Applied Computational Fluid Dynamics Using OpenFOAM

Value Added Course
College/University: KSR
Spring 2025

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Contents

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Introduction – About this course

- Course duration per session: 5 – 6 hrs (every Saturday)
- Total course duration: 30 – 35 hrs
- Requirements:
  - Virtual box and installing OS & softwares.
  - Interest to learn CFD using OpenFOAM & Octave
  - Interest to ask questions in discussion forum (GitHub)
- Exercises (equal weightages)

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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)

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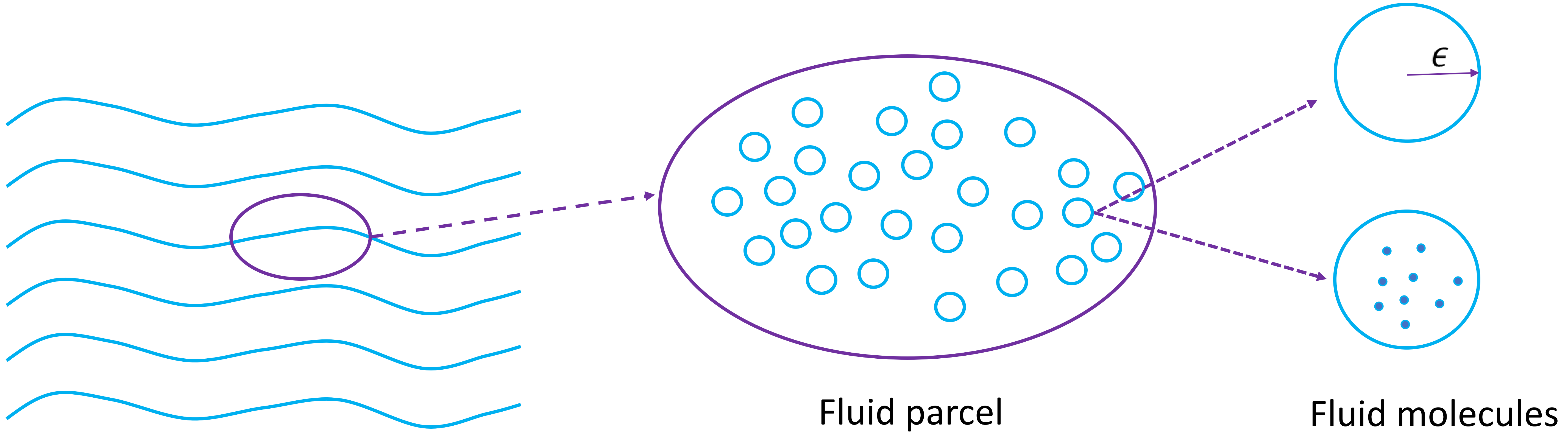
CFD fundamentals – Fluid

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



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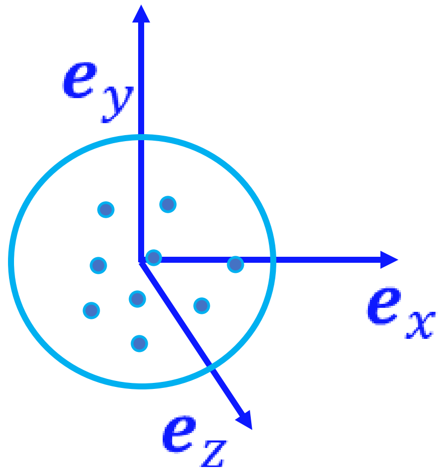
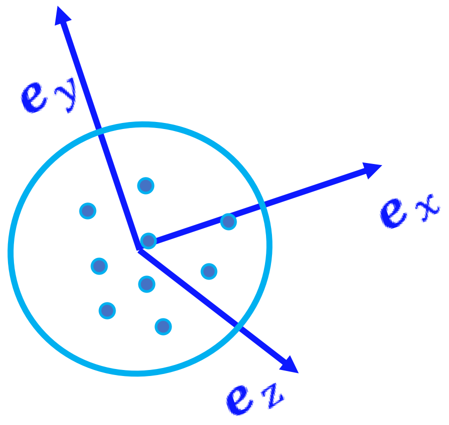
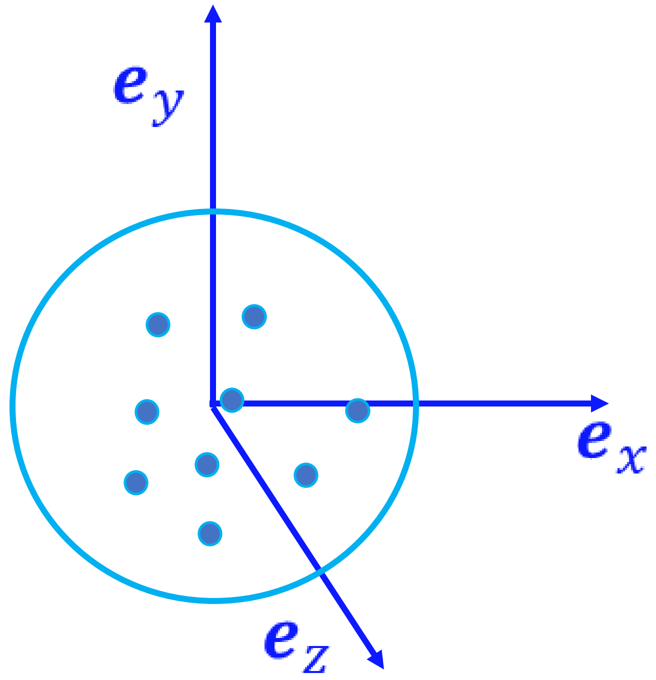


