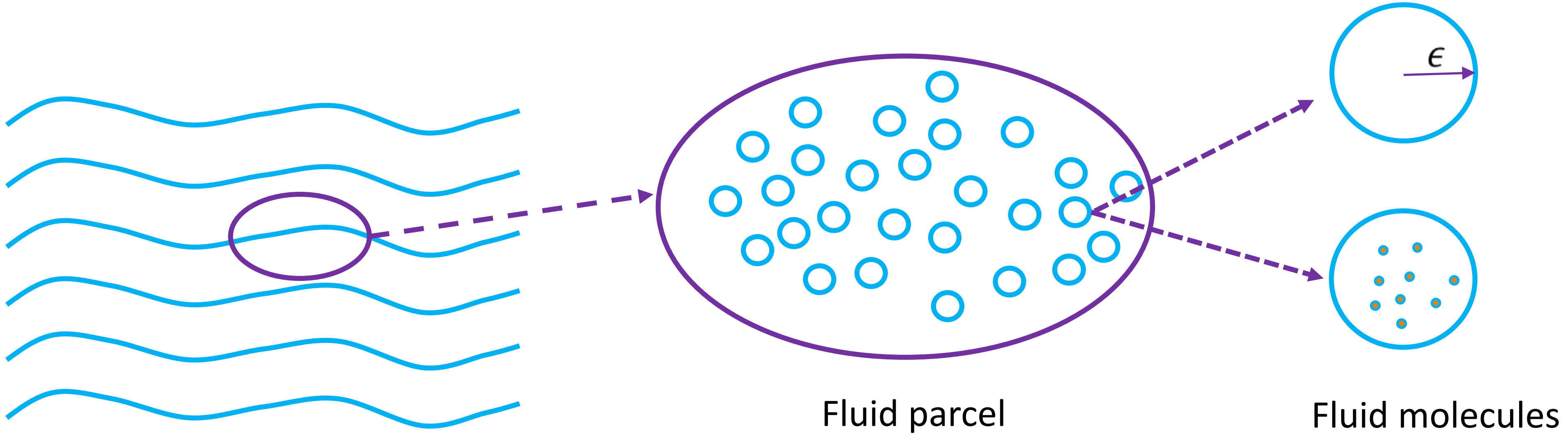
Introduction – References

- Ferziger and Peric; Computational Methods for Fluid Dynamics.
- S. Patankar; Numerical Heat Transfer and Fluid Flow.
- Tannehill et al.; Computational Fluid Mechanics and Heat Transfer.
- Versteeg, Malalasekera; An Introduction to Computational Fluid Dynamics.

- C.J. Greenshields, H.G. Weller; Notes on CFD: General Principles (OpenFOAM)

CFD fundamentals – Fluid

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



CFD fundamentals – Fluid

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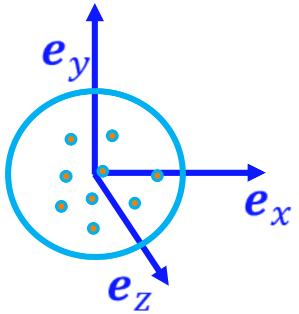
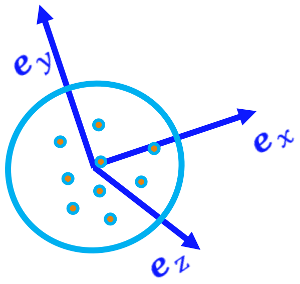
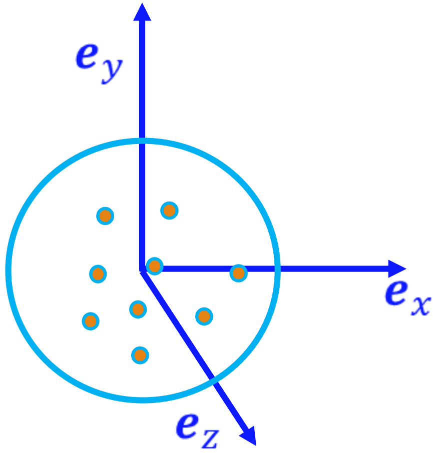


