

Applied Computational Fluid Dynamics with OpenFOAM

Day -2



ExaSlate

Develop \equiv Guide \equiv Collab

Contents

- Introduction
- CFD fundamentals
- Mathematical operations
- Governing Differential Equations
- Taylor series + FDM
- Exercise – 1 (Installations)
- Exercise – 2 (First order forward difference method)

Introduction – About this course

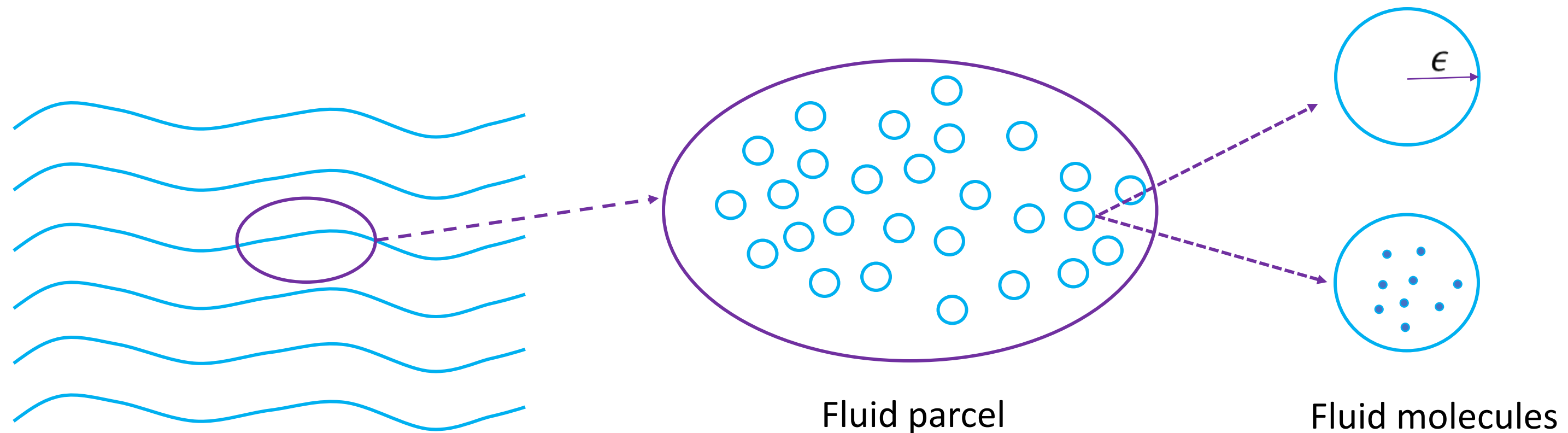
- Course duration per session: 2 hrs
- Total course duration: 30 – 35 hrs
- Requirements:
 - Virtual box and installing OS & softwares.
 - Interest to learn CFD using OpenFOAM & Octave
 - Interest to ask questions in discussion forum (GitHub)
- Exercises (equal weightages)

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)

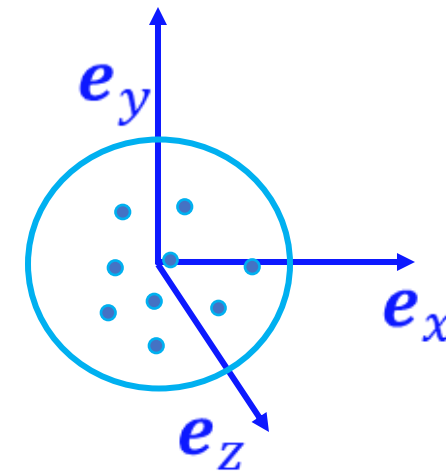
CFD fundamentals – Fluid

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

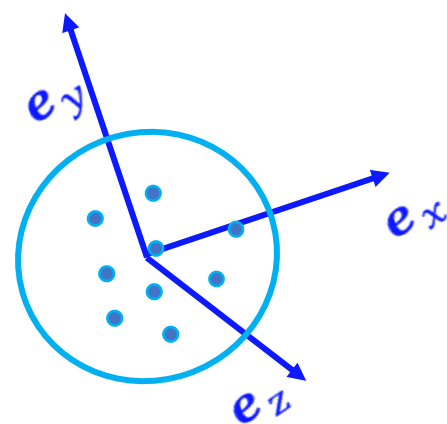


CFD fundamentals – Fluid

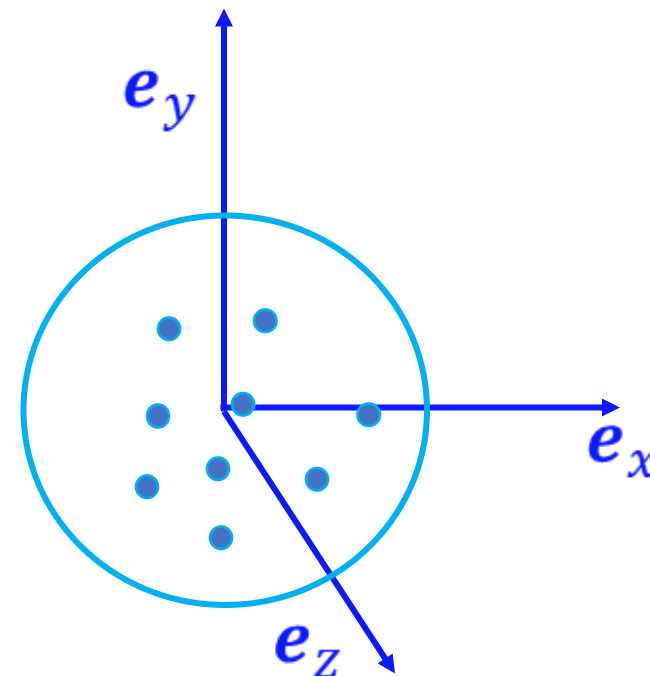
- A substance whose molecular structure offers no resistance to external forces -
Ferziger, Peric