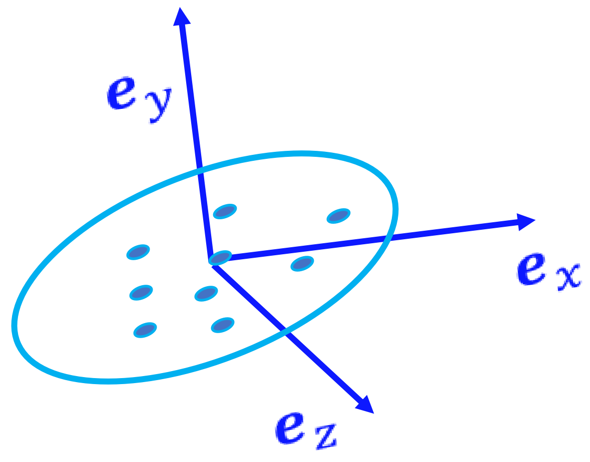
Fluid parcel



Rotation



Expansion



Deformation

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CFD fundamentals – Fluid

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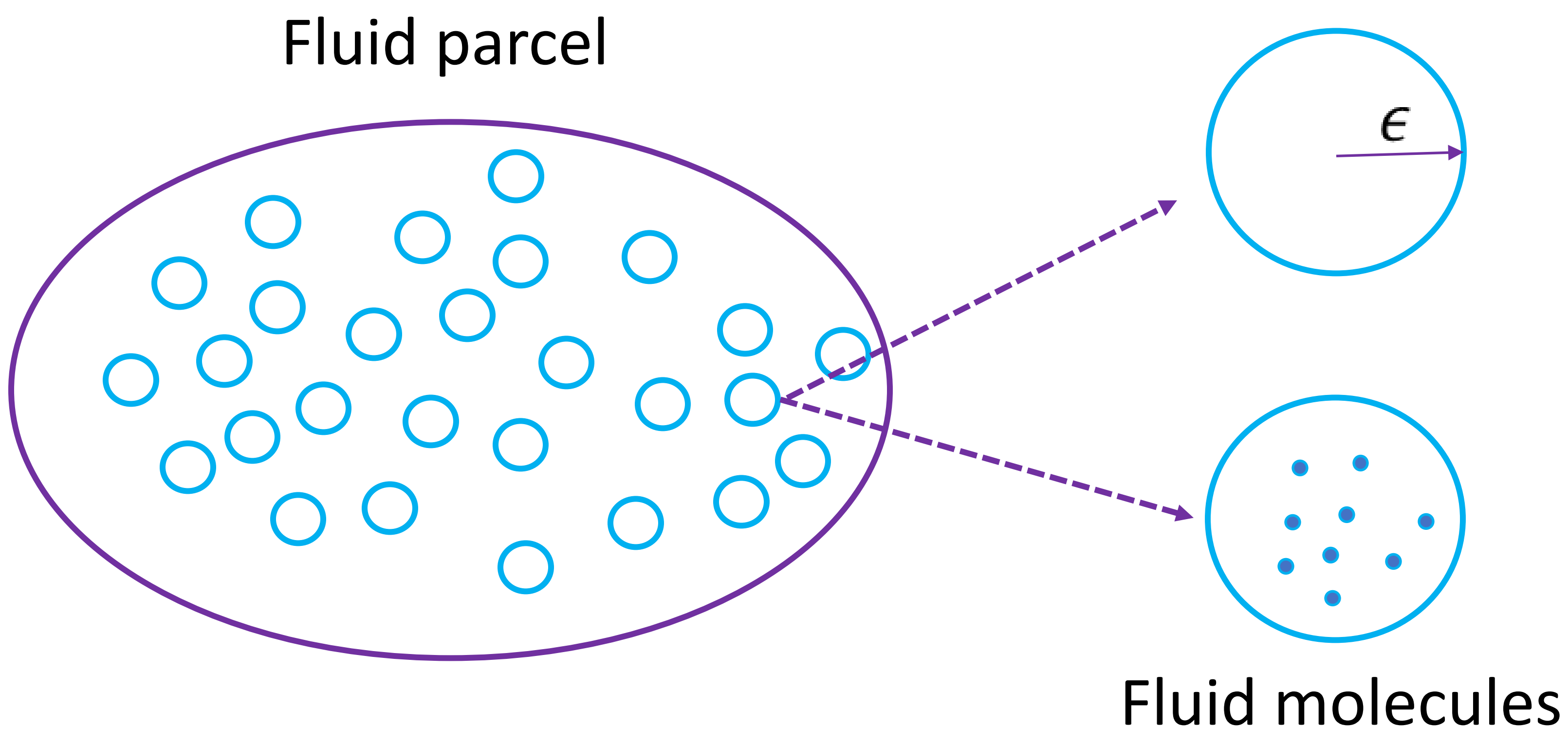
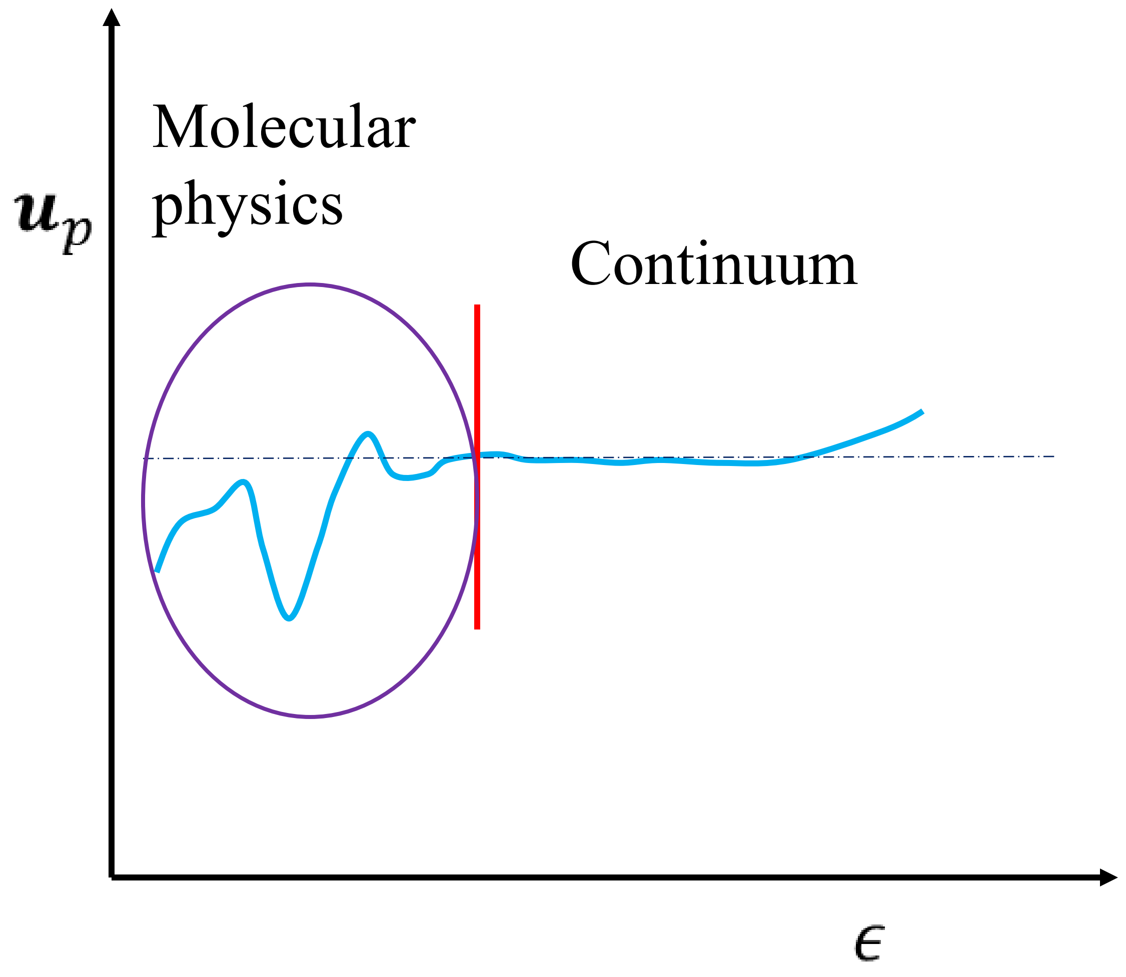


