Computational Fluid Dynamics: Lecture 2 (ME EN 6720)

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Mathematical representations

The first step:

- After identifying our physical process of interest we need to conceptualize it mathematically
- Most problems in fluid mechanics are described by a combination of:

  - Conservation of Mass: $$\left.\frac{dm}{dt}\right)_{sys} = 0$$

  - Conservation of Momentum: $$\sum \vec{F} = \left.\frac{d\left(m\vec{V}\right)}{dt}\right)_{sys}$$

  - Conservation of Energy: $$\dot{Q} - \dot{W} = \left.\frac{dE}{dt}\right)_{sys}$$

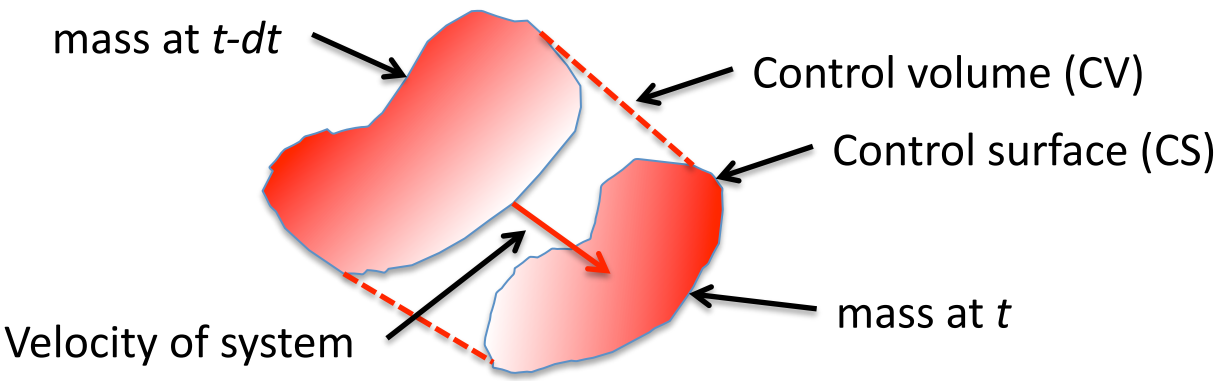
- No mass can enter or leave a system, it is a **Lagrangian** reference frame
- Typically in experiments and in CFD solutions we want a fixed **Eulerian** reference frame

Reynolds Transport Theorem

- How do we go from a system (Lagrangian) to a control volume (Eulerian) approach?

<u>Reynold’s Transport Theorem</u> (RTT):

RTT converts a Lagrangian reference frame to an Eulerian one



We can derive RTT by noting that the mass of the fluid at *t* and *t-dt* is the same and examining the geometric changes

See fluids text for full derivation (e.g., Fox et al., 2009 pg 95-99)

$$\left.\frac{dN}{dt}\right)_{sys} = \frac{\partial}{\partial t}\int_{CV} \rho\eta d\forall + \int_{CS} \rho\eta\vec{V}\cdot d\vec{A}$$

N = extensive property (mass, momentum, etc.)

η = intensive property (N per unit mass)

Conseravtion of mass

- We can apply RTT to the system formulation of conservation of mass

$$\left.\frac{dm}{dt}\right)_{sys} = 0 \qquad \text{set } N = m \Rightarrow \eta = \frac{\partial N}{\partial m} = \frac{\partial m}{\partial m} = 1$$

$$\Rightarrow \left.\frac{dm}{dt}\right)_{sys} = \boxed{\frac{\partial}{\partial t}\int_{CV} \rho d\forall + \int_{CS} \rho \vec{V} \cdot d\vec{A} = 0}$$

Finite Volumes

Use Gauss's theorem on the convective term to put both terms in volume form ➔

$$\frac{\partial}{\partial t}\int_{CV} \rho d\forall + \int_{CV} \nabla \cdot \left(\rho \vec{V}\right) d\forall = 0$$

We can move the time rate of change term inside the integral and then write

$$\int_{CV} \frac{\partial \rho}{\partial t} d\forall + \int_{CV} \nabla \cdot \left(\rho \vec{V}\right) d\forall = 0 \Rightarrow \int_{CV} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{V}\right)\right) d\forall$$

Finite Differences

If we shrink the CV to an infinitesimal size we get:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{V}\right) = 0 \ \text{ or in index notation } \ \boxed{\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i\right) = 0}$$

$$\text{sum repeated indexes: for } i = 1 \rightarrow 3,\ u_i u_i = u_1 u_1 + u_2 u_2 + u_3 u_3$$

Conservation of Momentum

- **Conservation of Momentum (Newton's 2nd law):**

-For a system: $$\sum \vec{F} = \left.\frac{d\left(m\vec{V}\right)}{dt}\right)_{sys}$$

-Or using RTT (same as above for mass):

$$\sum \vec{F} = \frac{\partial}{\partial t}\int_{CV} \rho \vec{V} d\forall + \int_{CS} \vec{V} \rho \vec{V}\, d\vec{A}$$

What are the forces for flow in a fluid volume?