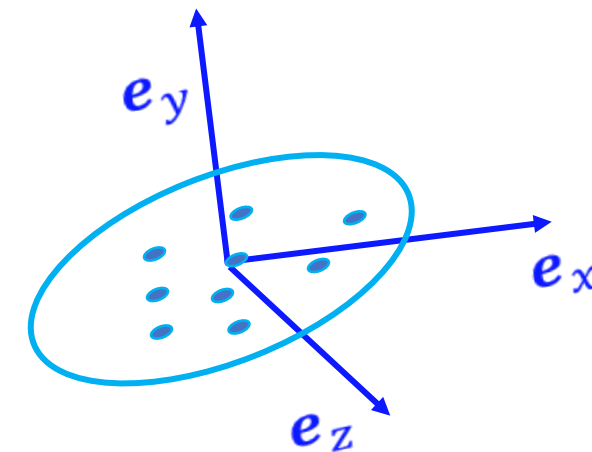
Fluid parcel



Rotation



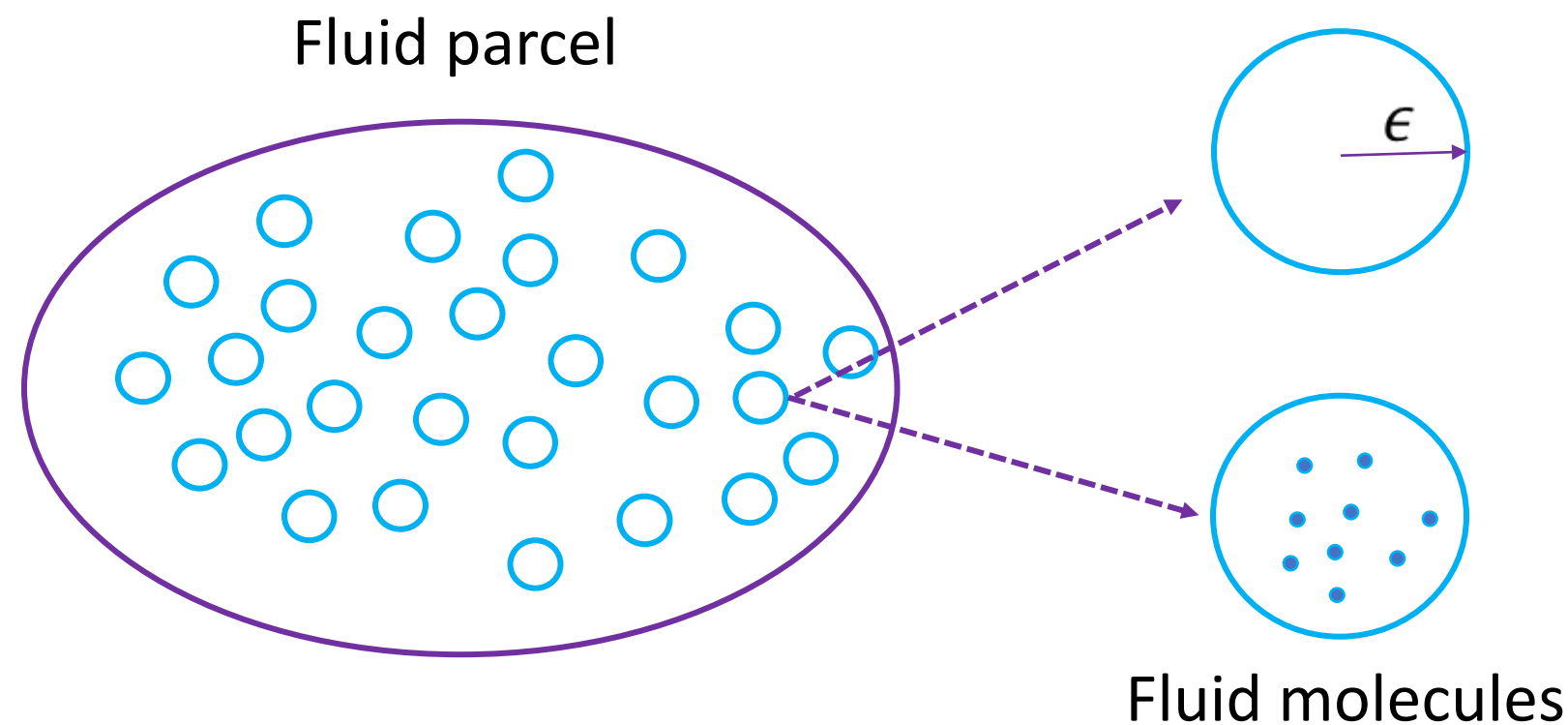
Expansion



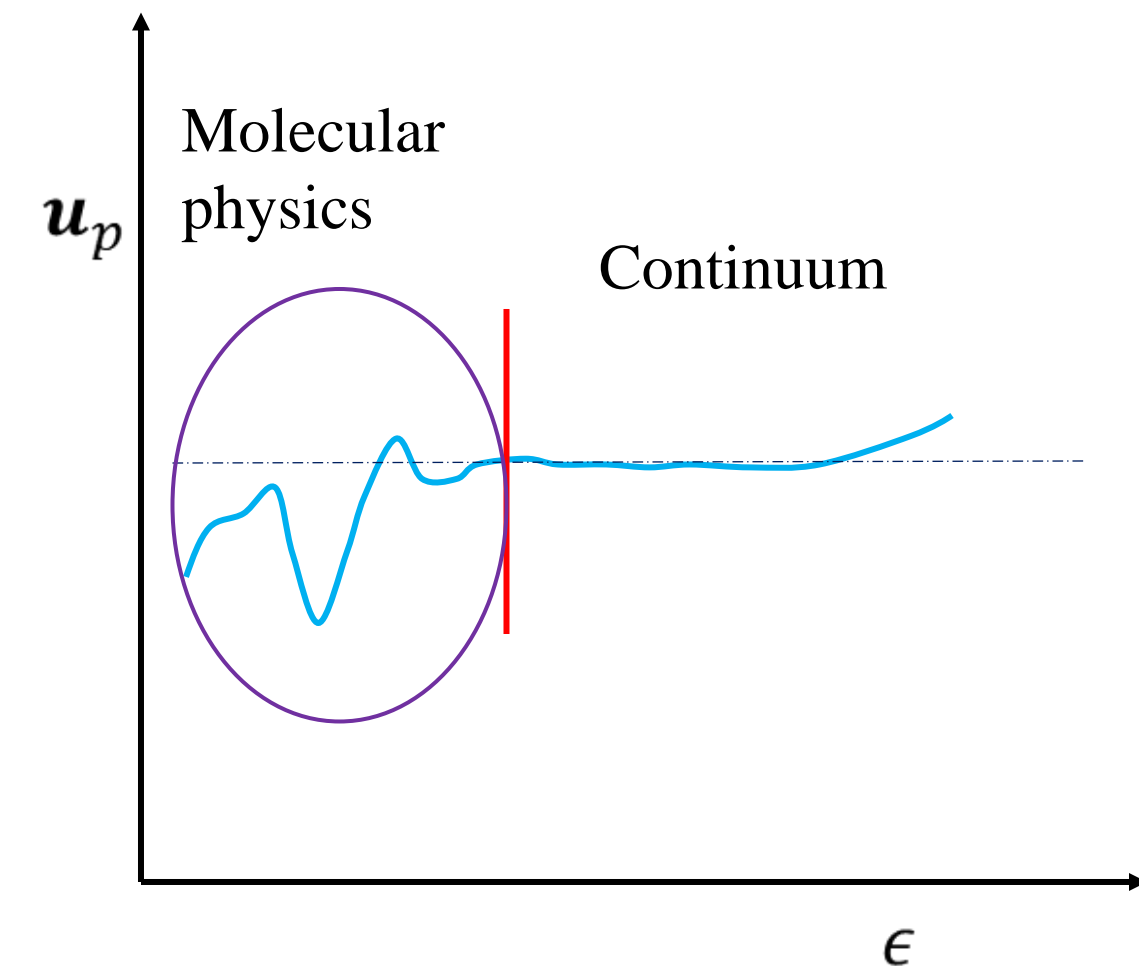
Deformation

CFD fundamentals – Fluid

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



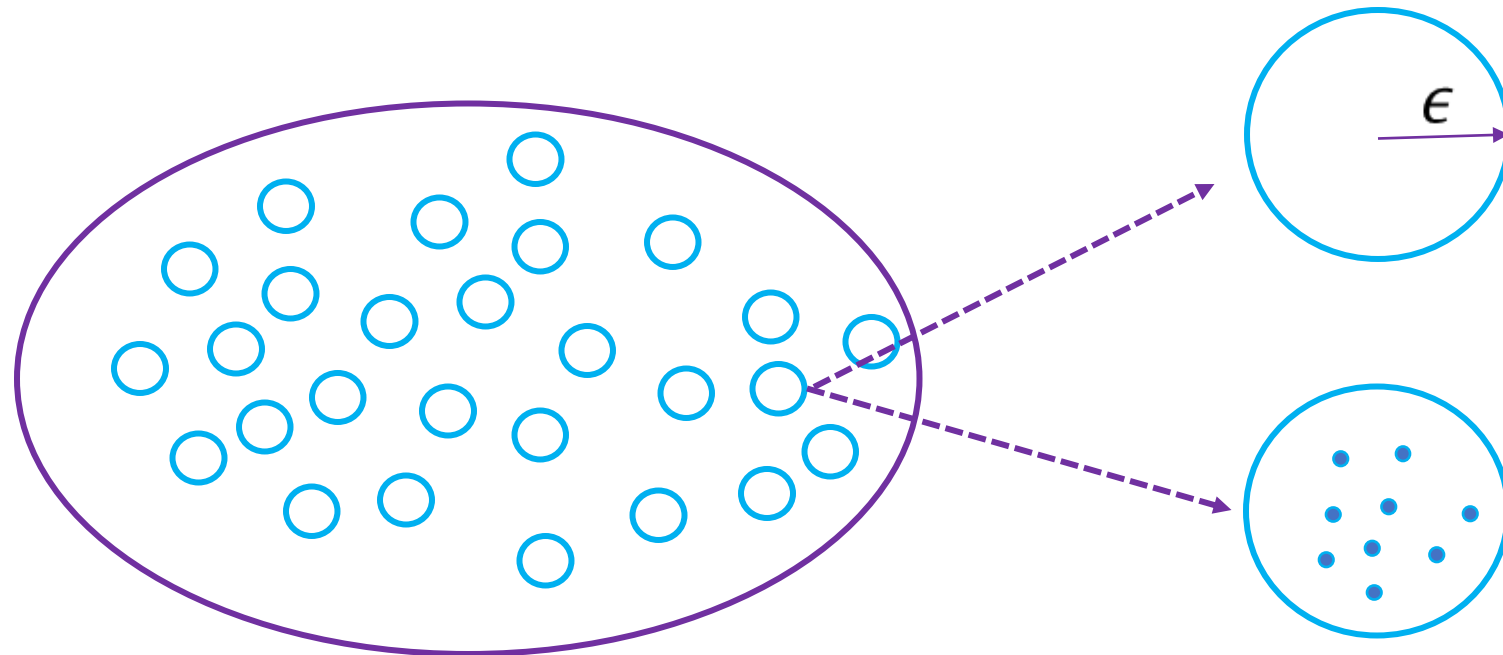
$$\mathbf{u}_p = \frac{\sum_{i=1}^{N_{mol}} \mathbf{u}_{mol}}{N_{mol}}$$



