Conservation Laws, Discretisation & Grids, part 1

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CFD: a game of approximation

1. Select a **mathematical model** that is an *approximation* of real-world fluid flow; eg. Navier-Stokes equations.
2. Use a **numerical** *approximation* to solve the equations of the mathematical model, particularly when there is no analytic solution available.

Approximations in mathematical models

'scale of reality' model individual particles or fluid elements

temporal approximation steady or unsteady; use of time-averaging over turbulent fluctuations to get mean flow properties (Reynolds-averaged Navier-Stokes); use of time-averaging over small-scale fluctuations only (large eddy simulation)

spatial approximation reduction from three-dimensions; 2-D (planar or axisymmetric); 1-D; quasi-1-D

We should decide in advance what mathematical model is appropriate for a given fluid simulation problem, either by research or experience. The process of checking whether the mathematical model is appropriate is called **validation**.

In this lecture...

- General form of a conservation law
- Fluxes of conserved quantities: convective & diffusive
- The conservation equations for fluid mechanics: mass, momentum & energy
- A taste of discretisation via finite volume method
- Introduction to gridding

General form of a conservation law

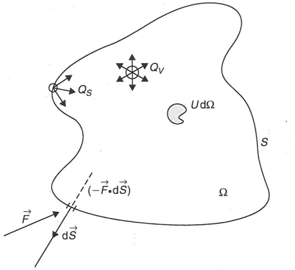
The variation of the total amount of a quantity U inside a given domain is equal to the balance between the amount of that quantity entering and leaving the considered domain, plus the contributions from possible sources generating that quantity.

Remarks

1. Not all fluid quantities obey a conservation law.
2. The conservation laws describing evolution of a fluid flow are:
    - conservation of mass
    - conservation of momentum
    - conservation of energy

General conservation law (for a scalar)

The variation of the ***total amount of a quantity*** *U* ***inside a given domain*** *is equal to the balance between the amount of that quantity entering and leaving the considered domain, plus the contributions from possible sources generating that quantity.*



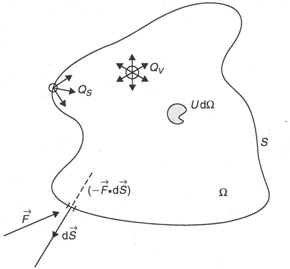
total amount of quantity U inside a given domain

$$\int_\Omega U d\Omega$$

$$\int_\Omega U d\Omega$$

General conservation law (for a scalar)

*The **variation** of the **total amount of a quantity** U **inside a given domain** is equal to the balance between the amount of that quantity entering and leaving the considered domain, plus the contributions from possible sources generating that quantity.*



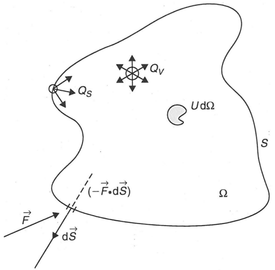
variation with time of the total amount of quantity *U* inside a given domain

$$\frac{\partial}{\partial t}\int_{\Omega} U d\Omega$$

$$\frac{\partial}{\partial t}\int_{\Omega} U d\Omega$$

General conservation law (for a scalar)

*The variation of the total amount of a quantity U inside a given domain is equal to the balance between **the amount of that quantity entering and leaving the considered domain**, plus the contributions from possible sources generating that quantity.*



the amount of that quantity U entering and leaving the considered domain

$$-\oint_S \vec{F}\cdot d\vec{S}$$

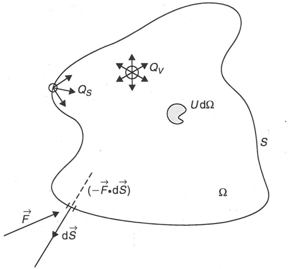
flux: the amount of U crossing the unit of surface per unit of time

$$F_n dS = \vec{F}\cdot d\vec{S}$$

$$\frac{\partial}{\partial t}\int_\Omega U d\Omega = -\oint_S \vec{F}\cdot d\vec{S} + \dots$$

General conservation law (for a scalar)

