- 1.1 What is computational fluid dynamics?
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- 1.5 The main discretisation methods

Appendices (A1: Notation; A2: Statics)

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 and heat transfer around electronic circuitry.

This range of applications is very broad and involves 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.

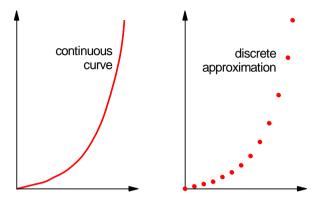
CFD 1-1 David Apsley

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*.

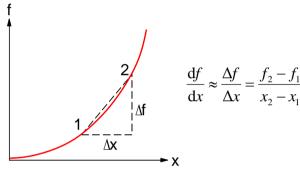
The fundamental elements of any CFD simulation are:

(1) The **flow field is discretised**; i.e. field variables $(\rho, u, v, w, p, \dots)$ 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:

- formulation of the problem (governing equations and boundary conditions);
- construction of a computational mesh (set of control volumes).

Solving:

- discretisation of the governing equations;
- solution of the resulting algebraic equations.

Post-processing:

- analysis of results (calculation of derived quantities: forces, flow rates, ...)
- visualisation (graphs and plots of the solution).

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 \times time
- energy: change of energy = work + heat

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

Additional equations may apply for *non-homogeneous* fluids (e.g. multiphase, or containing dissolved chemicals or suspended particles).

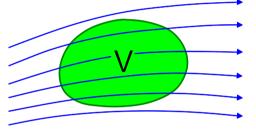
When applied to a fluid continuum these *conservation* principles may be expressed mathematically as either:

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

1.4.1 Integral (Control-Volume) Approach

This considers how the total amount of some physical quantity (mass, momentum, energy, ...) is changed within a finite region of space (*control volume*).

For an arbitrary control volume the balance of any physical quantity over an interval of time is



change = amount in - amount out + amount created

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

$$\begin{pmatrix} \mathbf{RATE \ OF \ CHANGE} \\ inside \ V \end{pmatrix} + \begin{pmatrix} \mathbf{NET \ FLUX} \\ throughboundary of \ V \end{pmatrix} = \begin{pmatrix} \mathbf{SOURCE} \\ inside \ V \end{pmatrix}$$
(1)

The *flux*, or rate of transport through a surface, is further subdivided into:

advection – movement with the fluid flow;

diffusion – net transport by random molecular or turbulent motion.

$$\begin{pmatrix} \text{RATE OF CHANGE} \\ inside V \end{pmatrix} + \begin{pmatrix} \text{ADVECTION} + \text{DIFFUSION} \\ throughboundary of } V \end{pmatrix} = \begin{pmatrix} \text{SOURCE} \\ inside V \end{pmatrix}$$
 (2)

The important point is that this is a **single, generic equation**, irrespective of whether the physical quantity concerned is mass, momentum, chemical content, etc. Thus, instead of dealing with lots of different equations we can consider the numerical solution of a generic *scalar-transport equation*. This we shall do in Section 4.

The *finite-volume* method, which is the subject of this course, is based on approximating these control-volume equations.

1.4.2 Differential Equations

In regions without shocks, interfaces or other discontinuities, the fluid-flow equations can also be written in equivalent **differential** forms. 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. This will be demonstrated in Section 2, where it will also be shown that there are several different ways of writing these differential equations.

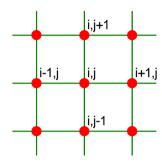
Finite-difference methods are based on the direct approximation of a differential form of the governing equations.

1.5 The Main Discretisation Methods

(i) Finite-Difference Method

Discretise the governing differential equations; e.g.

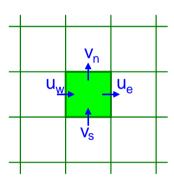
$$0 = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \approx \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + \frac{v_{i,j+1} - v_{i,j-1}}{2\Delta y}$$



(ii) Finite-Volume Method

Discretise the governing **integral** or **control-volume** equations; e.g.

net mass outflow =
$$(\rho uA)_e - (\rho uA)_w + (\rho vA)_n - (\rho vA)_s = 0$$



(iii) Finite-Element Method

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

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

Substitute into some form of the governing equations and solve for the coefficients (aka degrees of freedom or weights) u_{q} .

This course will focus on the finite-volume method.

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:

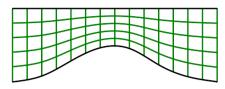
- it rigorously enforces **conservation**;
- it is **flexible** in terms of both **geometry** and the variety of **fluid phenomena**;
- it is directly relatable to **physical quantities** (mass flux, etc.).

In the finite-volume method ...

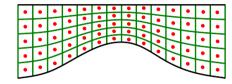
(1) A flow geometry is defined.



(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.

$$\begin{pmatrix} \begin{pmatrix} \\ \\ \\ \end{pmatrix} \end{pmatrix} \begin{pmatrix} \\ \\ \\ \\ \end{pmatrix} \end{pmatrix} = \begin{pmatrix} \\ \\ \\ \\ \\ \end{pmatrix}$$

APPENDICES

A1. Notation

Position/time:

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

Field variables:

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

Fluid properties:

 $\rho \qquad \qquad \text{density} \\ \mu \qquad \qquad \text{dynamic viscosity} \\ (v \equiv \mu/\rho \text{ is the } \textit{kinematic viscosity}) \\ \Gamma \qquad \qquad \text{diffusivity}$

A2. Statics

At rest, pressure forces balance weight. This can be written mathematically as

$$\Delta p = -\rho g \Delta z$$
 or $\frac{\mathrm{d}p}{\mathrm{d}z} = -\rho g$ (3)

The same equation also holds in a moving fluid if there is no vertical acceleration, or, as an approximation, if vertical acceleration is much smaller than g.

If density is constant, (3) can be written

$$p^* \equiv p + \rho gz = constant \tag{4}$$

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

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

$$p = \rho RT , \qquad R = R_0/m \tag{5}$$

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

$$e = c_{v}T$$
$$h = c_{p}T$$

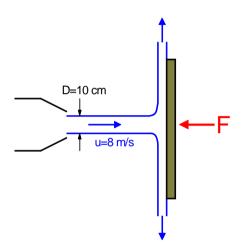
where c_v and c_p are the specific heat capacities at constant volume and constant pressure respectively.

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 ?





O2.

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: (a) the initial concentration of gas in ppm by mass; (b) 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?