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

CFD fundamentals – Continuum

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



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

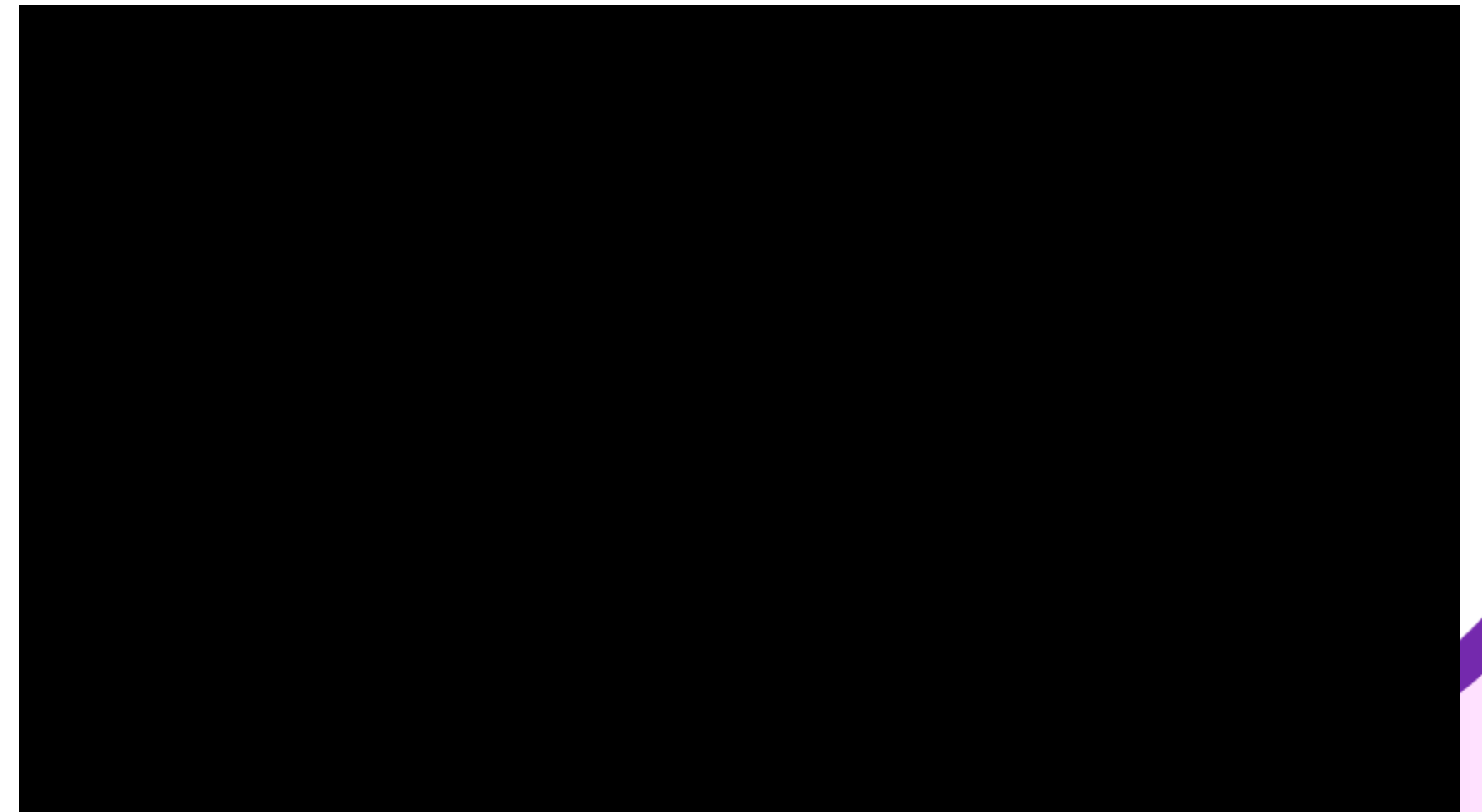
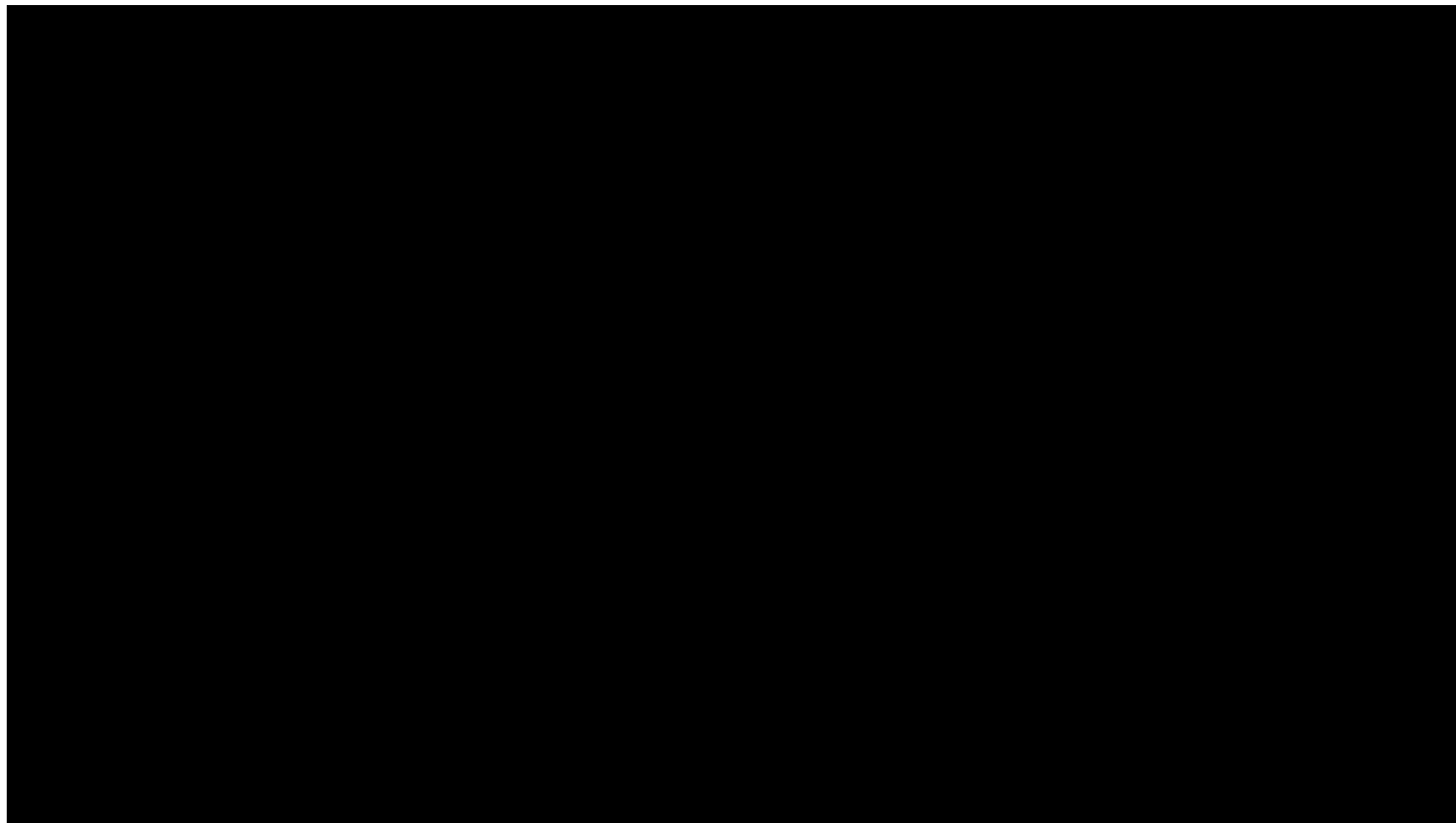
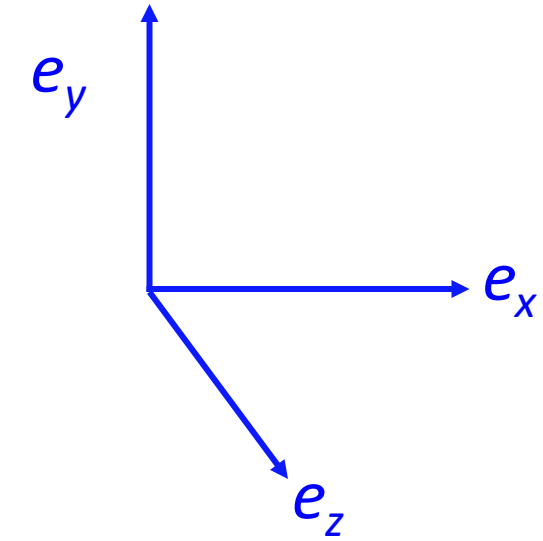
In physics, **mean free path** is the average distance over which a moving particle