- body forces: **gravity**, magnetism (for magnetohydrodynamics problems)
- surface forces: **stresses**, surface tension, etc.

We are mostly concerned with the pressure (normal stress) and shear stresses

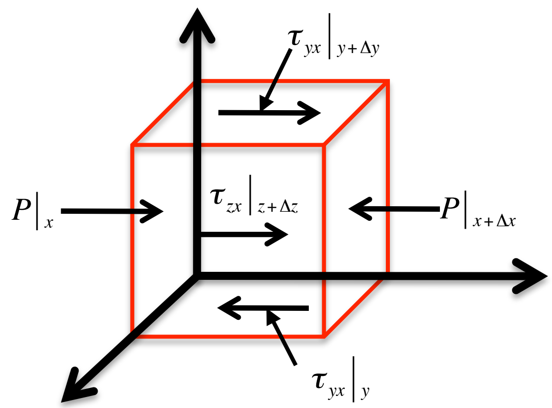
If we define our surface and body forces in integral forms we can write:

$$\frac{\partial}{\partial t}\int_{CV} \rho \vec{V} d\forall + \int_{CS} \vec{V} \rho \vec{V}\, d\vec{A} = \int_{CS} \mathbf{T} \cdot \hat{n}\, d\vec{A} + \int_{CV} \rho \vec{b} d\forall$$

Conservation of Momentum

- The stresses **T** depend on molecular processes
- To use conservation of momentum we have to <u>choose a form for the stress tensor</u> **T**

Recall "stress cube" for the x-direction:



T is a tensor (matrix) composed of all of the stress components in the x,y,z directions

The most common assumption is that the fluid is **Newtonian** (i.e. has a linear relation between stress and rate of strain)➔

$$\mathbf{T} = -\left(P + \frac{2}{3}\mu\nabla\cdot\vec{V}\right)\mathbf{I} + 2\mu\mathbf{D}$$

where $\mathbf{D} = \frac{1}{2}\left(\nabla\vec{V} + \nabla\vec{V}^T\right)$ is the deformation (rate of strain) tensor and **I** is the unit tensor (or identity matrix)

Conservation of Momentum

- The equivalent index-notation (differential) form of the momentum equation is:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = \frac{\partial(\tau_{ij})}{\partial x_j} - \frac{\partial(P)}{\partial x_i} + \rho g_i$$

where the stress has been split into shear (viscous) and normal (pressure) components using:

$$\tau_{ij} = 2\mu D_{ij} - \tfrac{2}{3}\mu\delta_{ij}\frac{\partial u_k}{\partial x_k} \quad \text{where } D_{ij} = \tfrac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \quad \text{and} \quad \delta_{ij} = \begin{cases} 1 \text{ for } i = j \\ 0 \text{ for } i \neq j \end{cases}$$

- <u>Forms of the Momentum Equation</u>
  - **Differential** vs. **Integral**
  - **Eulerian** vs. **Lagrangian**
  - **Conservative** vs. **Non conservative**

- For the integral equations, **conservative** means all terms are written in the form of a divergence (e.g.,$\nabla \cdot \vec{V}$)
- For Finite Volume formulations, using a conservative form instead of the non conservative form guarantees the velocity field will be divergent free (a requirement for realizeability)

Conservation of Energy

Conservation of Energy

Several forms of the conservation of energy exist (all mathematically equivalent)

- internal energy per volume
- internal energy per mass
- total energy ($e + \frac{1}{2} u_i u_i$)
- enthalpy

For a system conservation of energy is: $\dot{Q} - \dot{W} = \left.\frac{dE}{dt}\right)_{sys}$ or: **(in-out) + produced = stored**

- **(in-out)** is the convective flux of energy

-**Production** is the heat conducted in + the work done on the volume (e.g., thermal flux and shear stress)

- if we use $e = c_V T$ (specific internal energy)
- and define $q_i = -k \frac{\partial T}{\partial x_i}$ as the thermal conductive flux where c_V is the specific heat and

T is temperature. We can derive the following differential form for energy (see text for integral)

$$-\frac{\partial}{\partial x_j}\left[\rho u_j\left(e + \tfrac{1}{2} u_i u_i\right)\right] - \frac{\partial q_i}{\partial x_i} - \frac{\partial\left(P u_i\right)}{\partial x_j} + \frac{\partial\left(\tau_{ij} u_i\right)}{\partial x_j} = \frac{\partial}{\partial t}\left[\rho\left(e + \tfrac{1}{2} u_i u_i\right)\right]$$