The variation of the total amount of a quantity U inside a given domain is equal to the balance between the amount of that quantity entering and leaving the considered domain, ***plus the contributions from possible sources generating that quantity****.*



plus contributions from possible sources of quantity *U*
divide these into volume and surface sources

$$\int_\Omega Q_V d\Omega + \oint_S \vec{Q_s} \cdot \vec{dS}$$

$$\frac{\partial}{\partial t}\int_\Omega U d\Omega = -\oint_S \vec{F}\cdot\vec{dS} + \int_\Omega Q_V d\Omega + \oint_S \vec{Q_s}\cdot\vec{dS}$$

General conservation law (for a scalar)

The variation of the total amount of a quantity U inside a given domain is equal to the balance between the amount of that quantity entering and leaving the considered domain, ***plus the contributions from possible sources generating that quantity****.*

$$\frac{\partial}{\partial t}\int_{\Omega} U d\Omega = -\oint_{S} \vec{F}\cdot d\vec{S} + \int_{\Omega} Q_v d\Omega + \oint_{S} \vec{Q_s}\cdot d\vec{S} \tag{1}$$

or more typically written

$$\frac{\partial}{\partial t}\int_{\Omega} U d\Omega + \oint_{S} \vec{F}\cdot d\vec{S} = \int_{\Omega} Q_v d\Omega + \oint_{S} \vec{Q_s}\cdot d\vec{S} \tag{2}$$

This is **integral conservation form**

Remarks

- valid for any fixed surface S and volume Ω
- the internal variation of U, in the absence of volume sources, depends *only* on the flux contribution *through* the surface S

Differential form of the conservation law

Use Gauss' theorem to replace surface integrals:

$$\oint_S \vec{F} \cdot d\vec{S} = \int_\Omega \vec{\nabla} \cdot \vec{F} d\Omega$$

Recall the gradient operator, $\vec{\nabla}$, from vector calculus shown here in Cartesian coordinates:

$$\vec{\nabla} = \hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$$

$$\frac{\partial}{\partial t}\int_\Omega U d\Omega + \int_\Omega \vec{\nabla} \cdot \vec{F} d\Omega = \int_\Omega Q_v d\Omega + \int_\Omega \vec{\nabla} \cdot \vec{Q_s} d\Omega$$

Consider Ω to be arbitrarily small, therefore equations hold at a point:

$$\frac{\partial U}{\partial t} + \vec{\nabla} \cdot \vec{F} = Q_v + \vec{\nabla} \cdot \vec{Q_s} \tag{3}$$

$$\frac{\partial U}{\partial t} + \vec{\nabla} \cdot (\vec{F} - \vec{Q_s}) = Q_v \tag{4}$$

Convection-diffusion form

- We haven't yet said anything about the fluxes of quantity U
- In a fluid, fluxes come from two contributions:
  1. convective transport of the fluid
  2. molecular agitation

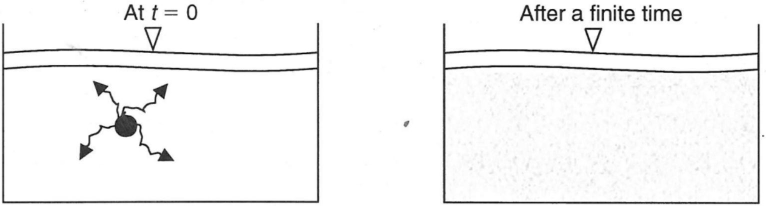
Convective flux, $\vec{F_c}$

the amount of U that is carried away or transported by the flow

$$\vec{F_C} = U\vec{v}$$

Convection-diffusion form: diffusive flux

flux contribution present in fluids at rest due to the macroscopic effect of the molecular thermal agitation



- proportional to the gradient of the concentration
- direction opposite to gradient because of the tendency towrds uniformity
- proportional to a diffusivity factor

Law of Fick

$$\vec{F_D} = -\kappa\rho\vec{\nabla}u$$

Convection-diffusion form

For $U = \rho u$,

$$\frac{\partial \rho u}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v} u) = \vec{\nabla} \cdot (\kappa \rho \vec{\nabla} u) + Q_v + \vec{\nabla} \cdot \vec{Q}_s \tag{5}$$