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

Mathematical operations

Gradient:

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



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

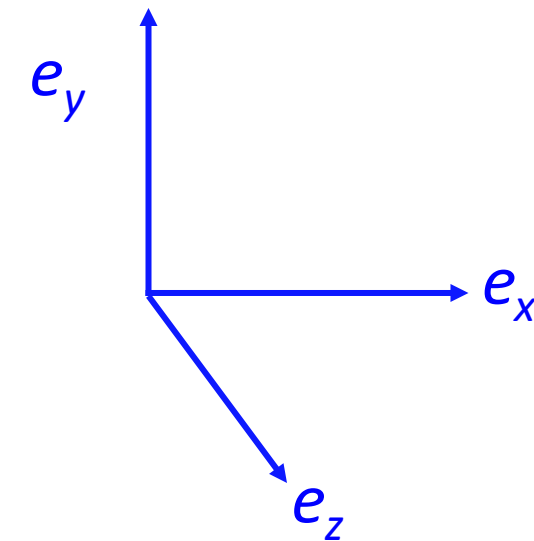
Mathematical operations

Gradient:

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

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

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



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

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.

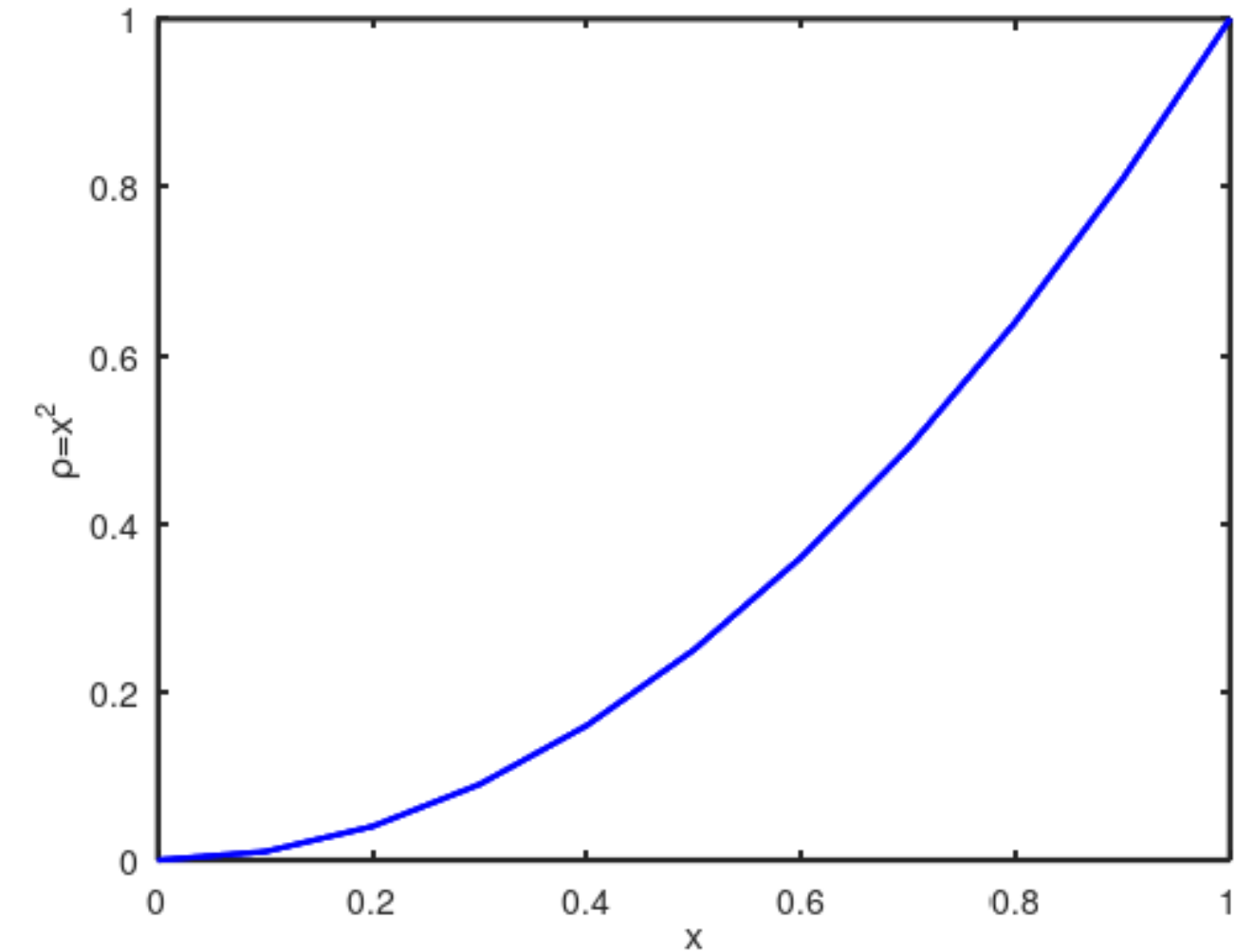
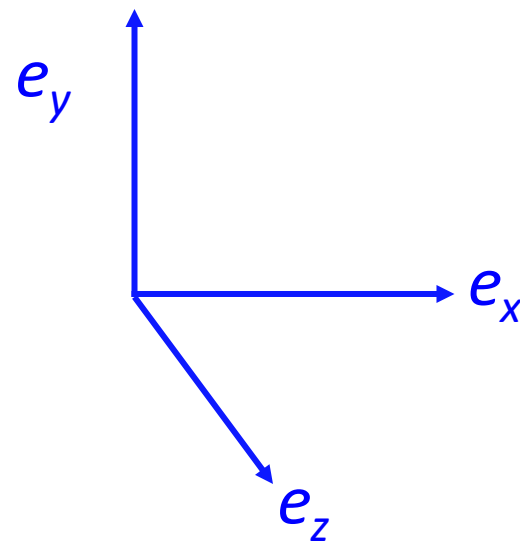
$$\nabla \cdot \mathbf{u} = \left(\frac{\partial}{\partial x} \mathbf{e}_x + \frac{\partial}{\partial y} \mathbf{e}_y + \frac{\partial}{\partial z} \mathbf{e}_z \right) (u \mathbf{e}_x + v \mathbf{e}_y + w \mathbf{e}_z) = \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial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

