

- 1.1 What is computational fluid dynamics?
 - 1.2 Basic principles of CFD
 - 1.3 Stages in a CFD simulation
 - 1.4 Fluid-flow equations
 - 1.5 The main discretisation methods
 - Appendices
 - Examples
-

1.1 What is Computational Fluid Dynamics?

Computational fluid dynamics (CFD) is the use of computers and numerical methods to solve problems involving fluid flow.

CFD has been successfully applied in many areas of fluid mechanics. These include aerodynamics of cars and aircraft, hydrodynamics of ships, flow through pumps and turbines, combustion and heat transfer, chemical engineering. Applications in civil engineering include wind loading, vibration of structures, wind and wave energy, ventilation, fire, explosion hazards, dispersion of pollution, wave loading on coastal and offshore structures, hydraulic structures such as weirs and spillways, sediment transport. More specialist CFD applications include ocean currents, weather forecasting, plasma physics, blood flow, biofluidics, heat transfer around electronic circuitry, metal casting.

These applications involve many different fluid phenomena. In particular, the CFD techniques used for high-speed aerodynamics (where compressibility is significant, but viscous and turbulent effects are often unimportant) are very different from those used to solve the incompressible, turbulent flows typical of mechanical and civil engineering.

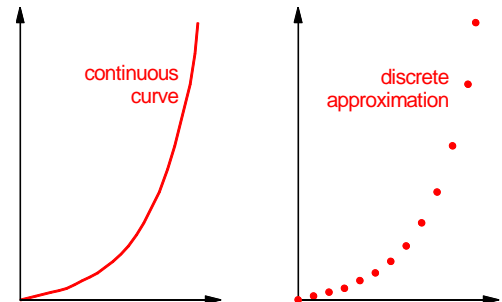
Although many elements of this course are widely applicable, the focus will be on simulating **viscous, incompressible** flow by the **finite-volume** method.

1.2 Basic Principles of CFD

The approximation of a continuously-varying quantity in terms of values at a finite number of points is called *discretisation*.

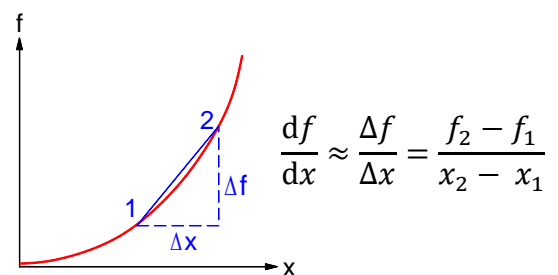
The following are common to any CFD simulation.

- (1) The flow field is discretised; i.e. field variables (ρ , u , v , w , p , ...) are approximated by their values at a finite number of *nodes*.



- (2) The equations of motion are discretised:

derivatives \rightarrow algebraic approximations
(*continuous*) (*discrete*)



- (3) The resulting system of algebraic equations is solved to give values at the nodes.

1.3 Stages in a CFD Simulation

The main stages in a CFD simulation are:

Pre-processing:

- formulate problem (geometry, equations, boundary conditions);
- computational mesh (set of control volumes).

Solving:

- discretise the governing equations;
- solve the resulting algebraic equations.

Post-processing:

- analyse (calculate derived quantities: forces, flow rates, ...);
- visualise (graphs and plots).

1.4 Fluid-Flow Equations

The equations of fluid flow are based on fundamental physical conservation principles:

- *mass*: change of mass = 0
- *momentum*: change of momentum = force × time
- *energy*: change of energy = work + heat

In fluid flow these are usually expressed as *rate* equations; i.e. *rate of change* = ...

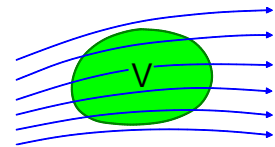
Additional equations may apply for *non-homogeneous* fluids (e.g. particle load, dissolved chemicals, multiple species, ...).

These *conservation* principles may be expressed mathematically as either:

- *integral (control-volume)* equations;
- *differential* equations.