$$\boldsymbol{u}_p = \frac{\sum_{i=1}^{N_{mol}} \boldsymbol{u}_{mol}}{N_{mol}}$$



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

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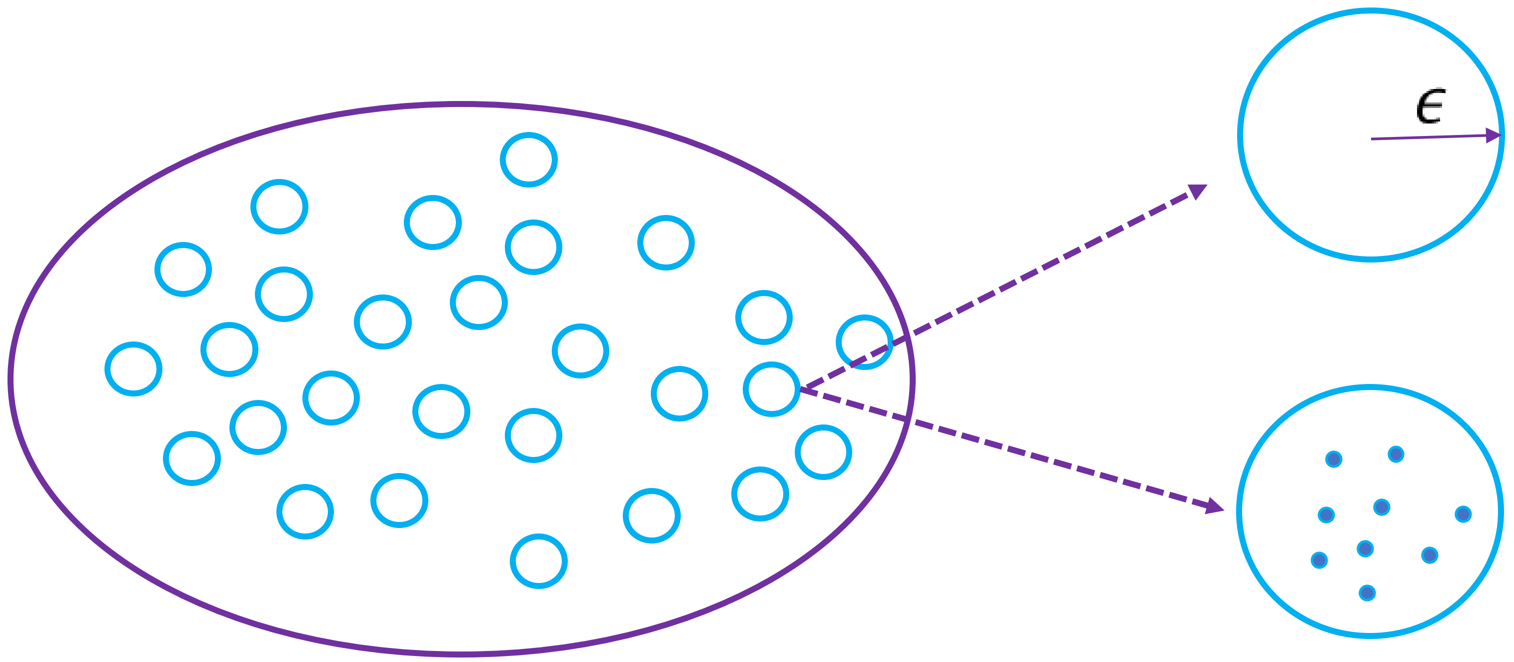
https://en.wikipedia.org/wiki/Knudsen_number#References

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

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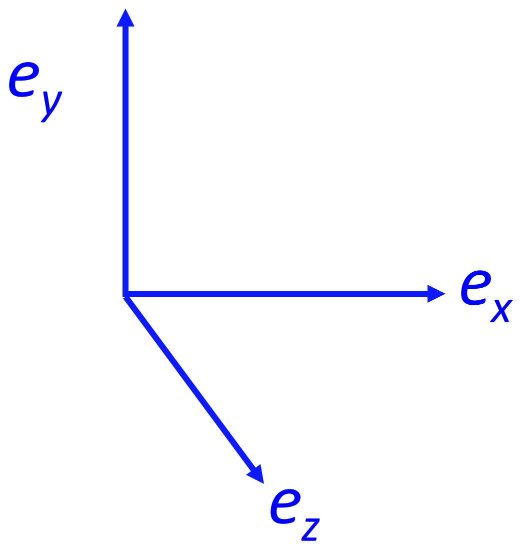
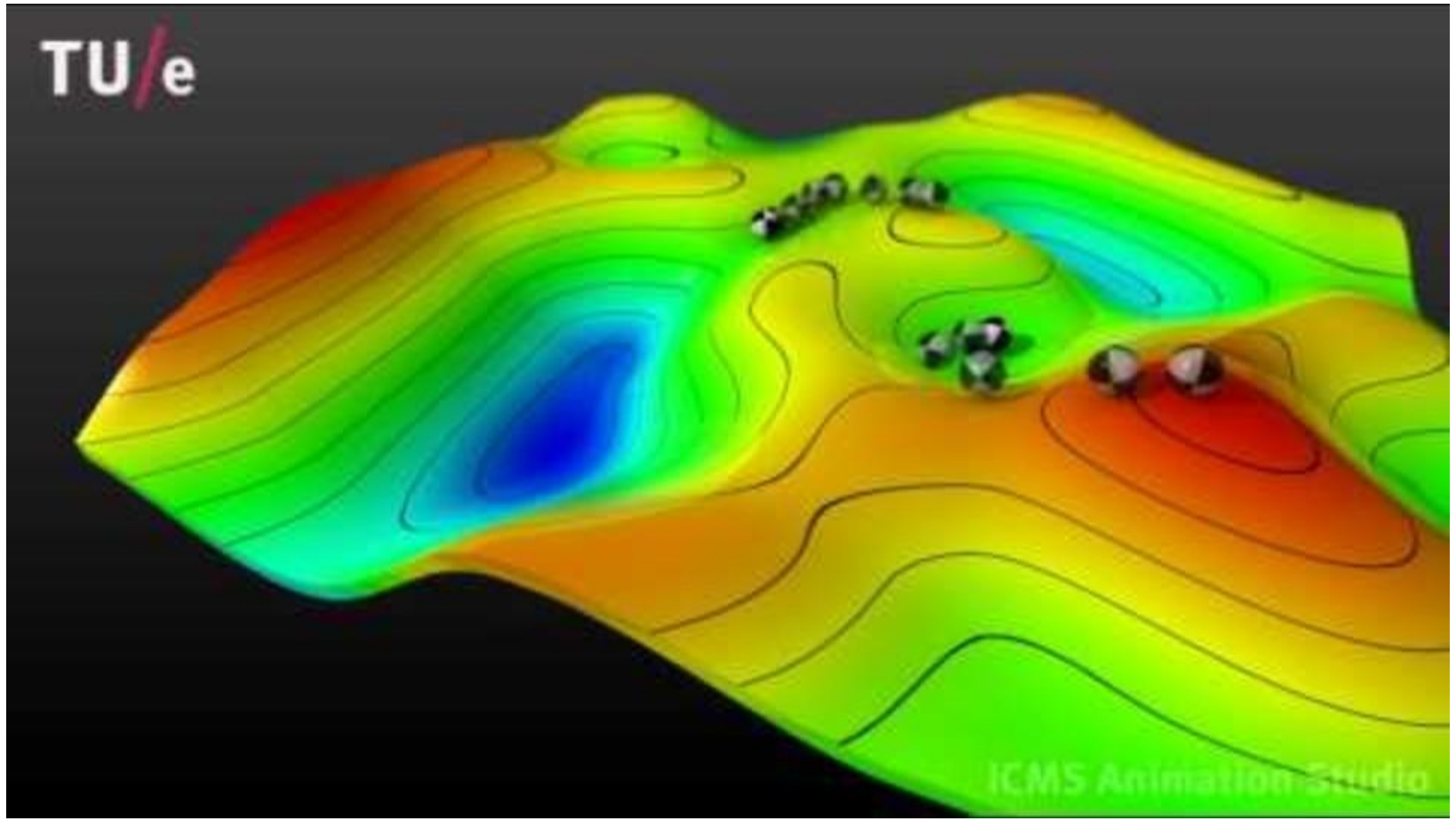
$$\frac{\partial}{\partial t}(\rho u)+\nabla\bullet(\rho \mathrm{u}u)=\nabla\bullet(\mu\,\nabla u)-\nabla p+S_u$$