Mathematical operations

Gradient

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

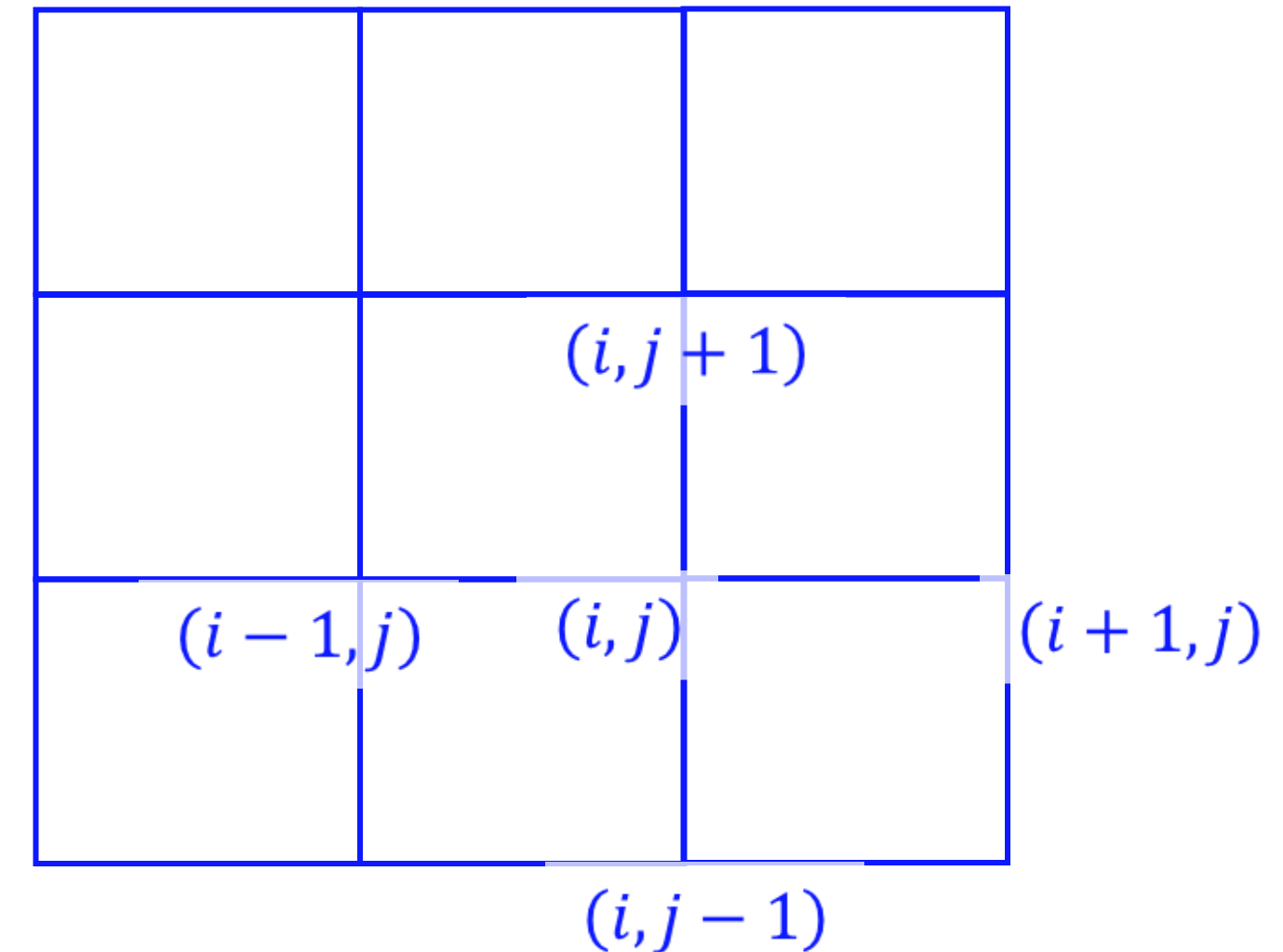
$$\frac{\partial \rho}{\partial x} = \frac{d\rho}{dx} (\text{in 1D})$$



