Conservation laws of Fluid motion and boundary Conditions

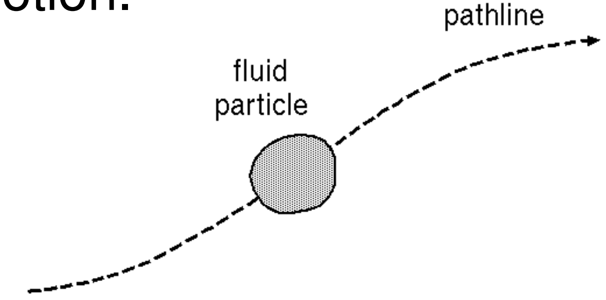
Governing equations

- The fluid is treated as a continuum. For length scales of about 1μm and larger, the molecular structure and motions may be ignored. A fluid element traced in space will stay a cohering fluid parcel with a conserved (constant) mass.

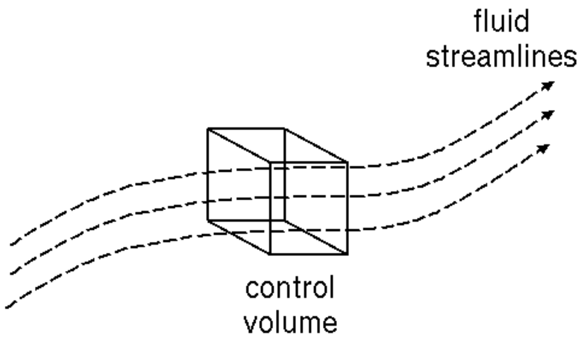
- The governing equations include the following conservation laws:
  - Conservation of mass.
  - Conservation of momentum: Newton's second law - the change of momentum equals the sum of forces on a fluid particle.
  - Conservation of energy: First law of thermodynamics - rate of change of energy equals the sum of rate of heat addition to and work done on fluid particle.
  - Conservation of an arbitrary scalar: Species concentration, …

Lagrangian vs. Eulerian description

A fluid flow field can be thought of as being comprised of a large number of finite sized fluid particles which have mass, momentum, internal energy, and other properties. Mathematical laws can then be written for each fluid particle. This is the Lagrangian description of fluid motion.



Another view of fluid motion is the Eulerian description. In the Eulerian description of fluid motion, we consider how flow properties change at a differential control volume that is fixed in space and time (x,y,z,t), rather than following individual fluid particles.

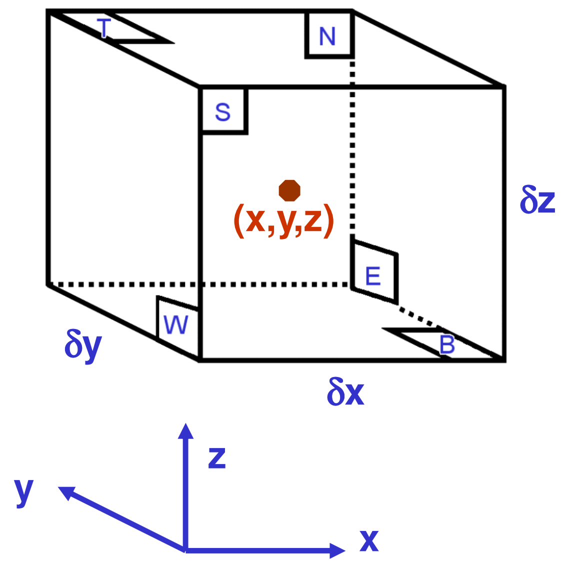


Governing equations can be derived using each method and converted to the other form.

Fluid volume fixed in space

- The behavior of the fluid is described in terms of macroscopic properties:
  - Velocity **u**
  - Density ρ
  - Specific energy e
  - Pressure p
  - Temperature T
- Properties are averages of a sufficiently large number of molecules.
- A differential control volume (fluid element) can be thought of as the smallest volume for which the continuum assumption is valid.