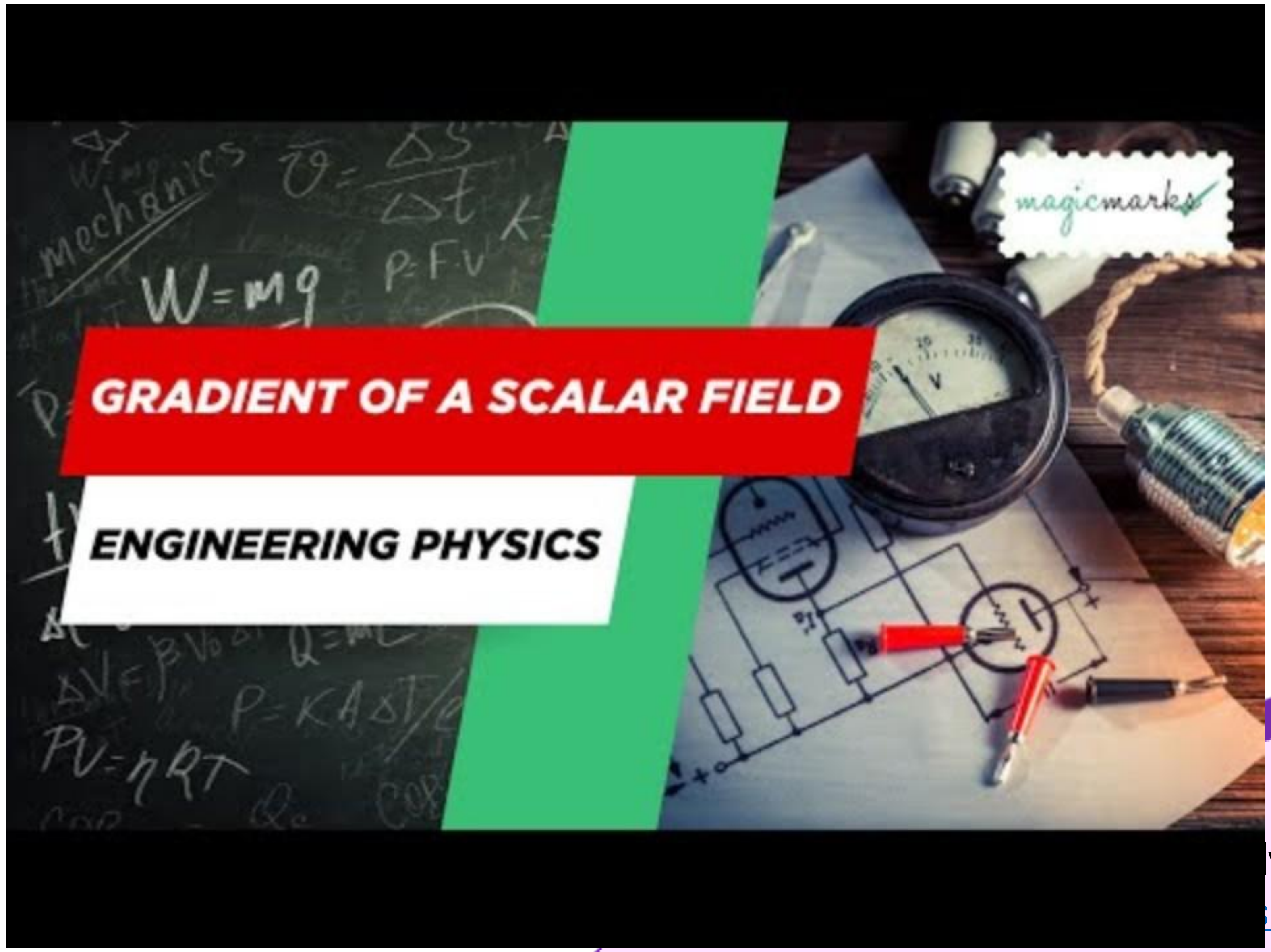
Mathematical operations



Gradient:

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





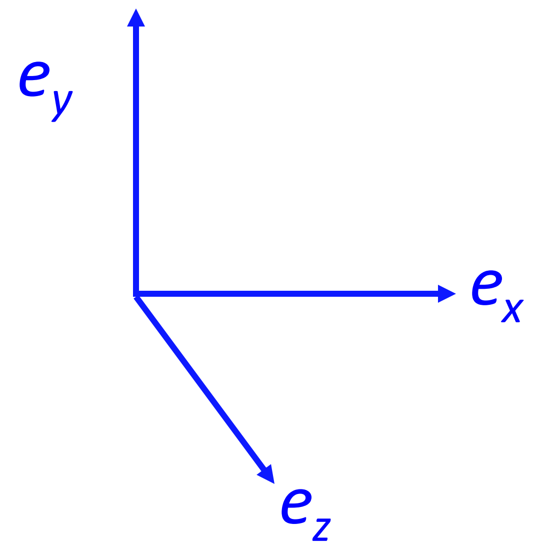
Source: https://www.youtube.com/watch?v=vWFjqgb-ylQ
https://www.youtube.com/watch?v=fZ231k3zsAA

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

Mathematical operations

Gradient:

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



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

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

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

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.