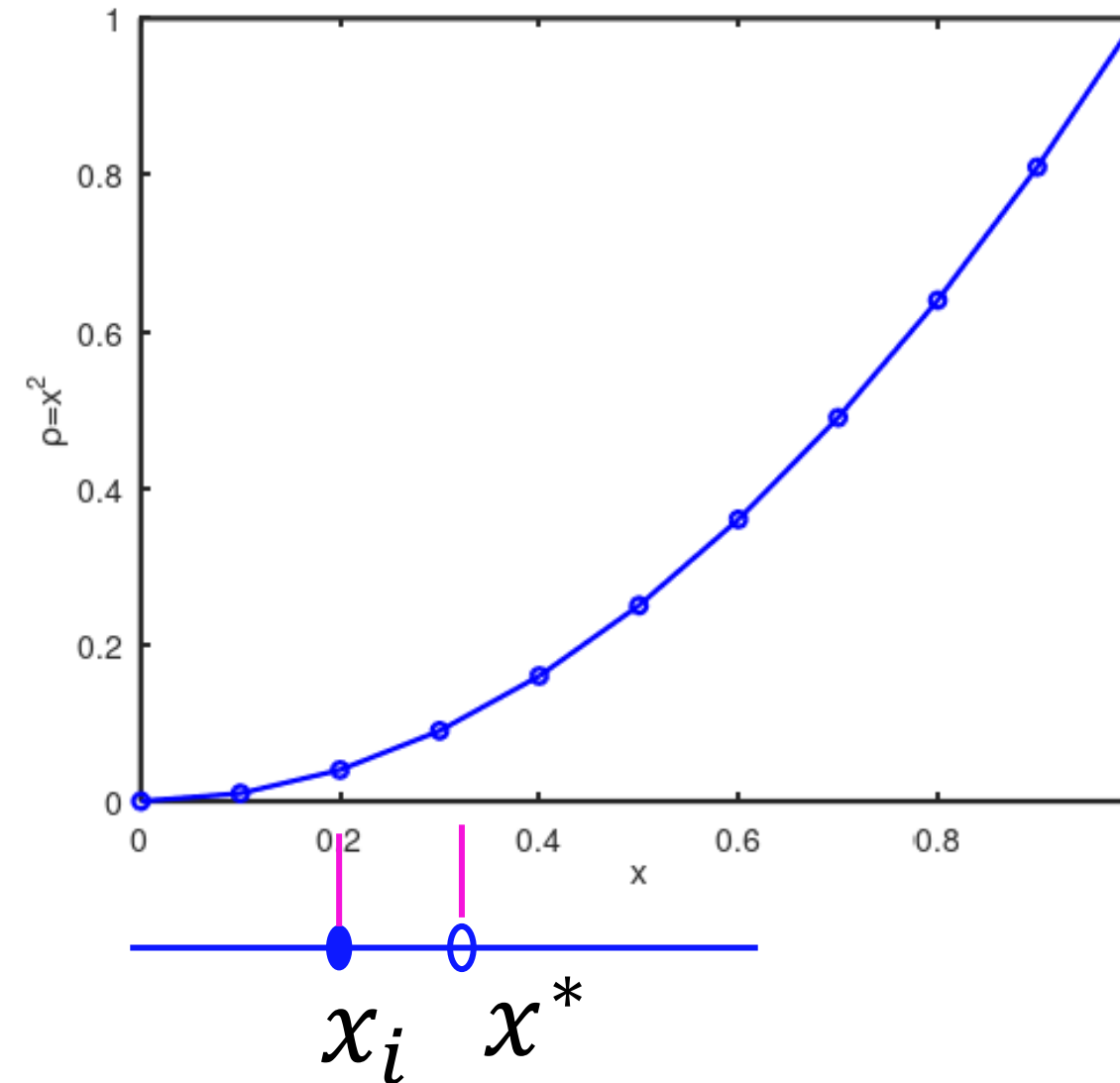
Finite Difference Method (FDM)

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

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



Taylor series expansion



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

Taylor series expansion



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

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

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

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

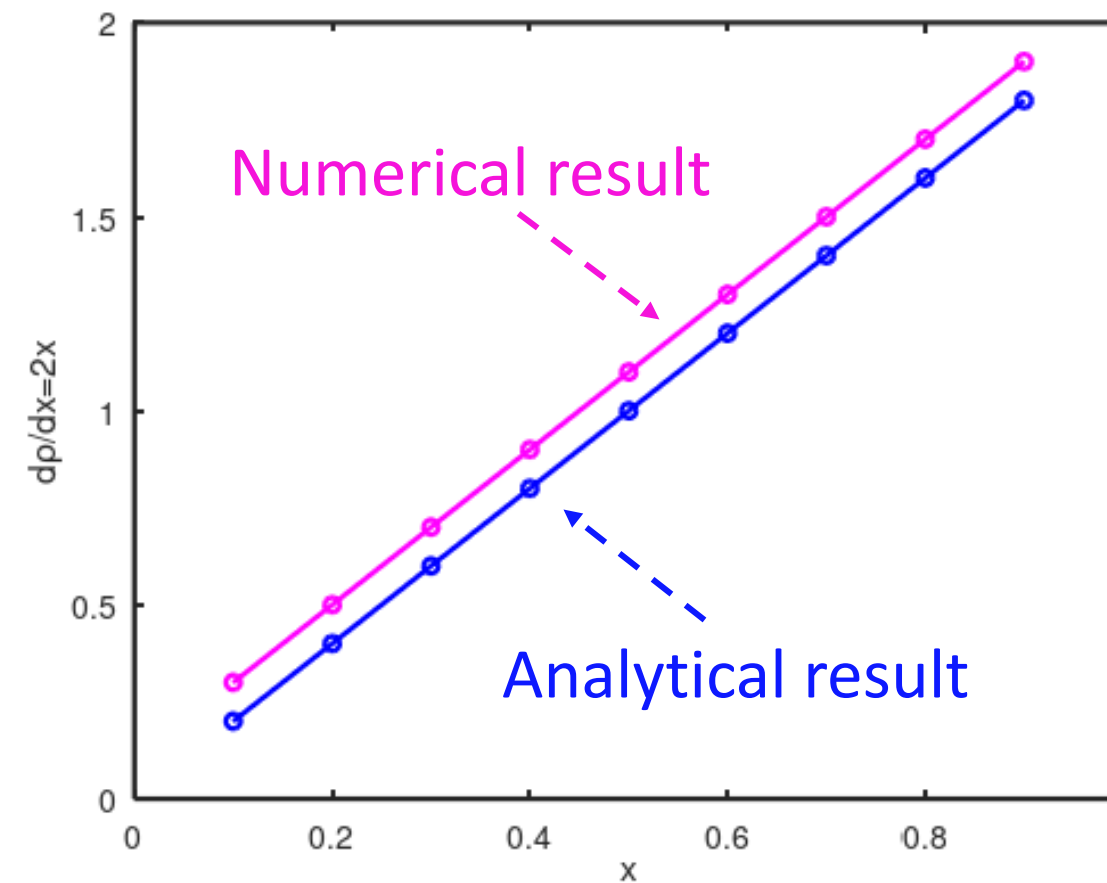
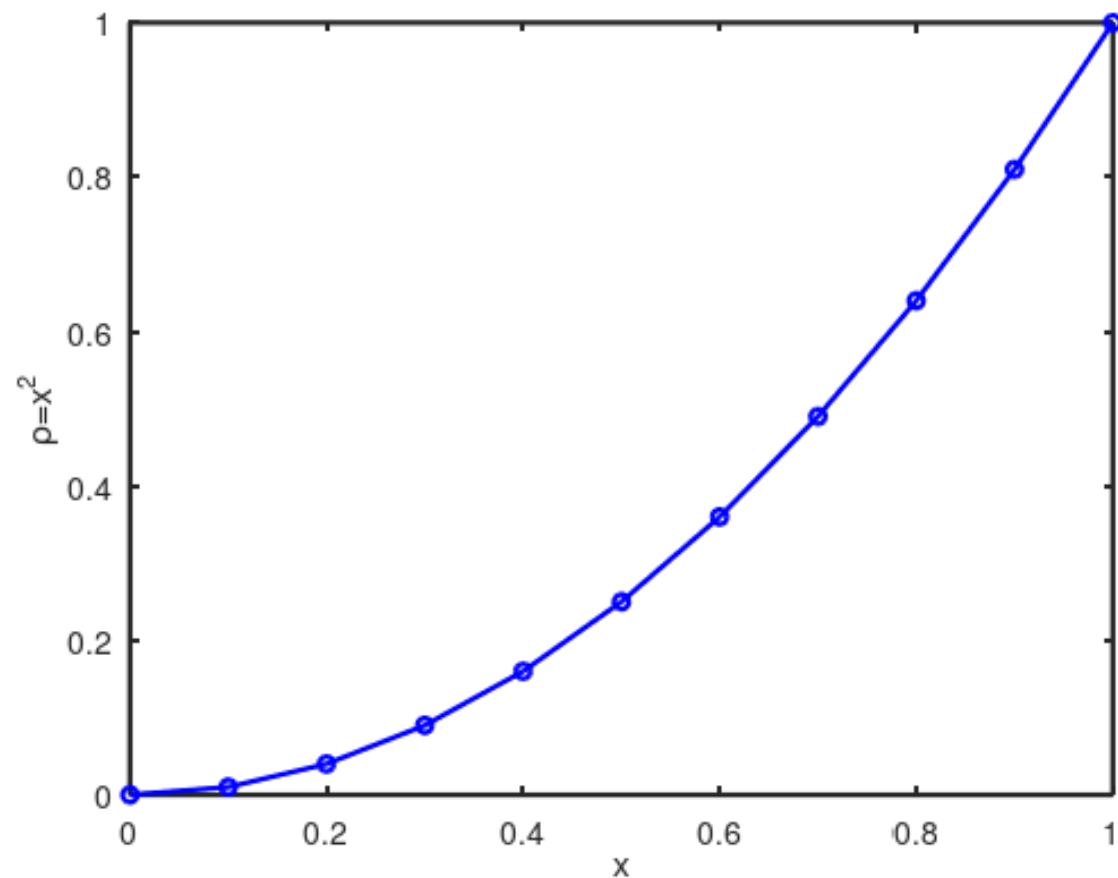
$$\nabla \rho = \left(\frac{\partial}{\partial x} \mathbf{e}_x + \frac{\partial}{\partial y} \mathbf{e}_y + \frac{\partial}{\partial z} \mathbf{e}_z \right) \rho = \left(\frac{\partial \rho}{\partial x} \mathbf{e}_x + \frac{\partial \rho}{\partial y} \mathbf{e}_y + \frac{\partial \rho}{\partial z} \mathbf{e}_z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