Convection	*Diffusion*
Expresses the transport of the considered quantity by the flow	Translates the effects of molecular collisions
Does not exist in a fluid at rest	Does exist in a fluid at rest
All quantities are convected by the flow	Not all quantities are subjected to diffusion
Directional behavior	Isotropic behavior
Leads to first order space derivatives in the conservation law	Leads to second order space derivatives in the conservation law
Is generally nonlinear, when the flow velocity depends on the transported variable	Is generally linear for constant fluid properties

Equations of fluid mechanics

A fluid field is described, at any instant in time, by knowledge of the velocity field and a minimum number of static properties, eg.

$$v_x, v_y, v_z, \rho, p$$

Use conservation laws for describe system of fluid flow:

- mass conservation $\rightarrow$ continuity equation
- momentum conservation $\rightarrow$ generalised Newton law giving equations of motion of a fluid
- energy conservation $\rightarrow$ first principle of thermodynamics

Mass conservation

$$\frac{\partial}{\partial t}\int_{\Omega} U d\Omega + \oint_S \vec{F}\cdot \vec{dS} = \int_{\Omega} Q_V d\Omega + \oint_S \vec{Q_s}\cdot \vec{dS}$$

With

$$U = \rho; \quad \vec{F_C} = \rho\vec{v}$$

$$\frac{\partial}{\partial t}\int_{\Omega} \rho d\Omega + \oint_S \rho\vec{v}\cdot \vec{dS} = 0 \tag{6}$$

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot(\rho\vec{v}) = 0 \tag{7}$$

Momentum conservation

With

$$\vec{U} = \rho\vec{v}; \quad \bar{\bar{F}}_C = \rho\vec{v} \times \vec{v}$$

$$\frac{\partial}{\partial t}\int_\Omega \rho\vec{v}d\Omega + \int_\Omega \vec{\nabla}\cdot(\rho\vec{v}\times\vec{v})\,d\Omega = \int_\Omega \rho\vec{f_e}d\Omega + \oint_S \left(-p\bar{\bar{I}} + \bar{\bar{\tau}}\right)\cdot d\vec{S} \tag{8}$$

$$\frac{\partial\rho\vec{v}}{\partial t} + \vec{\nabla}\cdot\left(\rho\vec{v}\times\vec{v} + p\bar{\bar{I}} - \bar{\bar{\tau}}\right) = \rho\vec{f_e} \tag{9}$$

Remarks:

- $p\bar{\bar{I}}$ is the pressure tensor, $\bar{\bar{\tau}}$ is the stress tensor, and $\vec{f_e}$ are any external body forces, such as gravity or electromagnetic.
- To derive this equation, start with the vector form of the general conservation law. This is not shown in this lecture series.

Energy conservation law

With

$$\vec{U} = \rho E; \quad E = e + \frac{\vec{v}^2}{2}; \quad \vec{F_C} = \rho \vec{v}\left(e + \frac{\vec{v}^2}{2}\right)$$

$$\vec{F_D} = -\gamma \rho \kappa \vec{\nabla} e = -k\vec{\nabla} T$$

$$\frac{\partial}{\partial t}\int_\Omega \rho E d\Omega + \oint_S \rho E \vec{v} \cdot \vec{dS} = \oint_S k\vec{\nabla} T \cdot \vec{dS} + \int_\Omega \rho \vec{f_e} \cdot \vec{v} d\Omega + \oint_S (\bar{\bar{\sigma}} \cdot \vec{v}) \cdot \vec{dS} \tag{10}$$

$$\frac{\partial \rho E}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v} E) = \vec{\nabla} \cdot (k \vec{\nabla} T) + \vec{\nabla} \cdot (\bar{\bar{\sigma}} \cdot \vec{v}) + W_f \tag{11}$$

where

$$W_f = \rho \vec{f_e} \cdot \vec{v}; \quad \bar{\bar{\sigma}} = -p\bar{\bar{I}} + \bar{\bar{\tau}}$$