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

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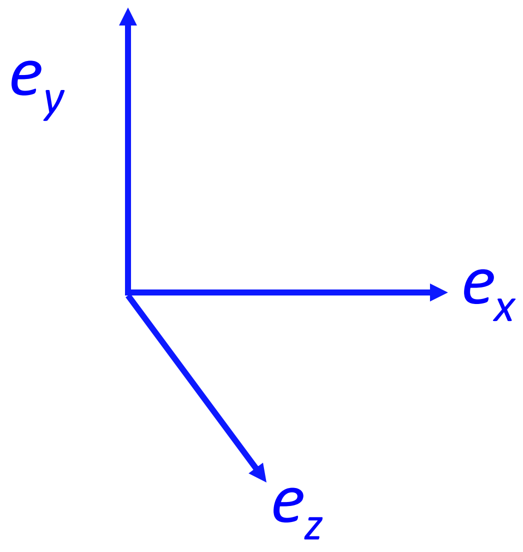
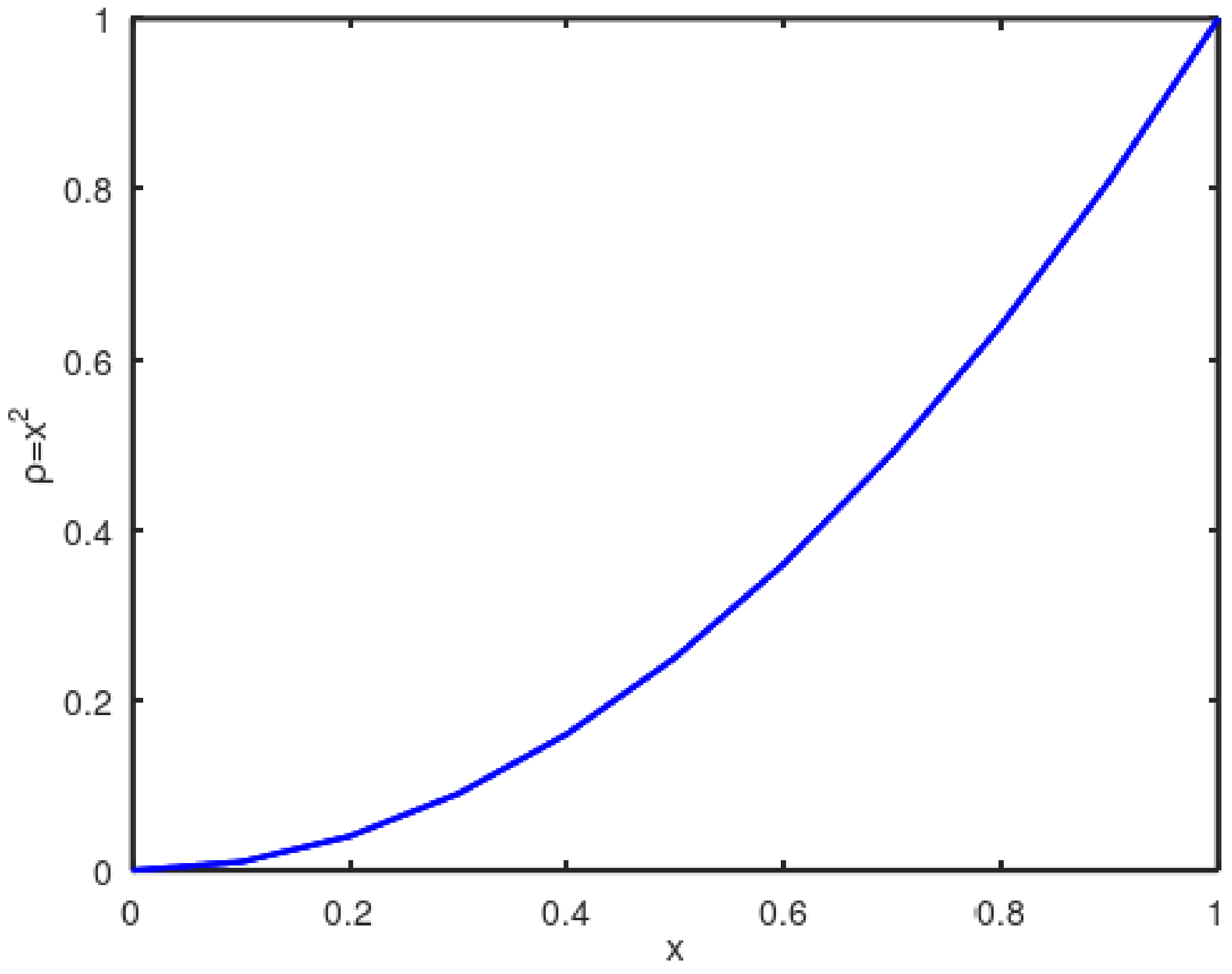
Mathematical operations

