Transport Equations

- Mass
- Momentum
- Energy
- Species

} Conservation Laws

Accumulation = in + out + Generation$_{net}$

Transport Eqns are Eulerian
Conservation Laws are for some <u>system</u> → Lagrangian

Link these with The Reynolds Transport theorem (RTT)

$$\frac{dB_{sys}}{dt} = \frac{d}{dt}\int_{CV} \rho b \, d\mathcal{V} + \int_{CS} \rho b \vec{V}_R \cdot \vec{n} \, dA$$

- B_{sys} is some extensive property of the system
    - Mass, energy, momentum, etc.
    - The system is some defined mass
- $b = B/\text{mass}$
- Read the equation as: "(The rate of change of B of the system) = (The rate of change of B in some Control Volume) + (The rate that B crosses out of the C.V.)"
- (Generation) ≡ (Accumulation) + (out − in)

Divergence Theorem

$$\int_{CV} \nabla \cdot \vec{V} \, d\mathcal{V} = \int_{CS} \vec{V} \cdot \vec{n} \, dA.$$

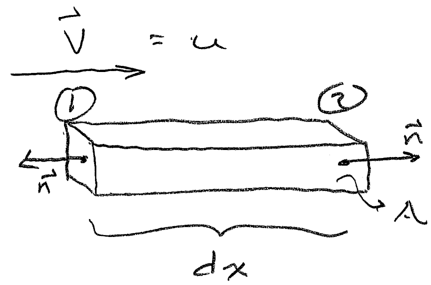
- Divergence is like a net outflow per unit volume. $(\nabla \cdot \vec{V})$

So $\int_{CV} \nabla \cdot \vec{V} \, d\mathcal{V}$ is the net out flow in the C.V.

$= (\text{out} - \text{in})$

$= \int_{C.S.} \vec{V} \cdot \vec{n} \, dA$

Example: 1-D



$$\int_{CV} \nabla \cdot \vec{V} \, d\mathcal{V} \Rightarrow \int_1^2 \frac{\partial}{\partial x} u \, A \, \cancel{dx} = A(u_2 - u_1)$$

$$\int_{CS} \vec{V} \cdot \vec{n} \, dA \Longrightarrow \int_{CS(2)} \vec{V} \cdot \vec{n} \, dA + \int_{CS(1)} \vec{V} \cdot \vec{n} \, dA$$

$$= A u_2 \quad - A u_1 \quad = A(u_2 - u_1)$$

at (1) $\vec{V} \cdot \vec{n} = -u_1$

at (2) $\vec{V} \cdot \vec{n} = u_2$

Mass

- $B_{sys} = M_{sys}$
- $b = 1 \qquad = B_s / M_s$
- Conservation Law: $\frac{dM_{sys}}{dt} = 0$; M_{sys} is const, not Created or Destroyed.
- $\frac{dB_{sys}}{dt} = \frac{d}{dt} \int_{CV} \rho b \, d\mathcal{V} + \int_{CS} \rho b \vec{V}_R \cdot \vec{n} \, dA$

$$0 = \underbrace{\frac{d}{dt} \int_{CV} \rho \, d\mathcal{V}}_{CV \neq CV(t)} + \underbrace{\int_{CS} \rho \vec{V}_R \cdot \vec{n} \, dA}_{\int_{CV} \nabla \cdot (\rho \vec{V}) d\mathcal{V}}$$

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

or $$\int_{cv} \frac{\partial}{\partial t}(\rho) + \nabla\cdot(\rho\vec{V})\, d\mathcal{V} = 0$$

- This is True for Any C.V. so

$$\boxed{\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\vec{V}) = 0}$$

- Differential form
- Mass Balance
- The integral form was $\frac{d}{dt}\int_{cv} \rho\, d\mathcal{V} + \int_{cs} \rho\vec{V}_R\cdot\vec{n}\,dA = 0$

Momentum

- $B_{sys} = \vec{Mom}_{sys} = M_{sys}\vec{V}_{sys}$
- $b = B_{sys}/M_{sys} = \vec{V}_{sys}$.
- Conservation Law ; Newton's 2^{nd} Law $\frac{d\vec{Mom}_{sys}}{dt} = \vec{F}_{ext,sys}$
- $\vec{F}_{ext,sys} = \frac{d}{dt}\int_{cv} \rho\vec{V}_s\, d\mathcal{V} + \int_{cs} \rho\vec{V}_s\vec{V}_R\cdot\vec{n}\,dA$
- $\vec{F}_{ext,s} = \int_{cv}\left[\frac{\partial}{\partial t}(\rho\vec{V}_s) + \nabla\cdot(\rho\vec{V}_s\vec{V}_R)\right] d\mathcal{V}$
- $\vec{F}_{ext,s}$: Pressure, Viscous, Body, etc.

