MA4110/MA5020: Computational Methods for Fluid Flow

Mathematical Prerequisites: Vector Calculus & PDE Foundations

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1 Introduction: The Mathematical Language of Fluids

Fluid motion is governed by physical conservation principles (conservation of mass, momentum, and energy). To translate these physical principles into mathematical equations that a computer can solve, we use two fundamental toolkits: **Vector Calculus** and **Partial Differential Equations (PDEs)**.

This lecture provides the essential mathematical foundations required before we derive the governing equations of fluid flow.

2 Essential Vector Differential Operators

Fluid fields are described by scalar quantities (density ρ, pressure p, temperature T) and vector quantities (velocity $\boldsymbol{v} = (u, v, w)$). The spatial changes in these fields are governed by four basic differential operators.

2.1 The Gradient

The **gradient** $\nabla\phi$ operates on a scalar field $\phi(x, y, z)$ and produces a vector pointing in the direction of the greatest rate of increase:

$$\nabla\phi = \left(\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z}\right) \tag{1}$$

Physical Intuition: A pressure difference creates a force. The pressure gradient term $-\nabla p$ represents the net force per unit volume driving fluid from high-pressure regions to low-pressure regions.

2.2 The Divergence

The **divergence** $\nabla \cdot \boldsymbol{v}$ operates on a vector field $\boldsymbol{v} = (u, v, w)$ and yields a scalar measuring the net volumetric expansion or contraction rate at a point:

$$\nabla \cdot \boldsymbol{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \tag{2}$$

Physical Intuition:

- $\nabla \cdot \boldsymbol{v} > 0$: Net expansion (fluid mass is leaving the volume element).
- $\nabla \cdot \boldsymbol{v} < 0$: Net compression (fluid mass is accumulating).
- $\nabla \cdot \boldsymbol{v} = 0$: **Incompressible flow** (volume of every fluid parcel remains constant).

2.3 The Curl

The **curl** $\nabla \times \boldsymbol{v}$ operates on a vector field $\boldsymbol{v}$ and produces a vector representing local rotation:

$$\nabla \times \boldsymbol{v} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ u & v & w \end{vmatrix} \tag{3}$$

Physical Intuition: In fluid dynamics, $\boldsymbol{\omega} = \nabla \times \boldsymbol{v}$ is called the **vorticity vector**. It measures twice the local angular velocity of a fluid element (spinning motion in vortices, shear layers, and boundary layers).

2.4 The Laplacian

The **Laplacian** $\nabla^2\phi$ is the divergence of the gradient ($\nabla^2\phi = \nabla \cdot (\nabla\phi)$):

$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2} \tag{4}$$

Physical Intuition: The Laplacian represents spatial diffusion and smoothing processes, such as viscous friction dissipating kinetic energy ($\nu\nabla^2\boldsymbol{v}$) or thermal conduction spreading heat ($k\nabla^2 T$).

3 The Divergence Theorem: Bridging Integral Laws to PDEs

Physical conservation laws are naturally stated over a finite region of space called a **Control Volume** (CV) bounded by a **Control Surface** (CS).

The Divergence Theorem (Gauss-Ostrogradsky)

For any smooth vector field $\mathbf{F}$ defined over a volume CV enclosed by surface CS:

$$\iint_{CS} (\mathbf{F} \cdot \mathbf{n})\, dA = \iiint_{CV} (\nabla \cdot \mathbf{F})\, dV \tag{5}$$

where $\mathbf{n}$ is the outward-facing unit normal vector.

Why this matters for numerical methods: This single theorem allows us to transform global boundary flux integrals ($\iint_{CS}$) into volume integrals ($\iiint_{CV}$). Because the choice of control volume is arbitrary, setting the integrand to zero yields the local **Partial Differential Equation (PDE)**.

4 Introduction to Partial Differential Equations (PDEs)

In single-variable calculus, an Ordinary Differential Equation (ODE) relates a function $u(x)$ to its derivatives with respect to a single variable x.

In fluid mechanics, physical variables change across both space (x, y, z) and time t. Therefore, fluid equations are **Partial Differential Equations (PDEs)**.

What is a PDE?

A **Partial Differential Equation** is an equation involving an unknown multivariable function $u(x, y, z, t)$ and its partial derivatives:

$$F\left(x, y, z, t, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial t}, \frac{\partial^2 u}{\partial x^2}, \dots\right) = 0 \tag{6}$$

4.1 Key Concepts of PDEs in Fluid Flow

1. **Independent Variables:** The spatial coordinates (x, y, z) and time t.
2. **Dependent Variables:** The fluid properties we solve for, such as density $\rho(x, y, z, t)$, velocity components (u, v, w), and pressure $p(x, y, z, t)$.
3. **Order of a PDE:** The order of the highest partial derivative present.
   - First-order advection: $\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} = 0$
   - Second-order diffusion: $\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2}$
4. **Linear vs. Non-linear PDEs:** A PDE is linear if the dependent variable and its derivatives appear only to the first power and are not multiplied together.
   - Fluid flow equations are predominantly **non-linear** due to convective acceleration terms like $u\frac{\partial u}{\partial x}$. This non-linearity gives rise to complex phenomena like shock waves and turbulence, making numerical methods essential!
5. **Initial and Boundary Conditions:** A PDE has infinitely many solutions. To find the specific physical solution, we must specify:
   - *Initial Conditions*: The state of the fluid at $t = 0$.
   - *Boundary Conditions*: Values or fluxes specified on the domain boundaries (e.g. no-slip wall $\boldsymbol{v} = 0$, inlet velocity).

Note: Detailed mathematical classification of PDEs (Hyperbolic, Parabolic, and Elliptic systems) will be formally covered in **Lecture 3**.

5 Summary

Mastering these vector differential operators, the divergence theorem, and the basic structure of PDEs prepares us to derive the fundamental equation of mass conservation (*the Continuity Equation*) in Lecture 1.

References

[1] John D. Anderson. *Computational Fluid Dynamics: The Basics with Applications.* McGraw-Hill, New York, NY, 1995.

[2] Randall J. LeVeque. *Finite Volume Methods for Hyperbolic Problems.* Cambridge University Press, Cambridge, UK, 2002.