Gradient

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

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





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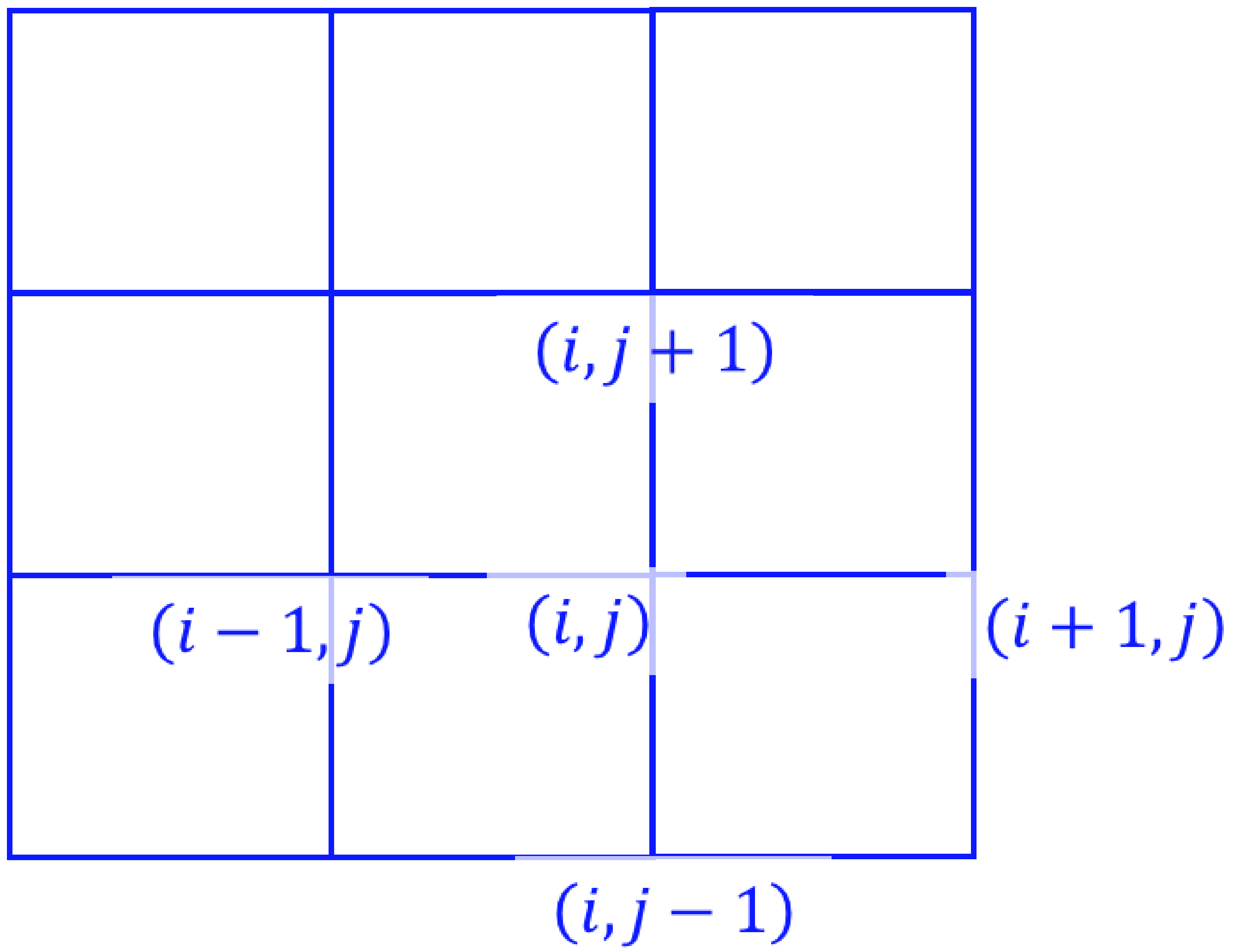
Finite Difference Method (FDM)

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

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



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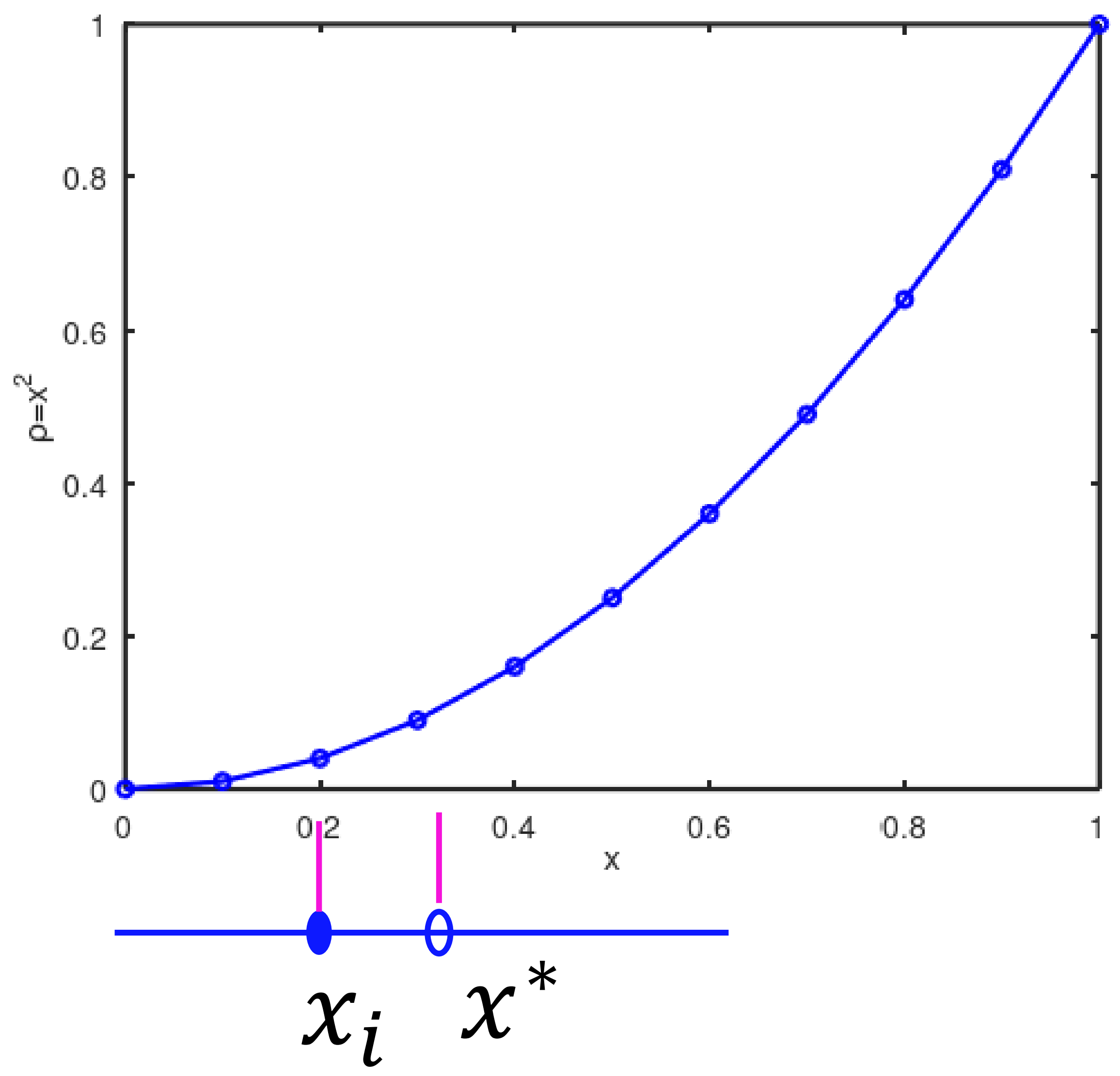
Taylor series expansion



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

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Taylor series expansion

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

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

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

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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