Pressure : $\int_{c.s.} -(p\,\vec{n})\,dA = \int_{cs} -\underline{\underline{\delta}}\cdot(p\,\vec{n})\,dA$

$$\underline{\underline{\delta}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \int_{cv} -\nabla\cdot(\underline{\underline{\delta}}\,p)\, d\mathcal{V}$$

Viscous: $-\int_{CS} \underline{\underline{\tau}} \cdot \vec{n}\, dA = -\int_{CV} \nabla \cdot \underline{\underline{\tau}}\, d\mathcal{V}$

Body: $\int_{CV} \rho \vec{g}\, d\mathcal{V}$

$$\rightarrow \int_{CV} \left[\frac{\partial}{\partial t}(\rho \vec{V}_s) + \nabla \cdot (\rho \vec{V}_s \vec{V}_R) \right] d\mathcal{V} = \int_{CV} -\nabla \cdot (P \underline{\underline{\delta}})\, d\mathcal{V} - \int_{CV} \nabla \cdot \underline{\underline{\tau}}\, d\mathcal{V} + \int_{CV} \rho \vec{g}\, d\mathcal{V}$$

$$\rightarrow \boxed{\frac{\partial}{\partial t}(\rho \vec{V}_s) + \nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla P - \nabla \cdot \underline{\underline{\tau}} + \rho \vec{g}}$$

- Differential form
- Integral form is

$$\frac{d}{dt}\int_{CV} \rho \vec{V}_s\, d\mathcal{V} + \int_{CS} \rho \vec{V}_s\, \vec{V}_R \cdot \vec{n}\, dA = \int_{CS} -P \vec{n}\, dA - \int_{CS} \underline{\underline{\tau}} \cdot \vec{n}\, dA + \int_{CV} \rho \vec{g}\, d\mathcal{V}$$

- u-mom:

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \vec{V}) = -\frac{\partial P}{\partial x} - \frac{\partial}{\partial x} \cdot \vec{\tau}_x + \rho g_x$$

- v-mom, w-mom likewise.
- Index notation.

$$\frac{\partial \rho V_j}{\partial t} + \frac{\partial}{\partial x_i}(\rho V_i V_j) = -\frac{\partial}{\partial x_j} P - \frac{\partial}{\partial x_i} \tau_{ij} + \rho g_j$$

- repeated indicies imply summation.
- lone indicies indicate a vector component.

Energy

- $B_{sys} = E_{tot}$: internal + kinetic
- $b = e_{tot} = u + \frac{1}{2}\vec{v}\cdot\vec{v}$ $\qquad u = h - \frac{P}{\rho}$
- Conservation Law: $\frac{dE_t}{dt} = \dot{Q} + \dot{W}$: heat + work.
- $\dot{Q} + \dot{W} = \int_{cv}\left[\frac{\partial}{\partial t}(\rho e_t) + \nabla\cdot(\rho\vec{V}_R e_t)\right]d\mathcal{V}$
   - $\dot{Q} = -\int_{c.s}\vec{q}\cdot\vec{n}\,dA = -\int_{cv}\nabla\cdot\vec{q}\,d\mathcal{V}$
   - $\dot{W} = -\int_{cs}\vec{F}\cdot\vec{v}\,dA = -\int_{cs}(P\underline{\underline{\delta}} + \underline{\underline{\tau}})\cdot\vec{v}\,dA + \int_{cv}\rho\vec{g}\cdot\vec{v}\,d\mathcal{V}$

$$= -\int_{cv}\nabla\cdot(P\underline{\underline{\delta}}\cdot\vec{v})\,d\mathcal{V} = -\int_{cv}\nabla\cdot(P\vec{v})\,d\mathcal{V}$$

$$-\int_{cv}\nabla\cdot(\underline{\underline{\tau}}\cdot\vec{v})\,d\mathcal{V} + \int\rho\vec{g}\cdot\vec{v}\,d\mathcal{V}$$

- $$\boxed{\frac{\partial}{\partial t}\rho e_t + \nabla\cdot(\rho\vec{v}e_t) = -\nabla\cdot\vec{q} - \nabla\cdot(P\vec{v}) - \nabla\cdot(\underline{\underline{\tau}}\cdot\vec{v}) + \rho\vec{g}\cdot\vec{v}}$$
   - Differential
   - Integral form is above.