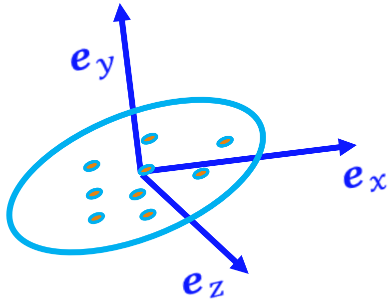
Fluid parcel



Rotation



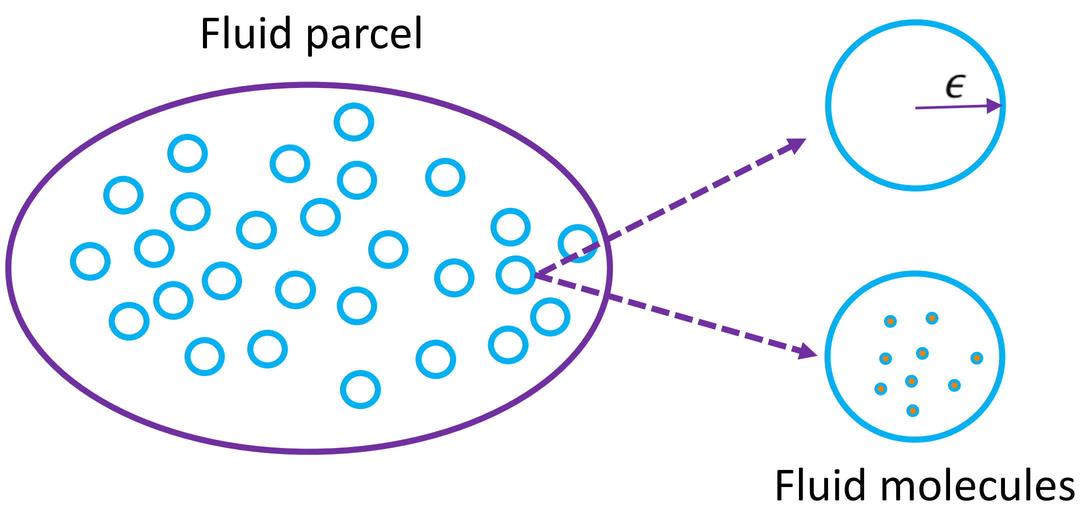
Expansion



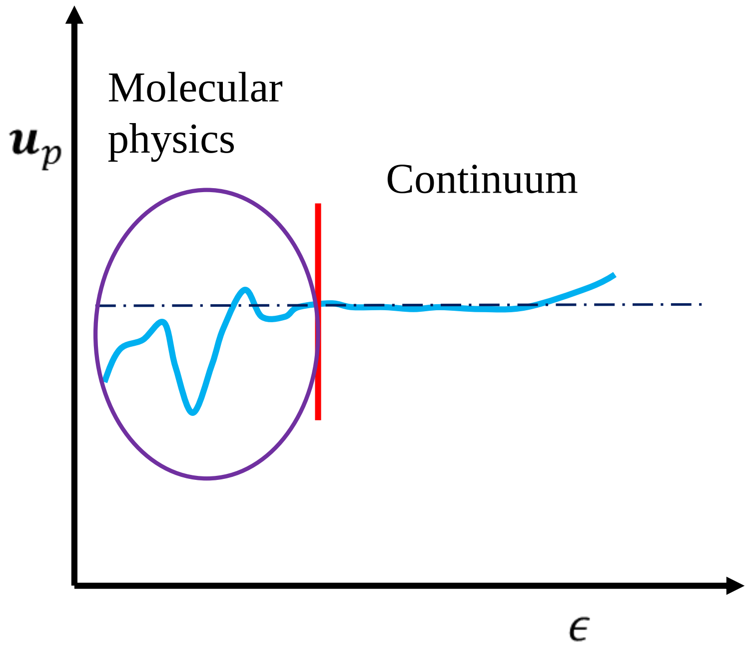
Deformation

CFD fundamentals – Fluid

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



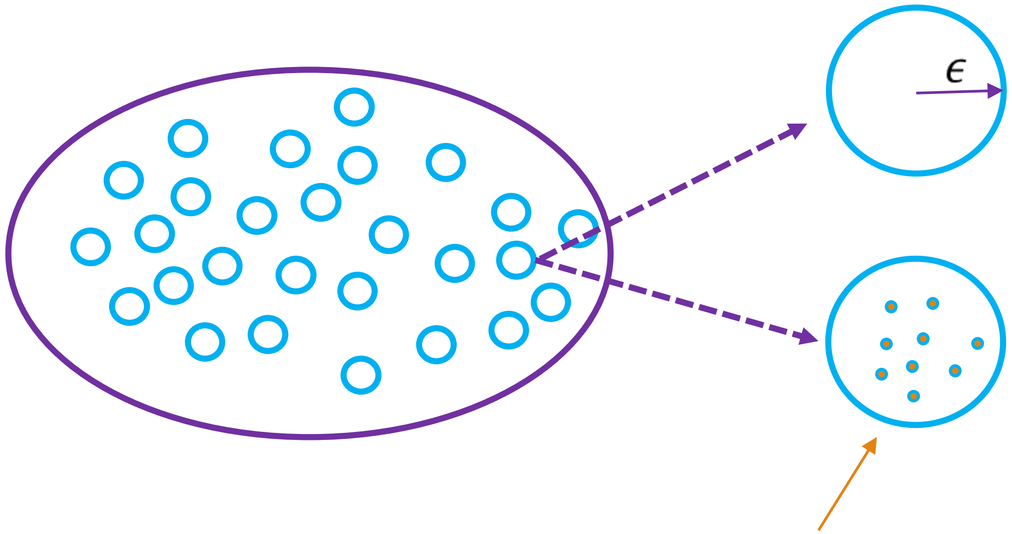
$$\boldsymbol{u}_p = \frac{\sum_{i=1}^{N_{mol}} \boldsymbol{u}_{mol}}{N_{mol}}$$



Fluid velocity: $\boldsymbol{u}(\boldsymbol{x}, t)$

CFD fundamentals – Continuum

Knudsen number: $$\mathrm{Kn} = \frac{\lambda}{L} = \frac{molecular\ mean\ free\ path\ length}{physical\ length}$$

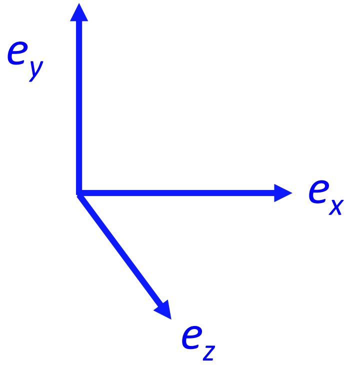


Kn < 0.01	Continuum flow
0.01 < Kn < 0.1	Slip flow
0.1 < Kn < 10	Transitional flow
Kn > 10	Free molecular flow

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

$$\frac{\partial}{\partial t}(\rho u) + \nabla \bullet (\rho \mathrm{uu}) = \nabla \bullet (\mu \, \nabla u) - \nabla p + S_u$$

Mathematical operations



Gradient:

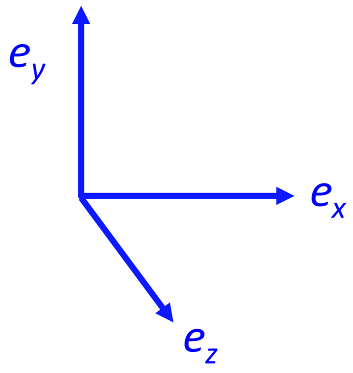
$$\nabla \rho = \left(\frac{\partial}{\partial x}\boldsymbol{e}_x + \frac{\partial}{\partial y}\boldsymbol{e}_y + \frac{\partial}{\partial z}\boldsymbol{e}_z \right) \rho = \left(\frac{\partial \rho}{\partial x}\boldsymbol{e}_x + \frac{\partial \rho}{\partial y}\boldsymbol{e}_y + \frac{\partial \rho}{\partial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

$$\frac{\partial}{\partial t}(\rho u) + \nabla \bullet (\rho \mathrm{u} u) = \nabla \bullet (\mu \nabla u) - \nabla p + S_u$$

Mathematical operations

Gradient:

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



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

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

$$\frac{\partial}{\partial t}(\rho u)+\nabla\bullet(\rho uu)=\nabla\bullet(\mu\ \nabla u)-\nabla p+S_u$$

Mathematical operations

Divergence:

- In vector calculus, divergence is a vector operator that operates on a vector field, producing a scalar field giving the **quantity of the vector field's source at each point**.

- More technically, the divergence represents the volume density of the outward flux of a vector field from an infinitesimal volume around a given point.

- As an example, consider air as it is heated or cooled. **The velocity of the air at each point defines a vector field**. While air is heated in a region, it expands in all directions, and thus the velocity field points outward from that region. **The divergence of the velocity field in that region would thus have a positive value**. While the air is cooled and thus contracting, the divergence of the velocity has a negative value.

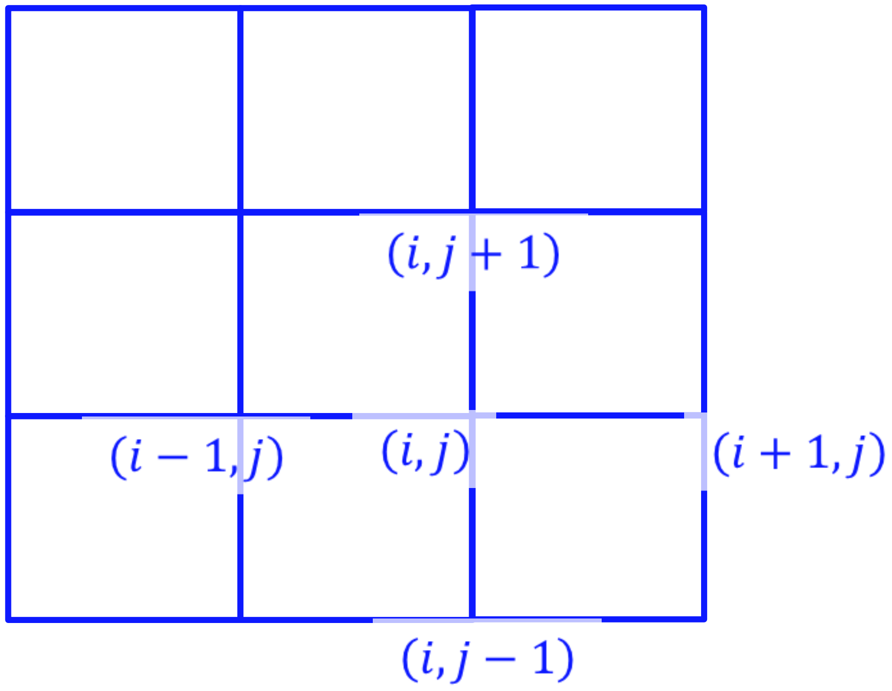
$$\nabla\cdot\boldsymbol{u}=\left(\frac{\partial}{\partial x}\boldsymbol{e}_x+\frac{\partial}{\partial y}\boldsymbol{e}_y+\frac{\partial}{\partial z}\boldsymbol{e}_z\right)(u\boldsymbol{e}_x+v\boldsymbol{e}_y+w\boldsymbol{e}_z)=\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial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