Conservation of a scalar

- **Conservation of Mass (revisited):**

- we can interpert density as $\rho = \dfrac{\text{mass}}{\text{volume}}$

- we can use the same basic definition for any scalar quantity ϕ if we interpert ϕ as a mass of the scalar per volume (concentration)

- we than have: $\dfrac{d\phi}{dt} = 0$ or using R.T.T.

$$\underbrace{\frac{\partial}{\partial t}\int_{CV} \phi d\forall}_{\text{accumulation}} + \underbrace{\int_{CS} \phi \vec{V}\, d\vec{A}}_{\text{flux}} = 0$$

accumulation = (inflow - outflow) + generation - degradation

Conservation of a scalar

accumulation = (inflow - outflow) + generation - degradation

$$\underbrace{\frac{\partial}{\partial t}\int_{CV}\phi d\forall}_{\text{net accumulation}} = -\underbrace{\int_{CS}\phi\vec{V}\cdot d\vec{A}}_{\text{flux}} + \underbrace{\int_{CV} r_g d\forall}_{\text{generation}} - \underbrace{\int_{CV} r_d d\forall}_{\text{degradation}}$$

- r_g = rate of generation of mass in the CV
- r_d = rate of degradation of mass in the CV
- note if $r_g = r_d$ (or $r_g = 0 = r_d$ etc.) we get our standard form if $\phi = \rho$

Conservation Equations

summing up our equations:

- conservation of mass
- conservation of momentum
- conservation of energy
- conservation of scalar concentration

Other equations of interest

-Inviscid flow equations in conservative form (Euler equations):

Continuity - $$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i)=0$$

Momentum - $$\frac{\partial(\rho u_i)}{\partial t}+\frac{\partial}{\partial x_j}(u_i u_j)=-\frac{\partial P}{\partial x_i}+\rho F_i$$

Energy - $$\frac{\partial(E)}{\partial t}+\frac{\partial}{\partial x_i}(E u_i)=\rho\dot{q}-\frac{\partial u_i P}{\partial x_i}+\rho F_i u_i \quad \text{where } E=\rho\left(e+\frac{1}{2}u_i u_i\right)$$

CFD Equations

<u>A few Notes</u>:

Each of these sets of equations are coupled nonlinear PDEs:

If we look at the N-S (or Euler) equations we have:

5 equations ➔ 6 unknowns therefore we need:

- Equations of state: (for air we can use the ideal gas law):

$$P = \rho R T$$

- we still need one more equation to close the set. We need a thermodynamic relation relating the different state variables.

- usually of the form: $e = f(T, \rho)$

- for a calorically perfect gas (constant specific heat) we have: $e = c_V T$

- The momentum, continuity, and energy equations combined are usually referred to as the Navier-Stokes (N-S) equations

Boundary and Initial Conditions

Boundary and Initial Conditions:

- in CFD we start with a physical process and then formulate a P.D.E
- we need to make sure we have a **well-posed** problem. What does this mean?
- A solution must exist and it must be unique!

We need proper **Initial Conditions** and **Boundary Conditions**

- 3 main types of B.C.s

- Direchlet: $u = a$ at the boundaries

- Neumann: $\dfrac{\partial u}{\partial n} = a$ at the boundaries

- Mixed (Robin): $a_1 u + a_2 \dfrac{\partial u}{\partial n} = a_3$ at the boundaries

More equations

- **Other equations** that we will discuss of interest to fluid mechanics and heat transfer:
  - 1st order linear (and nonlinear) wave equation:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$

  - Poisson equations (and Laplace equations):

$$\nabla^2\theta = \frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} = f(x,y)$$

  - Burger's equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \quad \text{(inviscid form is nonlinear wave)}$$

  - unsteady heat equation (Fourier's law)

$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2}$$

Classification of equations

- In general we can write the PDEs that we deal with in CFD (and many other fields) in the following form:

$$a\frac{\partial^2\phi}{\partial x^2}+b\frac{\partial^2\phi}{\partial x\partial y}+c\frac{\partial^2\phi}{\partial y^2}+d\frac{\partial\phi}{\partial x}+e\frac{\partial\phi}{\partial y}=g$$

- we can classify PDEs based on how they fit into this general form

Classification	discriminant	type of problems	example PDE
Elliptical	$b^2-4ac<0$	boundary value	Laplace equation
Parabolic	$b^2-4ac=0$	marching (IVP)	Heat equation
Hyperbolic	$b^2-4ac>0$	marching (IVP)	Wave equation

- for information on equation classification see Anderson chapter 3.