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

Analytical and Numerical solutions



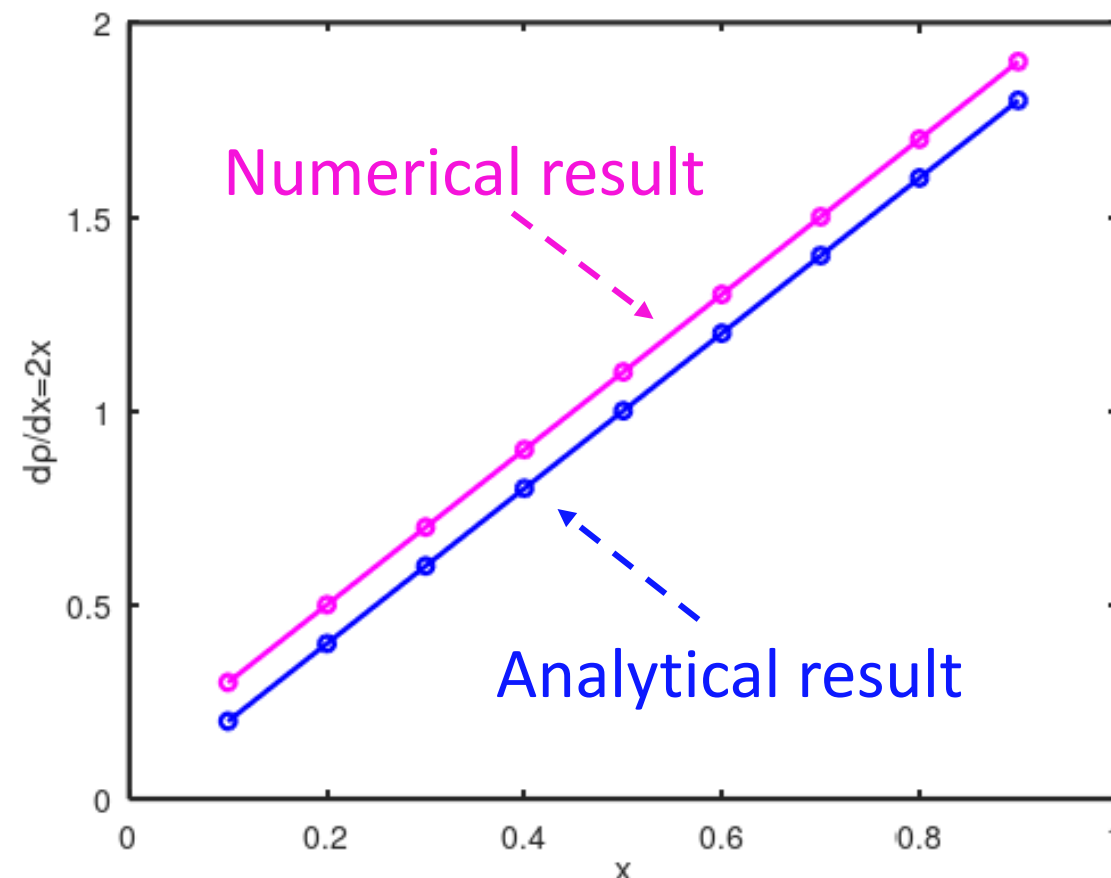
$$\left(\frac{\partial \rho}{\partial x}\right)_i = \frac{\rho(x_{i+1}) - \rho(x_i)}{\Delta x_i} + O(\Delta x_i)$$



Resolved in OCTAVE

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.



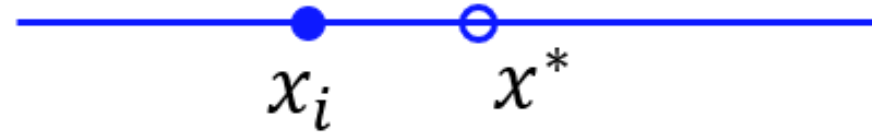
Exercise – 2 OCTAVE

```

1  %% Approximating derivative using first order numerical scheme.
2
3  clear all;
4  close all;
5
6  x = [0:0.1:1]';
7  y = x.^2;
8
9  n = length(x);
10
11 figure(1);
12 %plot(x, y, '-b', 'linewidth', 2);
13 plot(x, y, '-ob', 'linewidth', 2);
14 hold on;
15 xlabel('x');
16 ylabel('\rho=x^2');
17 set(gca, "linewidth", 2, "fontsize", 14)
18
19 % gradient
20 yp = 2*x; % Analytical expression
21
22 yp_n1 = zeros(size(y));
23
24 yp_n1(1, 1) = (y(2, 1) - y(1, 1)) / (x(2, 1) - x(1, 1));
25 yp_n1(n, 1) = (y(n, 1) - y(n-1, 1)) / (x(n, 1) - x(n-1, 1));
26
27 for i = 2 : length(y)-1
28     yp_n1(i, 1) = (y(i+1, 1) - y(i, 1)) / (x(i+1, 1) - x(i, 1));
29 end
30
31 figure(2);
32 hold on;
33 plot(x(2:n-1), yp(2:n-1), '-ob', 'linewidth', 2);
34 plot(x(2:n-1), yp_n1(2:n-1), '-om', 'linewidth', 2);
35 hold on;
36 xlabel('x');
37 ylabel('d\rho/dx=2x');
38 box on;
39 set(gca, "linewidth", 2, "fontsize", 14)
40 hold off;

```

Taylor series: Summary



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



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

First order forward difference

Exercise – 2

[Exercise-2] Solve using first order forward derivative scheme #3

kummi0402 started this conversation in General



kummi0402 27 minutes ago Maintainer

edited ...