Differential volume for conservation laws



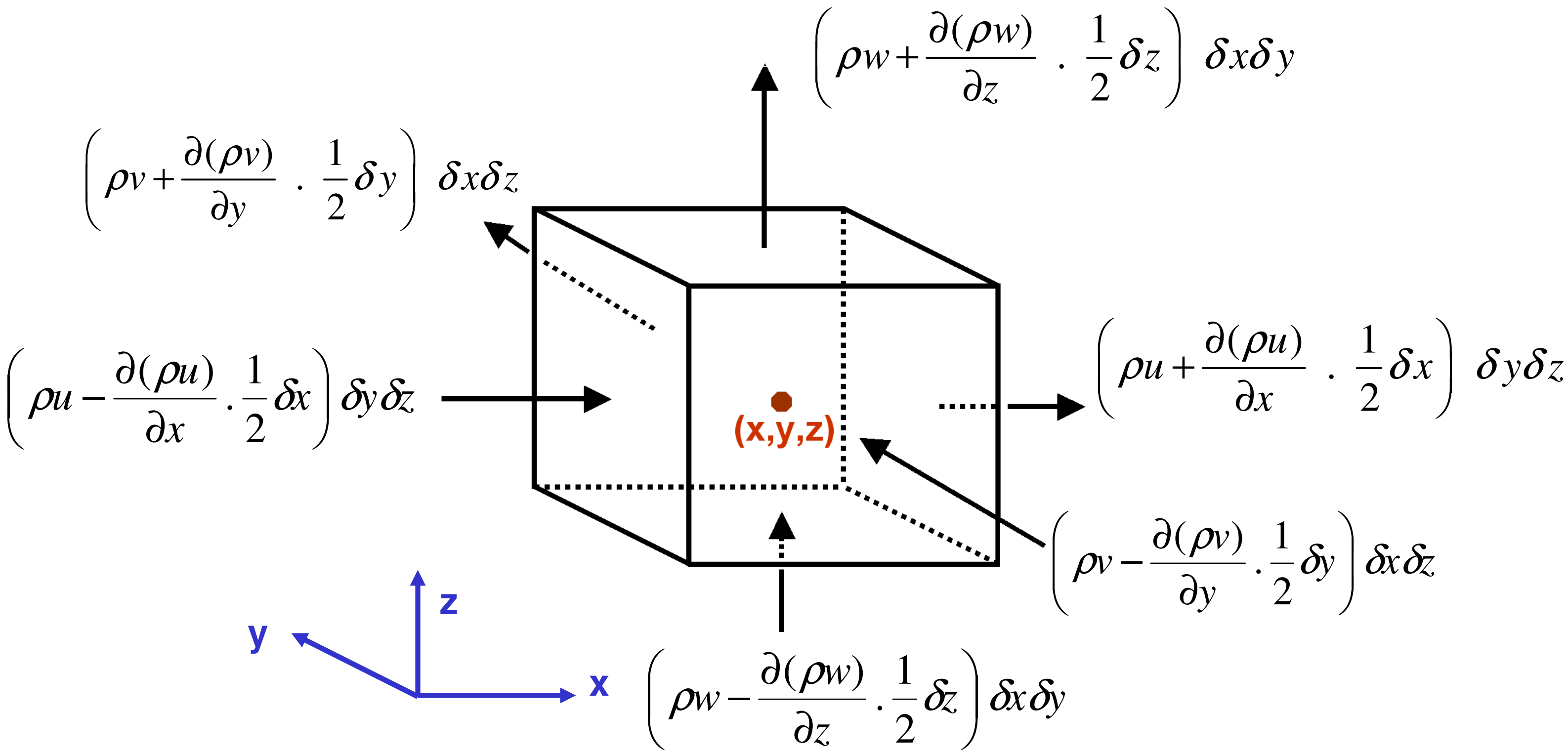
Faces are labeled North, East, West, South, Top and Bottom

Properties at faces are expressed as first two terms of a Taylor series expansion,

e.g. for ρ: $\rho_w = \rho_P - \frac{\partial \rho}{\partial x}\frac{1}{2}\delta x$ and $\rho_e = \rho_P + \frac{\partial \rho}{\partial x}\frac{1}{2}\delta x$

Mass balance (Eulerian Description)

- Rate of increase of mass in fluid element equals the net rate of flow of mass into element.
- Rate of increase is: $\frac{\partial}{\partial t}(\rho \delta x \delta y \delta z) = \frac{\partial \rho}{\partial t} \delta x \delta y \delta z$
- The inflows (positive) and outflows (negative) are shown here:



Continuity equation

- Summing all terms in the previous slide and dividing by the volume $\delta x \delta y \delta z$ results in:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial(\rho w)}{\partial z}=0$$

- In vector notation:

$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho \mathbf{u})=0$$

Change in density

Net flow of mass across boundaries
Convective term

- For incompressible fluids $\rho =$ const., and the equation becomes:

$$\nabla\cdot\mathbf{u}=0 \qquad \frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \qquad \frac{\partial u_i}{\partial x_i}=0$$

Path B: Fluid particle and fixed control volume

- We can derive the relationship between the equations for a fluid particle (Lagrangian) and a fluid element (Eulerian) as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\,\mathbf{u}) = \underbrace{\frac{\partial \rho}{\partial t} + (\mathbf{u} \cdot \nabla \rho)}_{\text{Substantial/total derivation}} + (\rho \nabla \cdot \mathbf{u}) = \frac{D\rho}{Dt} + (\rho \nabla \cdot \mathbf{u})$$