Mathematical operations

Finite difference:

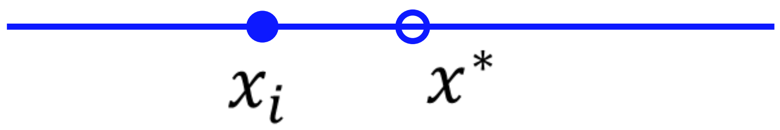
$$\nabla\rho = \left(\frac{\partial}{\partial x}\boldsymbol{e}_x + \frac{\partial}{\partial y}\boldsymbol{e}_y + \frac{\partial}{\partial z}\boldsymbol{e}_z\right)\rho = \left(\frac{\partial\rho}{\partial x}\boldsymbol{e}_x + \frac{\partial\rho}{\partial y}\boldsymbol{e}_y + \frac{\partial\rho}{\partial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

$$\left(\frac{\partial\rho}{\partial x}\right)_{i,j} = \frac{\rho_{i+1,j} - \rho_{i-1,j}}{2\Delta x}$$



Mathematical operations

Taylor series:



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

Mathematical operations

Taylor series:

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

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

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

Mathematical operations

Taylor series:

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

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

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

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

Finite difference

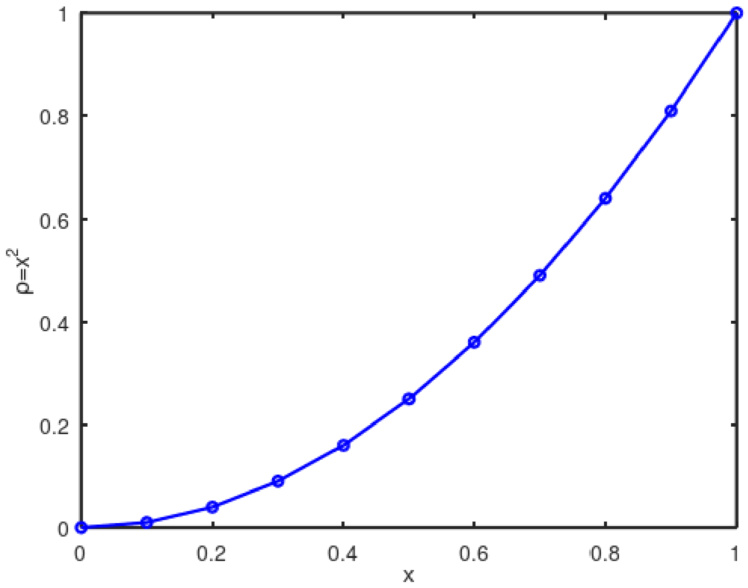
$$\nabla \rho = \left(\frac{\partial}{\partial x}\boldsymbol{e}_x + \frac{\partial}{\partial y}\boldsymbol{e}_y + \frac{\partial}{\partial z}\boldsymbol{e}_z\right)\rho = \left(\frac{\partial \rho}{\partial x}\boldsymbol{e}_x + \frac{\partial \rho}{\partial y}\boldsymbol{e}_y + \frac{\partial \rho}{\partial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

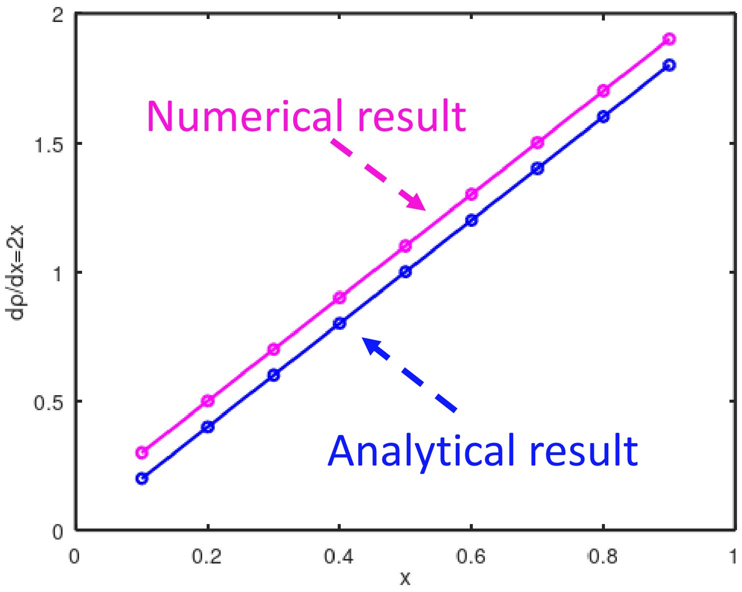
$$\left(\frac{\partial \rho}{\partial x}\right)_{i,j} = \frac{\rho_{i+1,j} - \rho_{i-1,j}}{2\Delta x}$$