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

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

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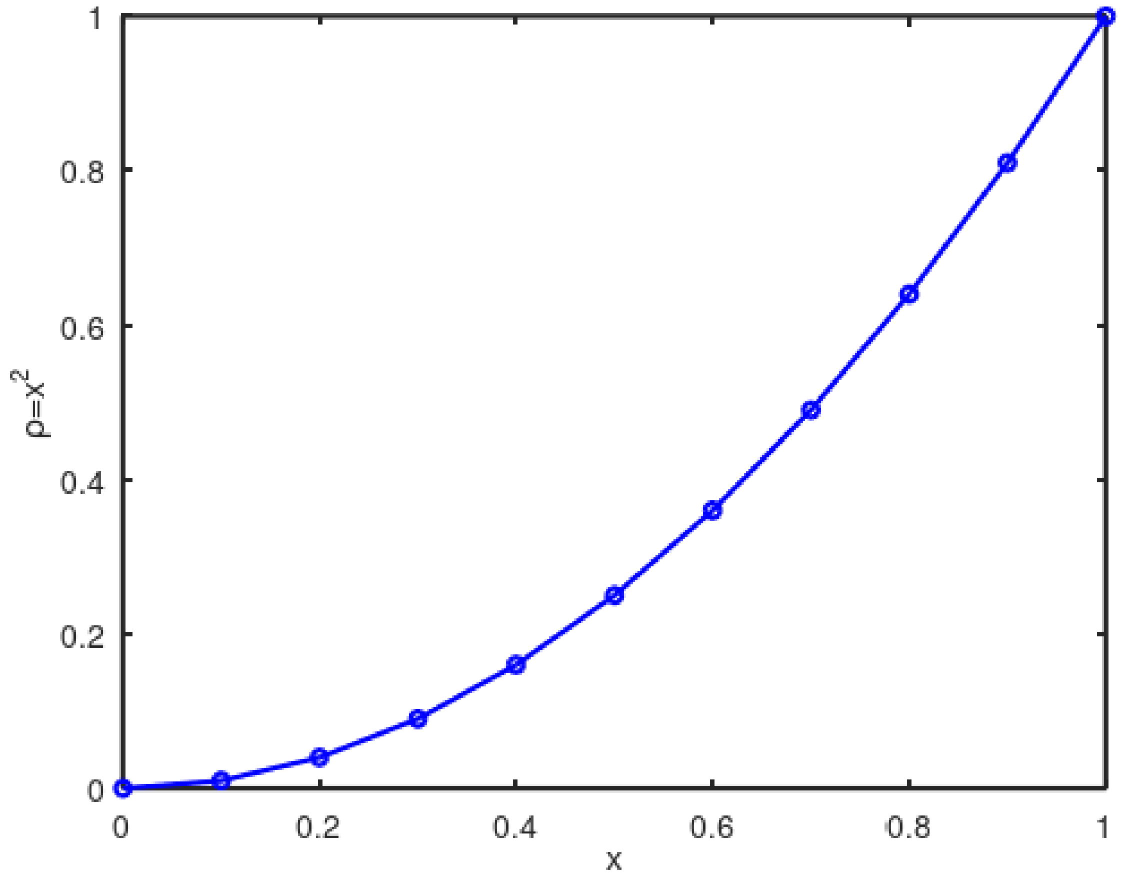
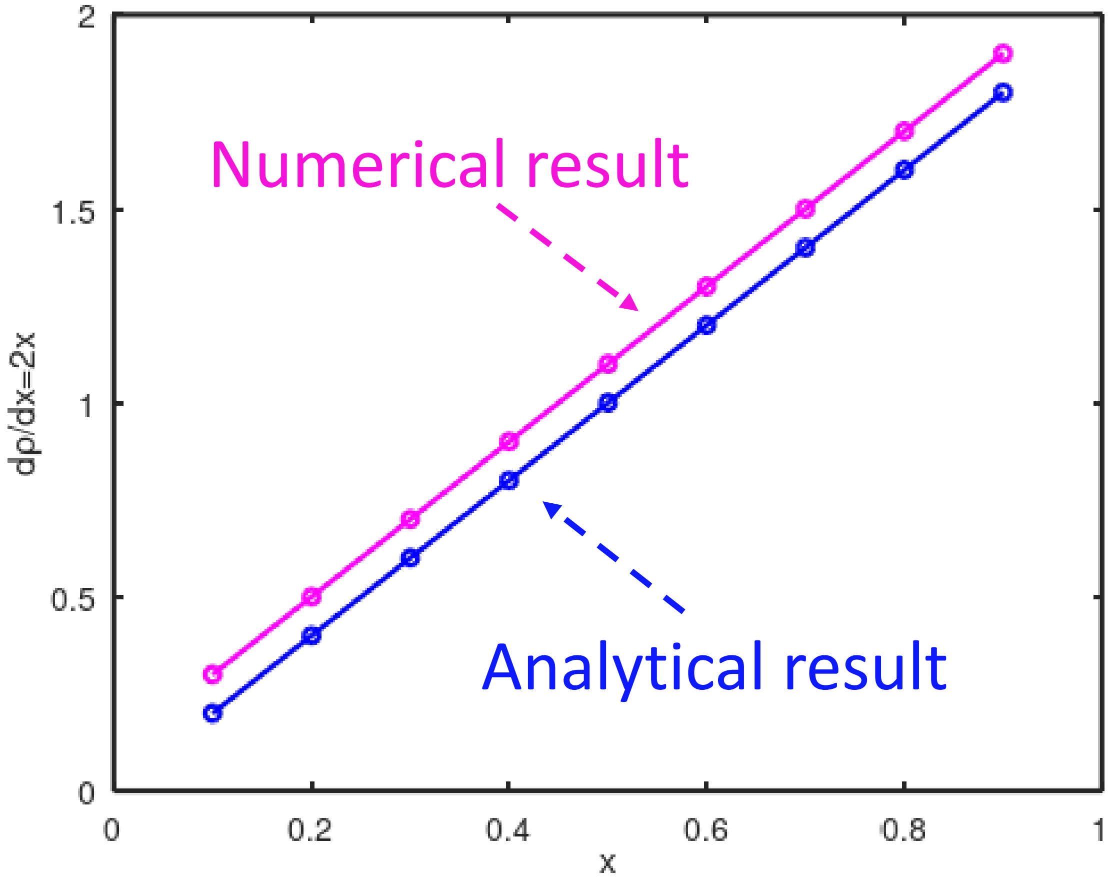
Analytical and Numerical solutions