Substantial/total derivation

$$\rho = \rho(t, x, y, z) \Rightarrow \frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial \rho}{\partial y}\frac{\partial y}{\partial t} + \frac{\partial \rho}{\partial z}\frac{\partial z}{\partial t}$$

$$\frac{\partial \rho}{\partial t} + \underbrace{\frac{\partial \rho}{\partial x} u_1 + \frac{\partial \rho}{\partial y} u_2 + \frac{\partial \rho}{\partial z} u_3}_{\text{convective derivation}}$$

local derivation

convective derivation

Momentum equation in three dimensions

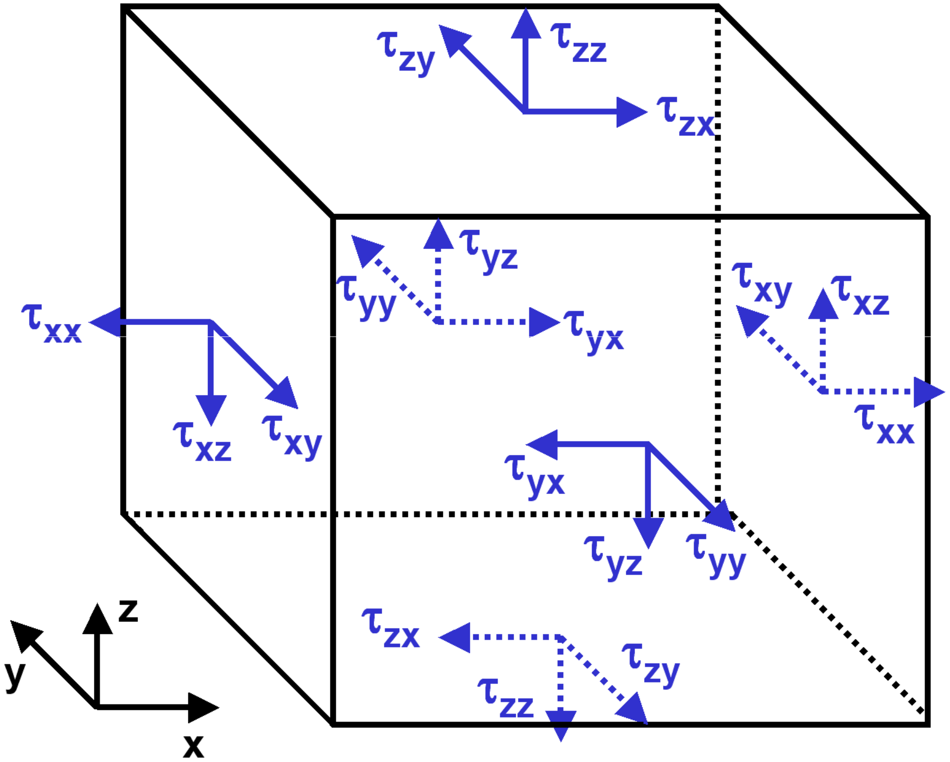
- We will first derive conservation equations for momentum and energy for fluid particles (Lagrangian frame of reference). Next, we will use the above relationships to transform those to an Eulerian frame (for a fixed control volume).
- Newton's second law: rate of change of momentum equals sum of forces (**F** = m.**a** for solid bodies).
- Rate of increased momentum:

$$\mathbf{F} = \frac{D\mathbf{I}}{Dt} = \frac{D(\rho\mathbf{u})}{Dt}$$

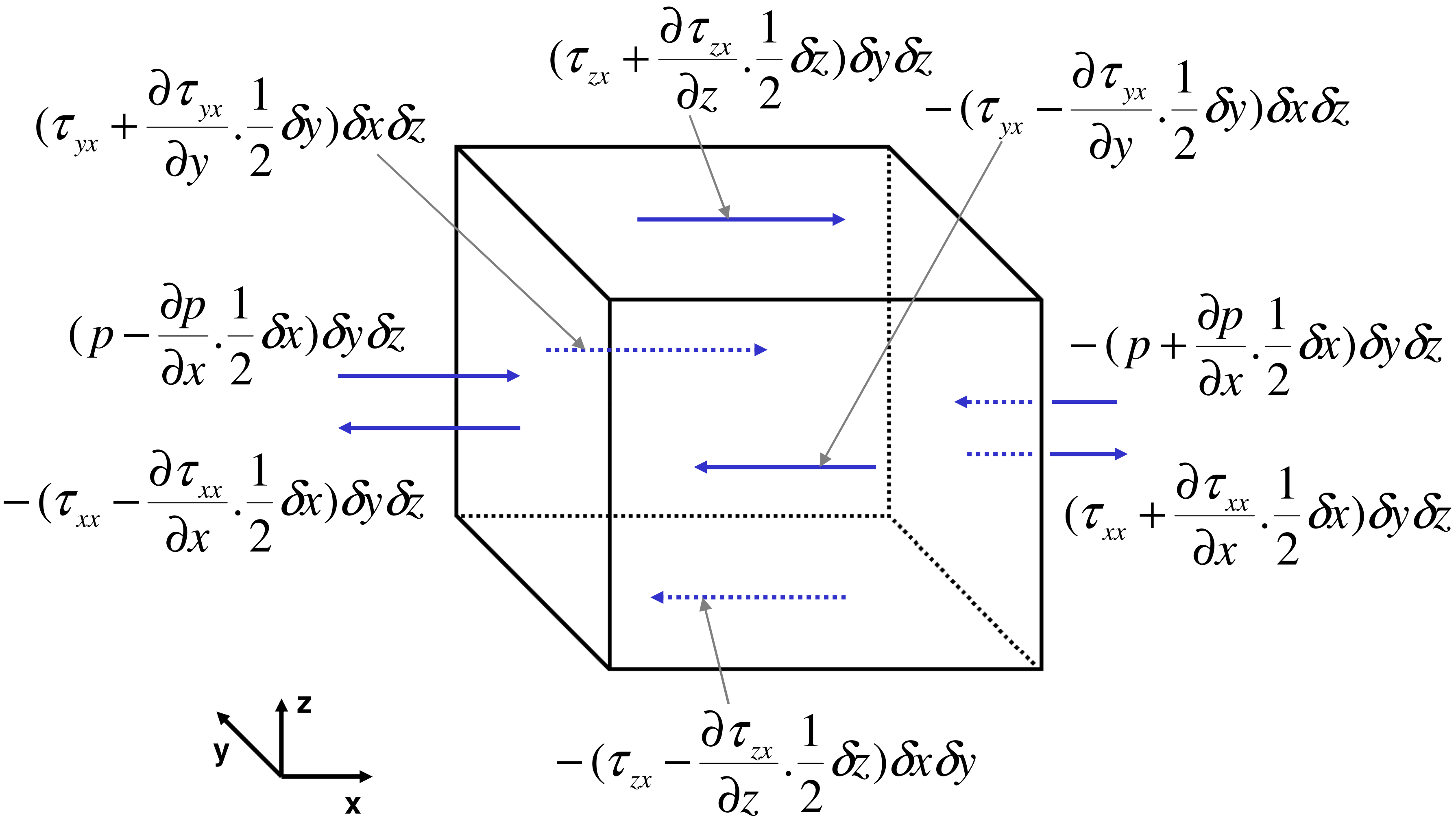
- Forces on fluid particles are:
  - Surface forces such as pressure and viscous forces.
  - Body forces, which act on a volume, such as gravity, centrifugal, Coriolis, and electromagnetic forces.

Viscous stresses

- Stresses are forces per area. Unit is N/m^2 or Pa.
- Viscous stresses denoted by τ.
- Suffix notation τ_{ij} is used to indicate direction.
- Nine stress components.
  - τ_{xx}, τ_{yy}, τ_{zz} are normal stresses. E.g. τ_{zz} is the stress in the z-direction on a z-plane.
  - Other stresses are shear stresses. E.g. τ_{zy} is the stress in the y-direction on a z-plane.
- Forces aligned with the direction of a coordinate axis are positive. Opposite direction is negative.



Forces in the x-direction



Net force in the x-direction is the sum of all the force components in that direction.

Momentum equation

- Set the rate of change of x-momentum for a Lagrangian fluid particle equal to:
  - the sum of the forces due to surface stresses shown in the previous slide, plus
  - the body forces. These are usually lumped together into a source term S_M:

$$\frac{D(\rho u)}{Dt} = \frac{\partial(-p+\tau_{xx})}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + S_{Mx}$$

- Written for a differential Eulerian contol volume:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \overbrace{\mathbf{S}_M}^{\rho \mathbf{g} + \ldots}$$

Viscous stresses

- A model for the viscous stresses τ_{ij} is required.
- We will express the viscous stresses as functions of the local deformation rate (strain rate) tensor.
- There are two types of deformation:
  - Linear deformation rates due to velocity gradients.
    - Elongating stress components (stretching).
    - Shearing stress components.
  - Volumetric deformation rates due to expansion or compression.
- All gases and most fluids are isotropic: viscosity is a scalar.