Mathematical operations

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

Governing Equations

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

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

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

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

1 2 3 4

1 → Unsteady/Transient term

2 → Advection/Convection term

3 → Diffusion term

4 → Source term

Governing Equations

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

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

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

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

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

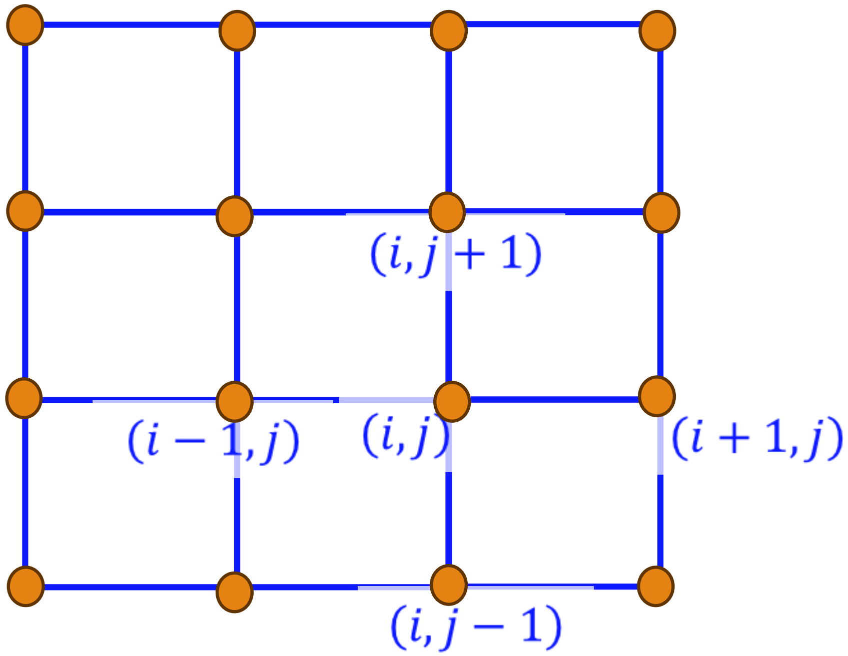
Turbulence equation: $\phi = k(\mathrm{or})\varepsilon, \Gamma = \Gamma_k(\mathrm{or})\Gamma_\varepsilon, S = S_k(\mathrm{or})S_\varepsilon$ ➔ $\boxed{\frac{\partial}{\partial t}(\rho k) + \nabla\bullet(\rho \mathrm{u}k) = \nabla\bullet(\ \Gamma_k\nabla k) + S_k}$