Make use of Octave code and plot for the forward first order derivative: when $\rho = x^2$ and x^3

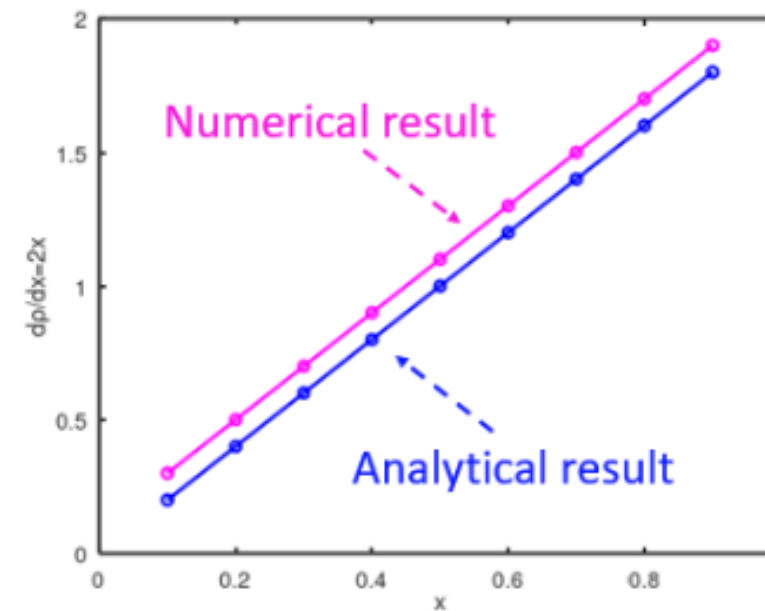
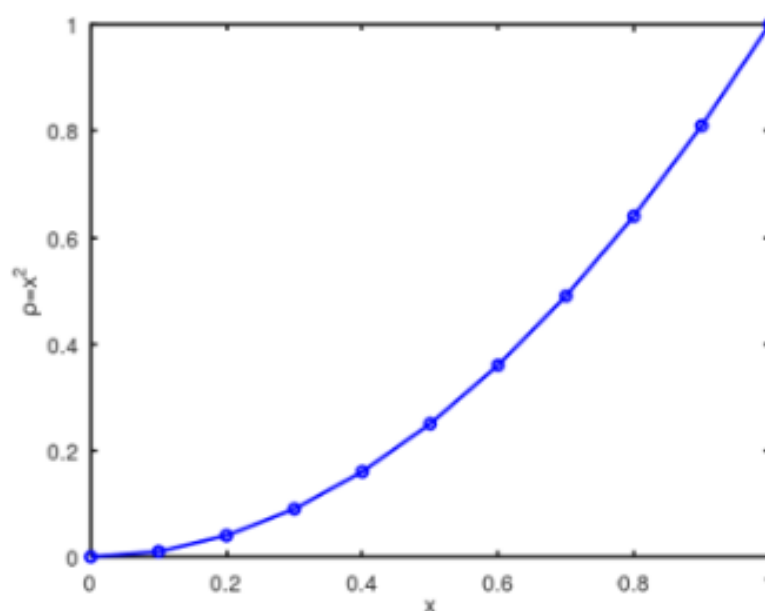
OCTAVE code:

<https://github.com/exaslate-learn/applied-cfd-using-openfoam-ksr-spring-2025/tree/main/day-2>

Analytical and Numerical solutions



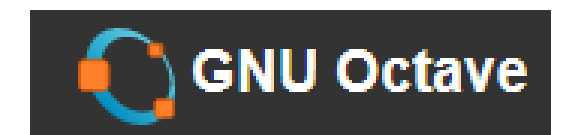
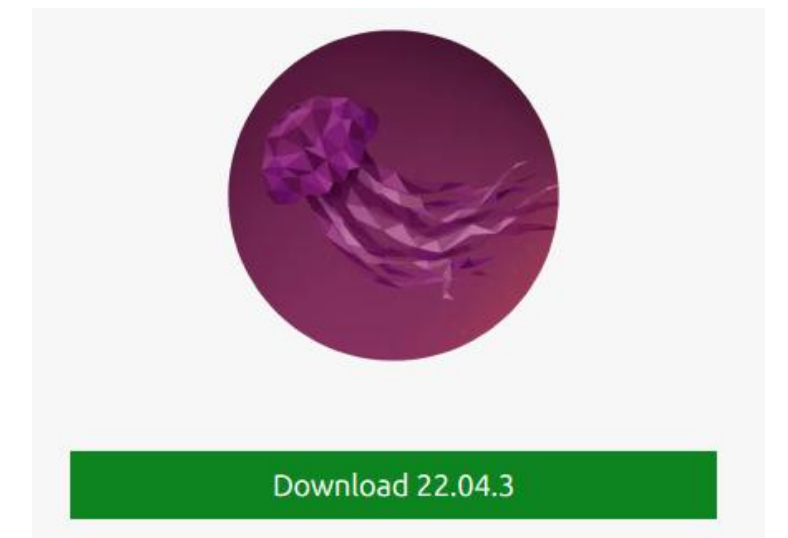
$$\left(\frac{\partial \rho}{\partial x}\right)_i = \frac{\rho(x_{i+1}) - \rho(x_i)}{\Delta x_i} + O(\Delta x_i)$$



Resolved in OCTAVE

Installations

- Preconfiguration packages:
 - <https://1drv.ms/f/s!AqT2YEB97-1RgP8MtsMPqoOGsq4ddg?e=IocXv0>
- List
 - Virtual Box [to create virtual machines]
 - Operating System: Ubuntu 24.04.1 [Install OpenFOAMv2412 & Octave]
 - AnyDesk [For remote access]
- Create a github account:
 - <https://github.com/exaslate-learn/applied-cfd-using-openfoam-ksr-spring-2025>
 - Discussion forum:
 - <https://github.com/exaslate-learn/applied-cfd-using-openfoam-ksr-spring-2025/discussions>



Exercise – 1 ➔ Install packages

[Exercise-1] Package installations #2

acrlakshman started this conversation in General



acrlakshman 4 days ago Maintainer

- Install OpenFOAM following the documentation in <https://1drv.ms/f/s!AqT2YEB97-1RgP8MtsMPqoOGsq4ddg?e=locXv0>
 - Follow instructions in `installation_steps.pdf`

↑ 1



Category

 General

Labels

None yet



VIMAL-SELVAN 2 days ago

```
openform VIMAL [Running] - Oracle VirtualBox
File Machine View Input Devices Help
Apr 20 23:57
vimalacer@vimalacer-VirtualBox: ~
vimalacer@vimalacer-VirtualBox:~$ which blockMesh
/home/vimalacer/OpenFOAM/openfoam/platforms/linux64GccDPInt32Opt/bin/blockMesh
vimalacer@vimalacer-VirtualBox:~$ blockMesh
*****
//
//      F ield      | OpenFOAM: The Open Source CFD Toolbox
//      O peration   | Version: 2412
//      A nd         | Website: www.openfoam.com
//      M anipulation|
//
*****
Build : d3949886ce-20241220 OPENFOAM=2412 version=v2412
Arch  : "LSB;label=32;scalar=64"
Exec  : blockMesh
Date  : Apr 20 2025
Time  : 23:57:48
Host  : vimalacer-VirtualBox
PID   : 3676
I/O   : uncollated
Case  : /home/vimalacer
nProcs : 1
trapFpe: Floating point exception trapping enabled (FOAM_SIGFPE).
fileModificationChecking: Monitoring run-time modified files using timeStampMaster (fileModificationSkew 5, maxFileModificationPolls 20)
allowSystemOperations: Allowing user-supplied system call operations
// ***** //
Create time

--> FOAM FATAL ERROR: (openfoam-2412)
cannot find file "/home/vimalacer/system/controlDict"

From virtual Foam::autoPtr<Foam::ISstream> Foam::fileOperations::uncollatedFileOperation::readStream(Foam::regIOobject&, const Foam::fileName&, const Foam::word&, bool) const
in file global/fileOperations/uncollatedFileOperation/uncollatedFileOperation.C at line 629.

FOAM exiting
vimalacer@vimalacer-VirtualBox:~$
```


THANK YOU