Viscous stress tensor

- Using an isotropic (first) dynamic viscosity μ for the linear deformations and a second viscosity λ=-2/3 μ for the volumetric deformations results in:

$$\boldsymbol{\tau} = \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{pmatrix} = \begin{pmatrix} 2\mu \frac{\partial u}{\partial x} - \frac{2}{3}\mu \nabla \cdot \mathbf{u} & \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) & \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \\ \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) & 2\mu \frac{\partial v}{\partial y} - \frac{2}{3}\mu \nabla \cdot \mathbf{u} & \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) \\ \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) & \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) & 2\mu \frac{\partial w}{\partial z} - \frac{2}{3}\mu \nabla \cdot \mathbf{u} \end{pmatrix}$$

$$= \mu\left[\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}\right) - \frac{2}{3}\nabla \cdot \mathbf{u}\ \mathbf{I}\right]$$

Note: ∇·u = 0 for incompressible fluids.

Navier-Stokes equation – differential and integral form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = S$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \overbrace{\boldsymbol{\tau}}^{\mu\left[\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}\right) - \frac{2}{3}\nabla \cdot \mathbf{u}\,\mathbf{I}\right]} + \mathbf{S}_M$$

$$\frac{\partial}{\partial t}\left(\int_{CV} \rho \, dV\right) + \int_A \rho \mathbf{u} \cdot \mathbf{dA} = \int_{CV} S \; dV$$

$$\frac{\partial}{\partial t}\left(\int_{CV} \rho \mathbf{u} \, dV\right) + \int_A \rho \mathbf{u}\mathbf{u} \cdot \mathbf{dA} = -\int_A p \mathbf{I} \cdot \mathbf{dA} + \int_A \boldsymbol{\tau} \cdot \mathbf{dA} + \int_{CV} \mathbf{S}_M \, dV$$

Energy equation

- First law of thermodynamics: rate of change of energy of a fluid particle is equal to the rate of heat addition plus the rate of work done.
- The total energy $E = i + \frac{1}{2}(u^2+v^2+w^2)$ comprises the internal (thermal) energy i and the kinetic (mechanical) energy $\frac{1}{2}(u^2+v^2+w^2)$. Usually, the potential energy (gravitation) is treated separately and included as a source term.
- The rate of increase total energy, DE/Dt, results out of work done by viscous stresses and the net heat conduction.
- We will derive the transport equation for the total energy. Next, we will subtract the kinetic energy equation to arrive at a conservation equation for the internal energy.

Work done by surfaces stresses in x-direction

$$\left(u\tau_{zx}+\frac{\partial(u\tau_{zx})}{\partial z}.\frac{1}{2}\delta z\right)\delta y\delta z$$

$$\left(u\tau_{yx}+\frac{\partial(u\tau_{yx})}{\partial y}.\frac{1}{2}\delta y\right)\delta x\delta z$$

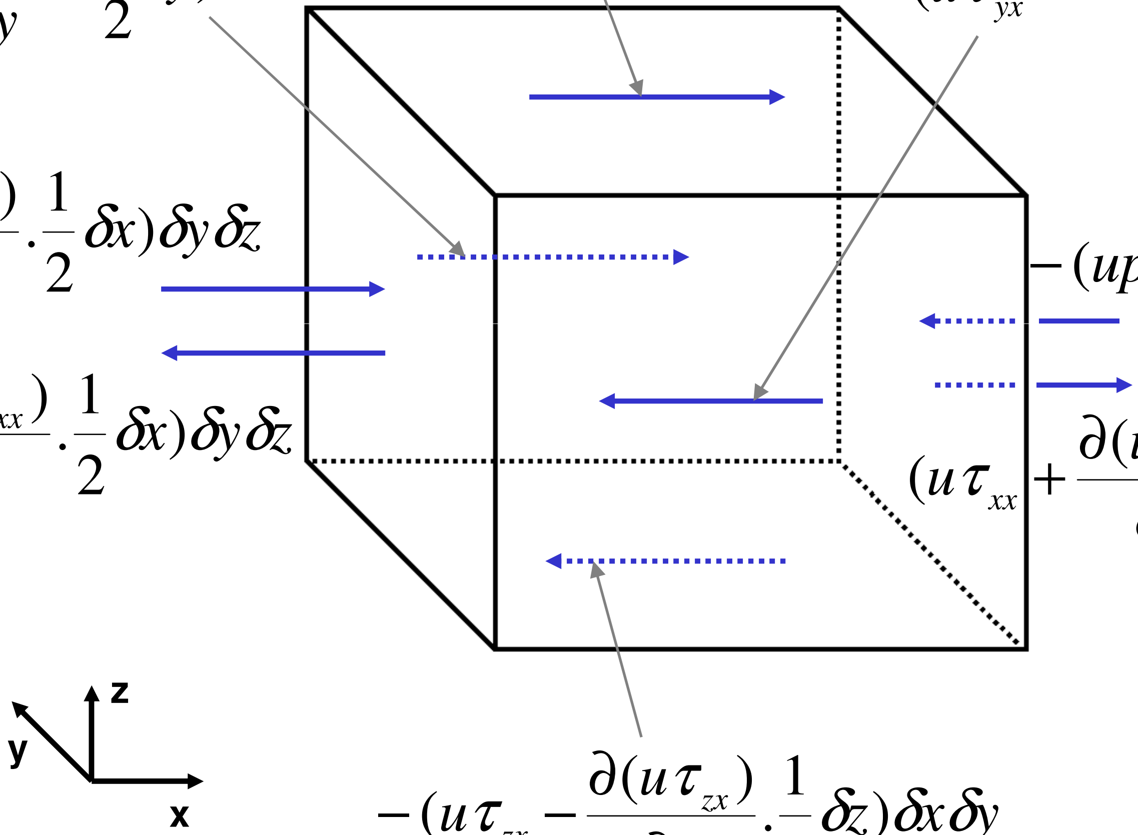
$$-\left(u\tau_{yx}-\frac{\partial(u\tau_{yx})}{\partial y}.\frac{1}{2}\delta y\right)\delta x\delta z$$