Species

- $B_s = m_i = mY_i$
- $b = Y_i$
- Conservation Law: $\frac{dmY_i}{dt} = S_i = \int_{cv}\dot{m}_i'''\,d\mathcal{V}$
- $\vec{V}_R = \vec{V}_i = \vec{v} + \vec{V}_i^D \longrightarrow \boxed{\frac{\partial}{\partial t}(\rho Y_i) + \nabla\cdot(\rho Y_i\vec{v}) + \nabla\cdot(\rho Y_i V_i^D) = \dot{m}_i'''}$

Constitutive Relations.

- $\vec{q} = -k\nabla T + \sum_k h_k \vec{j}_k + \vec{q}_{rad}$
- $P = \dfrac{\rho R T}{M}$ $\qquad M$ = molec. wt here.
- $\rho Y_i V_i^D = \vec{j}_i = -\dfrac{\rho Y_i D_i}{X_i}\nabla X_i = -\rho D_i \nabla Y_i - \dfrac{\rho D_i Y_i}{M}\nabla M$
- $\tau_{ij} = -\mu\left(\dfrac{\partial v_i}{\partial x_j} + \dfrac{\partial v_j}{\partial x_i} - \dfrac{2}{3}\delta_{ij}\dfrac{\partial v_l}{\partial x_l}\right)$

  - $\tau_{xx} = -2\mu\dfrac{\partial v_x}{\partial x} + \dfrac{2}{3}\mu\nabla\cdot\vec{v}$

    likewise for τ_{yy}, τ_{zz}
  - $\tau_{xy} = \tau_{yx} = -\mu\left[\dfrac{\partial v_y}{\partial x} + \dfrac{\partial v_x}{\partial y}\right]$

    likewise for $\tau_{y,z}$, τ_{zx}

Summary

Mass: $$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x_i}(\rho v_i)$$

Mom: $$\frac{\partial \rho v_i}{\partial t} = -\frac{\partial}{\partial x_j}(\rho v_i v_j) - \frac{\partial}{\partial x_i}P - \frac{\partial}{\partial x_i}\tau_{ij} + \rho g_i$$

Energy: $$\frac{\partial \rho e_t}{\partial t} = -\frac{\partial}{\partial x_i}(\rho v_i e_t) - \frac{\partial}{\partial x_i}q_i - \frac{\partial}{\partial x_i}(P v_i) - \frac{\partial}{\partial x_i}(\tau_{ij} v_j) + \rho g_i v_i$$

Species: $$\frac{\partial \rho Y_k}{\partial t} = -\frac{\partial}{\partial x_i}(\rho v_i Y_k) - \frac{\partial}{\partial x_i} j_{k,i} + \dot{m}_i'''$$

$$\frac{\partial Q}{\partial t} = -\frac{\partial}{\partial x_i}(v_i Q) - \frac{\partial}{\partial x_i} f + S$$

$$Q = \begin{bmatrix} \rho \\ \rho v_j \\ \rho e_t \\ \rho Y_k \end{bmatrix} \qquad f = \begin{bmatrix} 0 \\ P + \tau_{ij} \\ q_i + P v_i + \tau_{ij} v_j \\ J_{k,i} \end{bmatrix} \qquad S = \begin{bmatrix} 0 \\ \rho g_i \\ \rho g_i v_i \\ \dot{m}_i''' \end{bmatrix}$$

For use in an ODE Solver, we do

- $$\frac{dQ}{dt} = R(Q, t)$$
- Code the R function,

Discretize the equations on a 3-D Grid.

→ $Q = Q^{ijk}$

→ Solve via Method of lines.

- 1 PDE : $\frac{\partial Q}{\partial t} = \ldots$

  becomes n_{grid} ODE's