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





Resolved in OCTAVE

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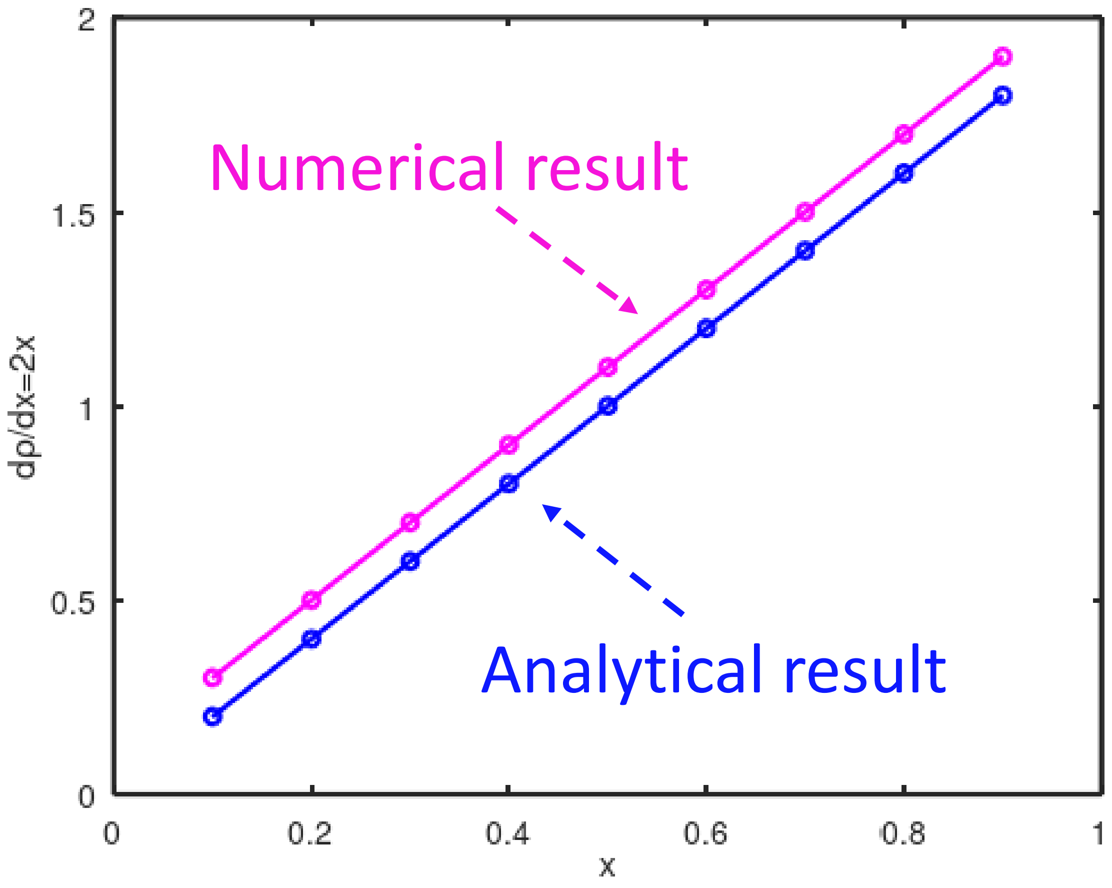
Analytical and Numerical solutions

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 – 4
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;
```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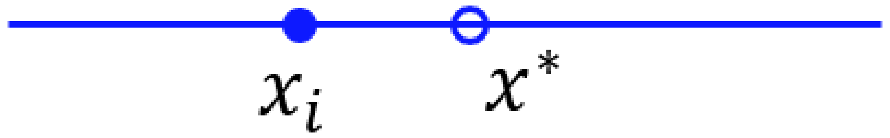
Taylor series: Summary



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

First order forward difference

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Exercise – 4

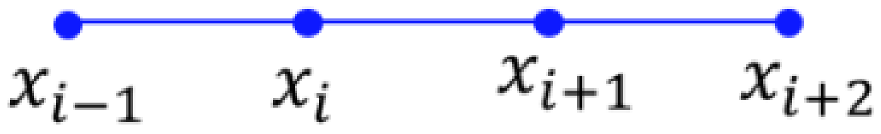
[Exercise-4] Solve using first order forward derivative scheme #5

kummi0402 started this conversation in General

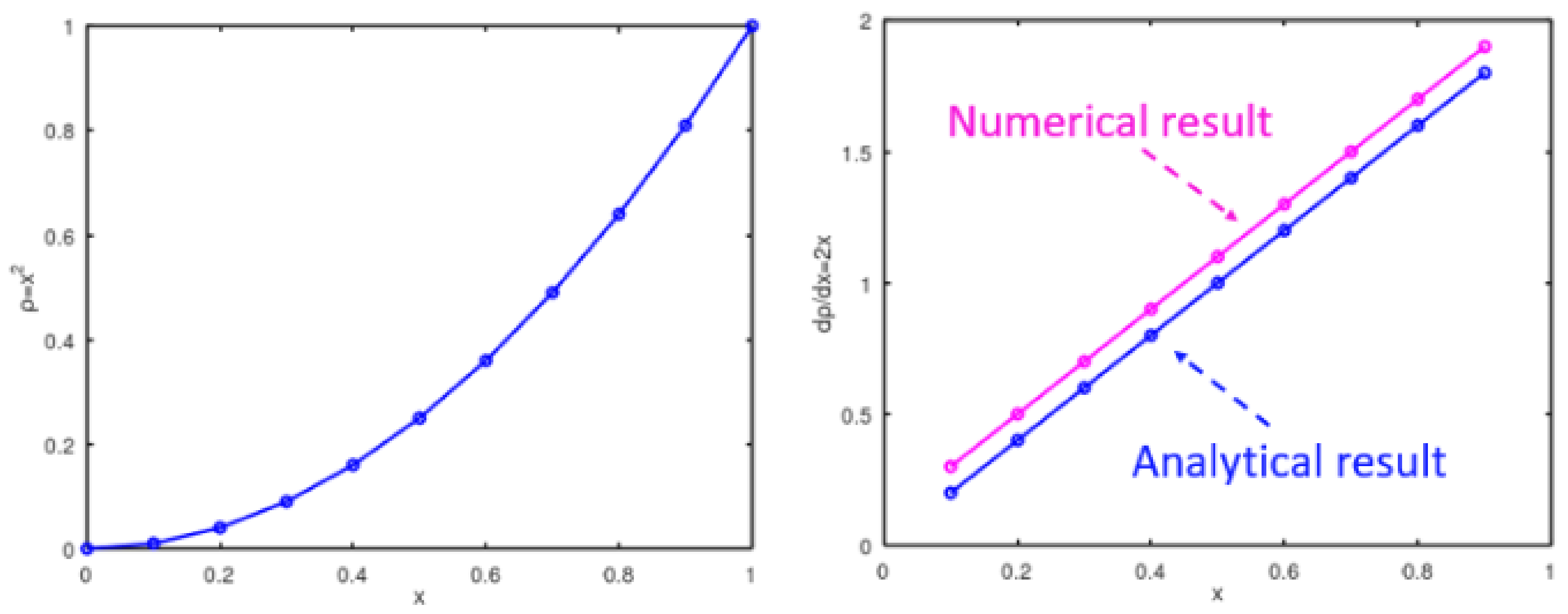
kummi0402 now Maintainer

Make use of Octave code and plot for the forward first order derivative: when $\rho = x^2$ and x^3
OCTAVE code: https://github.com/exaslate-learn/applied-cfd-using-openfoam-aec-2025/tree/main/DAY1-1

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

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THANK YOU