$$\left(up-\frac{\partial(up)}{\partial x}.\frac{1}{2}\delta x\right)\delta y\delta z$$

$$-\left(up+\frac{\partial(up)}{\partial x}.\frac{1}{2}\delta x\right)\delta y\delta z$$

$$-\left(u\tau_{xx}-\frac{\partial(u\tau_{xx})}{\partial x}.\frac{1}{2}\delta x\right)\delta y\delta z$$

$$\left(u\tau_{xx}+\frac{\partial(u\tau_{xx})}{\partial x}.\frac{1}{2}\delta x\right)\delta y\delta z$$



$$-\left(u\tau_{zx}-\frac{\partial(u\tau_{zx})}{\partial z}.\frac{1}{2}\delta z\right)\delta x\delta y$$

Work done (energy flux) is force times velocity.

Work done by surface stresses

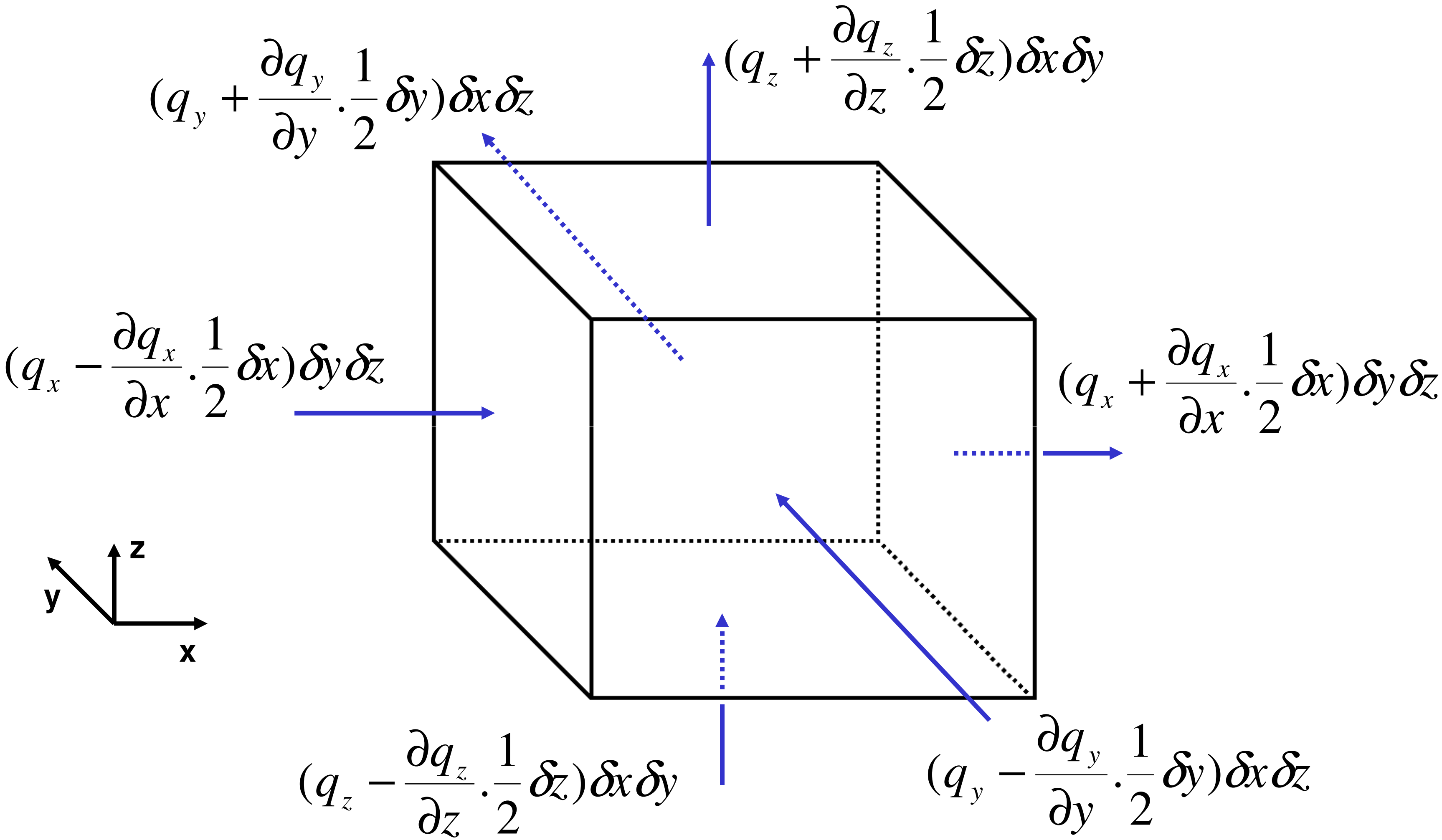
- Add all and divide by $\delta x \delta y \delta z$ to get the work done per unit volume by the surface stresses:

$$-\nabla \cdot (p\mathbf{u}) + \frac{\partial (u\tau_{xx})}{\partial x} + \frac{\partial (u\tau_{yx})}{\partial y} + \frac{\partial (u\tau_{zx})}{\partial z} + \frac{\partial (v\tau_{xy})}{\partial x}$$

$$+ \frac{\partial (v\tau_{yy})}{\partial y} + \frac{\partial (v\tau_{zy})}{\partial z} + \frac{\partial (w\tau_{xz})}{\partial x} + \frac{\partial (w\tau_{yz})}{\partial y} + \frac{\partial (u\tau_{zz})}{\partial z}$$

$$= -\nabla \cdot (p\mathbf{u}) + \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u})$$

Energy flux due to heat conduction



The heat flux vector q has three components, q_x, q_y, and q_z.

Energy flux due to heat conduction

- Summing all terms and dividing by $\delta x \delta y \delta z$ gives the net rate of heat transfer to the fluid particle per unit volume:

$$-\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} - \frac{\partial q_z}{\partial z} = -\nabla \cdot \mathbf{q}$$

- Fourier's law of heat conduction relates the heat flux to the local temperature gradient:

$$\mathbf{q} = -\lambda \nabla T$$

Total energy equation

- Setting the total derivative for the energy in a Lagrangian fluid particle equal to the previously derived work and energy flux terms, results in the following energy equation:

$$\rho \frac{DE}{Dt} = -\nabla \cdot (p\mathbf{u}) + \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u}) + \nabla \cdot (\lambda \nabla T) + S_E$$

- Note that we also added a source term S_E that includes sources (potential energy, sources due to heat production from chemical reactions, etc.).

Kinetic energy equation

- Separately, we can derive a conservation equation for the kinetic energy of the fluid.
- In order to do this, we multiply the u-momentum equation by u, the v-momentum equation by v, and the w-momentum equation by w. We then add the results together.
- This results in the following equation for the kinetic energy:

$$\rho \frac{D[\frac{1}{2}(u^2+v^2+w^2)]}{Dt} = -\mathbf{u}\nabla p + u\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}\right)$$

$$+ v\left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z}\right) + w\left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}\right) + \mathbf{u}.\mathbf{S}_M$$

Internal energy equation

- Subtract the kinetic energy equation from the energy equation.
- Define a new source term for the internal energy as $S_i = S_E - \mathbf{u}.\mathbf{S_M}$. This results in:

$$\frac{Di}{Dt} = -p\,\nabla \cdot \mathbf{u} + \nabla \cdot (\lambda\,\nabla\,T) + \Phi + S_i$$

- Here Φ is the viscous dissipation term. This term is always positive and describes the conversion of mechanical energy to heat.

$$\Phi = \mu\left\{2\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2\right] + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)^2\right\} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})^2$$