Closure of equation system

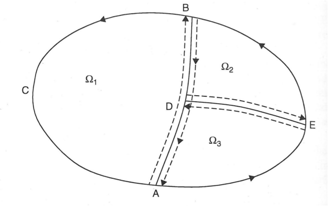
For a perfect gas in compressible flow, we can close the system of conservation laws with equations of state:

$$e = e(T)$$

$$p = p(\rho, T)$$

A taste of discretisation using finite volumes

$$\frac{\partial}{\partial t}\int_{\Omega} U d\Omega + \oint_S \vec{F}\cdot d\vec{S} = \int_{\Omega} Q d\Omega$$



Summation of individual control volumes within larger domain

$$\begin{aligned}
\frac{\partial}{\partial t}\int_{\Omega_1} U d\Omega + \oint_{ABCA} \vec{F}\cdot d\vec{S} &= \int_{\Omega_1} Q d\Omega \\
\frac{\partial}{\partial t}\int_{\Omega_2} U d\Omega + \oint_{DEBD} \vec{F}\cdot d\vec{S} &= \int_{\Omega_2} Q d\Omega \\
\frac{\partial}{\partial t}\int_{\Omega_3} U d\Omega + \oint_{AEDA} \vec{F}\cdot d\vec{S} &= \int_{\Omega_3} Q d\Omega
\end{aligned}$$

Basics of finite-volume method

We use direct discretisation of the integral form of the consevation laws

1. Subdivide the domain into finite (small) volumes
2. Apply the integral conservation laws to each of these finite volumes

The key idea is that it should be "easy" to apply the conservation laws to these individual finite volumes, as compared to the domain as a whole.

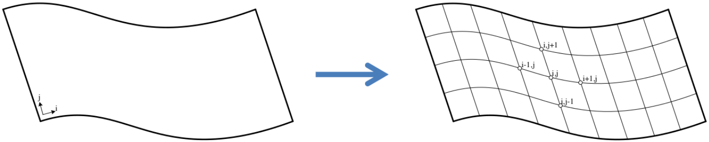
$$\frac{\partial}{\partial t}\int_{\Omega} U d\Omega + \oint_{S} \vec{F} \cdot d\vec{S} = \int_{\Omega} Q d\Omega$$

when discretised becomes

$$\frac{\partial}{\partial t}(U_j \Omega_j) + \sum_{\text{faces}} \vec{F} \cdot \Delta\vec{S} = Q_j \Omega_j$$

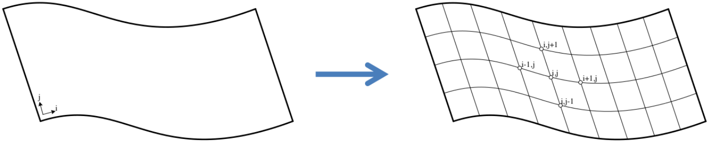
Subdividing a domain: gridding

The first step in the finite-volume method was to subdivide the domain into small finite volumes. This process is known as gridding or meshing.



Structured grids in two dimensions

- Let's restrict our attention at the moment to two dimensions and domains with 4 edges.
- With 4 connecting edges, it is possible to arrange quadrilateral-shaped finite volumes in a regular array across the domain.
- Due to the regularity of how the finite volumes are laid out, we call this grid type a structured grid.



Documentation for gridding in MECH4480/7480

Throughout MECH4480/7480, we will make use of the Geometry package that comes with Eilmer4 for building two-dimensional meshes. The report on the Geometry package is available at:

`cfcfd.mechmining.uq.edu.au/eilmer/pdfs/geometry-user-guide.pdf`

To use the Geometry package to generate grids suitable for OpenFOAM, we have created the foamMesh tool:

`cfcfd.mechmining.uq.edu.au/eilmer/pdfs/foammesh-user-guide.pdf`

Top-down view of geometric elements

`StructuredGrid` this object accepts a `Patch` object and discretises the surface in a form ready for use as a grid

`Patch` this object is a surface constructed from four joining `Paths`

`Path` this object is a curve or path through space; used to represent a single edge of a `Patch`

`Vector3` this object represents a point in 3D space; used in construction of `Paths`

Demonstration of building grids for simple domains