1.4.1 Integral (Control-Volume) Approach

This describes how the *total amount* of a physical quantity (mass, momentum, energy, ...) is changed within a finite region of space (*control volume*). Over an interval of time:



$$\text{CHANGE} = (\text{AMOUNT ENTERING} - \text{AMOUNT LEAVING}) + \text{AMOUNT CREATED}$$

In fluid mechanics this is usually expressed in rate form by dividing by the time interval (and transferring net transfer through the boundary to the LHS):

$$\left(\begin{array}{c} \text{TIME DERIVATIVE} \\ \text{of amount in } V \end{array} \right) + \left(\begin{array}{c} \text{NET FLUX} \\ \text{through boundary of } V \end{array} \right) = \left(\begin{array}{c} \text{SOURCE} \\ \text{inside } V \end{array} \right) \quad (1)$$

The *flux* (rate of transport through a surface) is further subdivided into:

*advection*¹ – movement with the flow;

diffusion – net transport by random molecular or turbulent motion.

$$\left(\begin{array}{c} \text{TIME DERIVATIVE} \\ \text{of amount in } V \end{array} \right) + \left(\begin{array}{c} \text{ADVECTION+DIFFUSION} \\ \text{through boundary of } V \end{array} \right) = \left(\begin{array}{c} \text{SOURCE} \\ \text{inside } V \end{array} \right) \quad (2)$$

This is a generic equation, independent of whether the physical quantity is mass, momentum, chemical content, etc. Thus, instead of lots of different equations, we can consider the numerical solution of a generic *scalar-transport equation* (Section 4).

The *finite-volume* method is based on approximating these control-volume equations.

¹ Some authors – but not this one – prefer the term *convection* to *advection*.

1.4.2 Differential Equations

In regions without shocks, interfaces or other discontinuities, fluid-flow equations can also be written in differential forms (Section 2). These describe what is going on at a point rather than over a whole control volume. Mathematically, they can be derived by making the control volumes infinitesimally small. There are many ways of writing these differential equations.

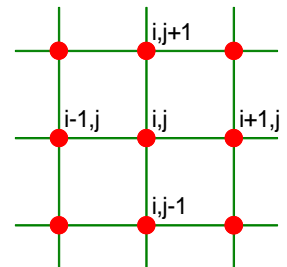
Finite-difference methods approximate some differential form of the governing equations.

1.5 The Main Discretisation Methods

(i) Finite-Difference Method

Discretise *differential* equations; e.g. for mass:

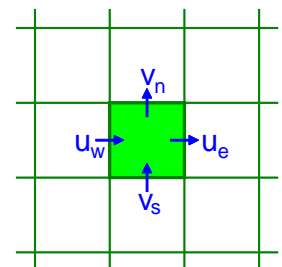
$$0 = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \approx \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + \frac{v_{i,j+1} - v_{i,j-1}}{2\Delta y}$$



(ii) Finite-Volume Method

Discretise *integral* (control-volume) equations; e.g.

$$0 = \text{net mass outflow} = (\rho u A)_e - (\rho u A)_w + (\rho v A)_n - (\rho v A)_s$$



(iii) Finite-Element Method

Express the solution as a weighted sum of *shape functions* $S_\alpha(\mathbf{x})$; e.g. for velocity:

$$u(\mathbf{x}) = \sum u_\alpha S_\alpha(\mathbf{x})$$

Substitute into one of several forms of the governing equations and solve for the coefficients (aka *degrees of freedom*, or *weights*) u_α .

The finite-element method is popular in solid mechanics (geotechnics, structures) because:

- it has considerable geometric flexibility;
- general-purpose software can be used for a wide variety of physical problems.

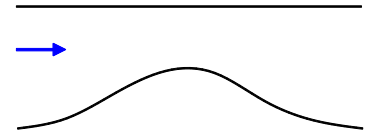
The finite-volume method is popular in fluid mechanics because:

- it rigorously enforces conservation;
- it is flexible in terms of both geometry and fluid phenomena;
- it is directly relatable to physical quantities (mass flux, etc.).

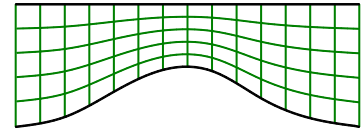
This course will focus on the *finite-volume* method.

In the finite-volume method ...