Summary of equations in differential form

$$Mass: \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\, \mathbf{u}) = 0$$

$$Momentum: \quad \frac{\partial\, \rho\, \mathbf{u}}{\partial t} + \nabla \cdot \left(\rho\, \mathbf{uu}\right) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{S}_M$$

$$Internal\ energy: \quad \frac{\partial(\rho i)}{\partial t} + \nabla \cdot (\rho i \mathbf{u}) = -\, p\, \nabla \cdot \mathbf{u} + \nabla \cdot (\lambda\, \nabla T) + \Phi + S_i$$

$$Equations\ of\ state: \quad p = p(\rho, T) \quad and \quad i = i(\rho, T)$$

$$e.g.\ for\ perfect\ gas: p = \rho R T \quad and \quad i = C_v T$$

General transport equations

- The system of equations is now closed, with seven equations for seven variables: pressure, three velocity components, enthalpy, temperature, and density.
- There are significant commonalities between the various equations. Using a general variable ϕ, the conservative form of all fluid flow equations can usefully be written in the following form:

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla\cdot(\rho\phi\mathbf{u}) = \nabla\cdot(\Gamma\nabla\phi) + S_\phi$$

- Or, in words:

Rate of increase of ϕ of fluid element + **Net rate of flow of ϕ out of fluid element (convection)** = **Rate of increase of ϕ due to diffusion** + **Rate of increase of ϕ due to sources**

Integral form

- The key step of the finite volume method is to integrate the differential equation shown in the previous slide, and then to apply Gauss' divergence theorem, which for a vector **a** states:

$$\int_{CV} \nabla \cdot \mathbf{a}\, dV = \int_{A} \mathbf{n} \cdot \mathbf{a}\, dA$$

- This then leads to the following general conservation equation in integral form:

$$\frac{\partial}{\partial t}\left(\int_{CV} \rho\phi\, dV\right) + \int_{A} \mathbf{n}\cdot(\rho\phi\mathbf{u})\, dA = \int_{A} \mathbf{n}\cdot(\Gamma\nabla\phi)\, dA + \int_{CV} S_{\phi}\, dV$$

Rate of increase of ϕ	+	Net rate of decrease of ϕ due to convection across boundaries	=	Net rate of increase of ϕ due to diffusion across boundaries	+	Net rate of creation of ϕ

- This is the actual form of the conservation equations solved by finite volume based CFD programs

Navier-Stokes equation – differential and integral form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = S$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \overbrace{\boldsymbol{\tau}}^{\mu\left[\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}\right) - \frac{2}{3}\nabla \cdot \mathbf{u}\ \mathbf{I}\right]} + \mathbf{S}_M$$

$$\frac{\partial}{\partial t}\left(\int_{CV} \rho\, dV\right) + \int_A \rho \mathbf{u} \cdot \mathbf{dA} = \int_{CV} S\ dV$$

$$\frac{\partial}{\partial t}\left(\int_{CV} \rho \mathbf{u}\, dV\right) + \int_A \rho \mathbf{u}\mathbf{u} \cdot \mathbf{dA} = -\int_A p\, \mathbf{I} \cdot \mathbf{dA} + \int_A \boldsymbol{\tau} \cdot \mathbf{dA} + \int_{CV} \mathbf{S}_M\, dV$$

Summary of equations in differential form

$$Mass: \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$Momentum: \quad \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \left(\rho \mathbf{u}\mathbf{u}\right) = -\nabla p + \underbrace{\nabla \cdot \boldsymbol{\tau}}_{\mu\left[\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}\right) - \frac{2}{3}\nabla \cdot \mathbf{u}\, \mathbf{I}\right]} + \mathbf{S}_M$$

$$Internal\ energy: \quad \frac{\partial (\rho i)}{\partial t} + \nabla \cdot (\rho i \mathbf{u}) = -\, p\, \nabla \cdot \mathbf{u} + \nabla \cdot (\lambda\, \nabla T) + \Phi + S_i$$

$$Equations\ of\ state\ (e.g.\ for\ perfect\ gas): p = \rho RT \quad and \quad i = C_v T$$

Summary of equations in differential form (constant fluid properties)

$$Mass: \quad \nabla \cdot \mathbf{u} = 0$$

$$Momentum: \quad \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{uu}) \right) = -\nabla p + \mu \Delta \mathbf{u} + \mathbf{S}_M$$

$$Internal\ energy: \quad \rho c_p \left(\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u} T) \right) = \lambda \Delta T + \Phi + S_i$$

$$Species\ concentration: \quad \rho \left(\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{u} c_i) \right) = \Gamma \Delta c_i + S_{i,react}$$