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

Finite Difference – Finite Volume

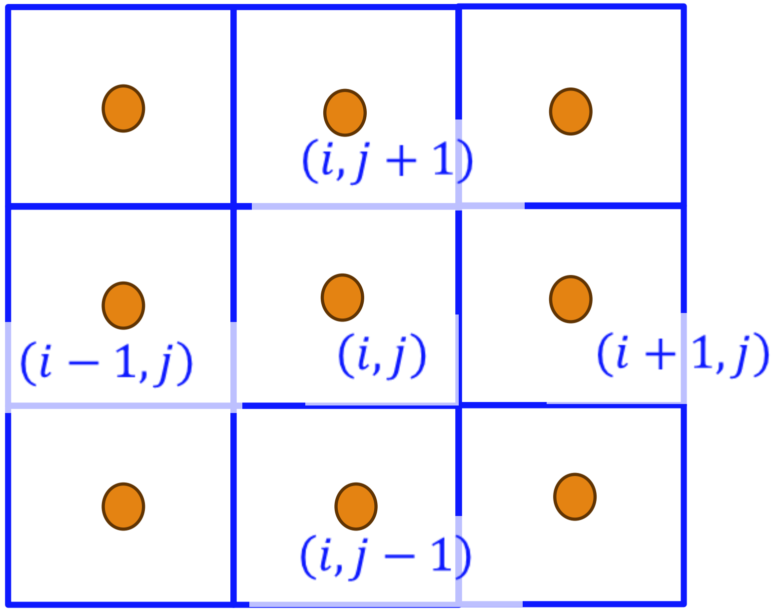
Differential form

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



Integral form

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

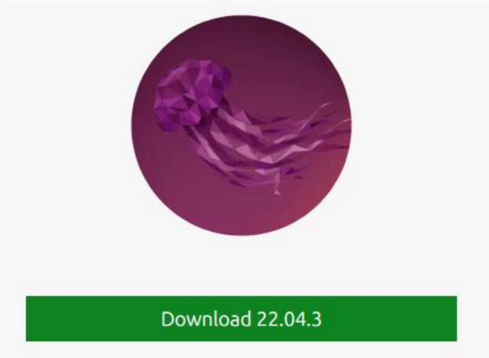


Installations

- Preconfiguration packages:
    - https://1drv.ms/f/s!AqT2YEB97-1RgP8MtsMPqoOGsq4ddg?e=IocXv0

- List
    - Virtual Box [to create virtual machines]
    - <u>Operating System:</u> Ubuntu 22.04 [Install OpenFOAMv2306 & Octave]
    - AnyDesk [For remote access]

- Create a github account:
    - https://github.com/Kumaresh0402/ComputationalThermalEngineering
    - Discussion forum:
        - https://github.com/Kumaresh0402/ComputationalThermalEngineering/discussions



GNU Octave

What is OpenFOAM and it's importance ?

https://www.youtube.com/watch?v=3BOwFAA0ISw

Exercises

Exercise – 1 ➔ Install packages

- Preconfiguration packages:
  - https://1drv.ms/f/s!AqT2YEB97-1RgP8MtsMPqoOGsq4ddg?e=IocXv0
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  - Virtual Box [to create virtual machines]
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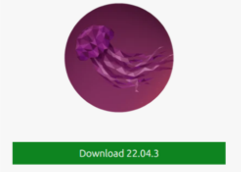


OpenFOAM®

OpenFOAM-v2306 openfoam

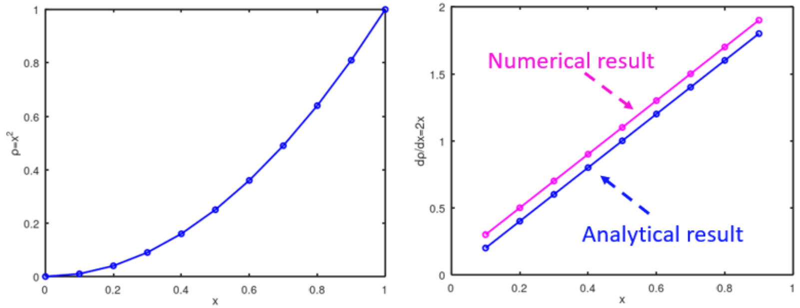
GNU Octave

Exercise – 2 ➔ Test Octave

Analytical and Numerical solutions

x_{i-1} x_i x_{i+1} x_{i+2}

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



Resolved in OCTAVE