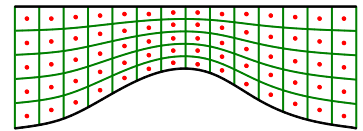
(1) A flow geometry is defined.



(2) The flow domain is decomposed into a set of *control volumes* or *cells* called a *computational mesh* or *grid*.



(3) The *control-volume* equations are *discretised* – i.e. approximated in terms of values at *nodes* – to form a set of *algebraic* equations.



(4) The discretised equations are solved numerically.

$$\begin{pmatrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{pmatrix} \begin{pmatrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{pmatrix} \phi = \begin{pmatrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{pmatrix} \mathbf{b}$$

APPENDICES

A1. Notation

Position/time:

$\mathbf{x} \equiv (x, y, z)$ or (x_1, x_2, x_3) position; (z usually vertical when gravity is important)
 t time

Field variables:

$\mathbf{u} \equiv (u, v, w)$ or (u_1, u_2, u_3) velocity
 p pressure
($p - p_{\text{atm}}$ is *gauge pressure*; $p^* = p + \rho g z$ is *piezometric pressure*)
 T temperature
 ϕ concentration (amount per unit mass or volume)

Fluid properties:

ρ density
 μ dynamic viscosity
($\nu \equiv \mu/\rho$ is the *kinematic viscosity*)
 Γ diffusivity

A2. Hydrostatics

At rest, pressure forces balance weight. This hydrostatic relation can be written

$$\Delta p = -\rho g \Delta z \quad \text{or} \quad \frac{dp}{dz} = -\rho g \quad (3)$$

The same equation also holds in a moving fluid if vertical acceleration is much smaller than g .

If density is constant, (3) can be written as either

$$\Delta(p + \rho g z) = 0$$
$$p^* \equiv p + \rho g z = \text{constant} \quad (4)$$

p^* is the *piezometric pressure*. For a constant-density flow without a free surface, gravitational forces can be eliminated entirely from the equations by working with the piezometric pressure.

A3. Equation of State

In compressible flow, pressure, density and temperature are connected by an *equation of state*. The most common is the *ideal gas law*:

$$p = \rho R T, \quad R = R_0/m \quad (5)$$

where R_0 is the universal gas constant, m is the molar mass and T is the absolute temperature. For ideal gases, temperature is related to internal energy e or enthalpy h (per unit mass) by

$$e = c_v T, \quad h = c_p T \quad (6)$$

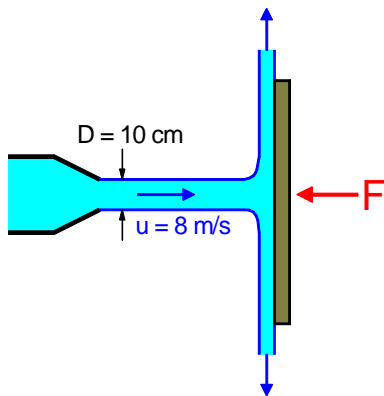
c_v and c_p are specific heat capacities at constant volume and constant pressure respectively.

Examples

The following simple examples develop the control-volume notation to be used in the rest of the course.

Q1.

Water (density 1000 kg m^{-3}) flows at 2 m s^{-1} through a circular pipe of diameter 10 cm . What is the mass flux C across the surfaces S_1 and S_2 ?



Q2.

A water jet strikes normal to a fixed plate as shown. Compute the force F required to hold the plate fixed.

Q3.

An explosion releases 2 kg of a toxic gas into a room of dimensions $30 \text{ m} \times 8 \text{ m} \times 5 \text{ m}$. Assuming the room air to be well-mixed and to be vented at a speed of 0.5 m s^{-1} through an aperture of 6 m^2 , calculate:

- the initial concentration of gas in ppm by mass;
 - the time taken to reach a safe concentration of 1 ppm .
- (Take the density of air as 1.2 kg m^{-3} .)

Q4.

A burst pipe at a factory causes a chemical to seep into a river at a rate of 2.5 kg hr^{-1} . The river is 5 m wide, 2 m deep and flows at 0.3 m s^{-1} . What is the average concentration of the chemical (in kg m^{-3}) downstream of the spill?