

CFD Course Formula Student Bizkaia 2017

# The equations of fluid motion and their discretization

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# 1. Governing Equations and their Discretization

# Conservation law

# Conservation law

## Conservation law

A measurable property of an isolated physical system does **not change over time**



Mikhail Lomonosov, discovered the law of mass conservation in 1756 by experiments, concluding that phlogiston theory is incorrect.

Antoine Lavoisier's discovery of the Law of Conservation of Mass led to many new findings in the 19th century.

Source: (left) <https://en.wikipedia.org> (right) <https://commons.wikimedia.org>

# Derivation: conservation law

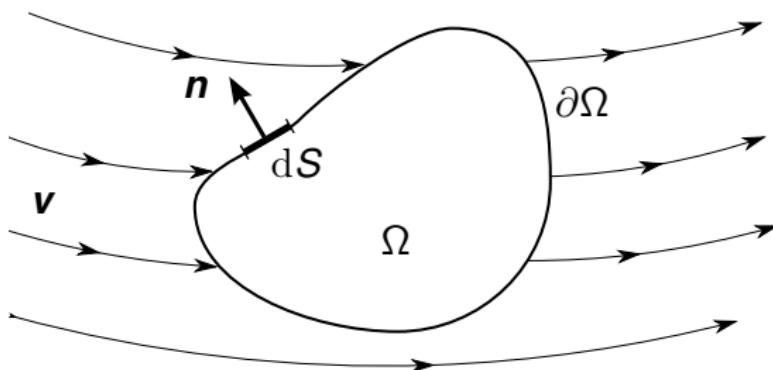
## Some hypothesis on “fluid dynamics”

1. We are interested in the motion of a large number of individual particles: atoms and molecules!
2. We **assume** that the density of the fluid is high enough so that the motion can be **approximated as continuum**  $\Rightarrow$  we are in the field of **continuum mechanics**
3.  $\Rightarrow$  An infinitesimally small fluid element (in the sense of **differential calculus**) still contains enough particles, allowing us to prescribe **mean** quantities such as velocity, energy etc.
4. We are thus able to define all this quantities at each point of the fluid

# Control volume

We will use the **Eulerian** approach. We thus naturally divide the flow field into fluid elements, or **volumes**, and try to develop a mathematical description of their physics.

We define the **finite control volume** (fixed in space):



where  $\Omega$  is the control volume with boundary is  $\partial\Omega$ ,  $n$  is the outwarding unit normal vector, and  $v$  is the velocity field.

# Derivation: conservation law (cont.)

Applying the conservation law to a scalar  $\phi$ , we state that the following quantities are in equilibrium within a control volume  $\Omega$ :

- Variation in time  $t$ :

$$\frac{d}{dt} \int_{\Omega} \phi d\Omega$$

- Amount due to the velocity  $\mathbf{v}$  (**convective flux**):

$$-\oint_{\partial\Omega} \phi (\mathbf{v} \cdot \mathbf{n}) dS$$

- Amount due to the diffusion (**diffusive flux**), expressed by the

generalized Fick's gradient law:

$$\oint_{\partial\Omega} \kappa \rho [\nabla (\phi/\rho) \cdot \mathbf{n}] dS,$$

where  $\kappa$  is the thermal diffusivity coefficient, and  $\rho$  is the density

- Volume** and **surface** sources  $Q_V, \mathbf{Q}_S$ :

$$\int_{\Omega} Q_V d\Omega + \oint_{\partial\Omega} (\mathbf{Q}_S \cdot \mathbf{n}) dS$$

## Derivation: conservation law (cont.)

After summing the contributions, we end up with the general conservation law for a **scalar quantity**:

$$\frac{d}{dt} \int_{\Omega} \phi d\Omega + \oint_{\partial\Omega} \phi (\mathbf{v} \cdot \mathbf{n}) - \kappa \rho [\nabla(\phi/\rho) \cdot \mathbf{n}] dS = \int_{\Omega} Q_V d\Omega + \oint_{\partial\Omega} (\mathbf{Q}_S \cdot \mathbf{n}) dS \quad (1)$$

## Derivation: conservation law (cont.)

**NOTE:** if we consider a **vector** as conserved quantity, the previous conservation law (1) would still be valid.

But differing in the **order** of the geometrical objects:

1. Convective and diffusive fluxes become **tensors**  $\bar{\bar{F}}_C, \bar{\bar{F}}_D$
2. The volume source becomes a **vector**  $\mathbf{Q}_V$
3. The surface source becomes a **tensor**  $\bar{\bar{\bar{Q}}}_S$

We can rewrite the conservation law for a **vector quantity  $u$**  as

$$\frac{d}{dt} \int_{\Omega} \mathbf{u} d\Omega + \oint_{\partial\Omega} \left[ (\bar{\bar{F}}_C - \bar{\bar{F}}_D) \cdot \mathbf{n} \right] dS =$$

$$\int_{\Omega} \mathbf{Q}_V d\Omega + \oint_{\partial\Omega} (\bar{\bar{\bar{Q}}}_S \cdot \mathbf{n}) dS \quad (2)$$

## Derivation: conservation law (cont.)

Equations (1) and (2) express the conservation law in the **integral formulation**, and are characterized by two very important and desirable properties:

- 1. Conservation:** in absence of sources, the variation of  $\phi$  and  $\mathbf{u}$  is only due to fluxes across the boundary  $\partial\Omega$ , and **no** flux is created inside  $\Omega$   
⇒ both **local** and **global** conservation
- 2. Generality:** the integral form remains valid even in presence of shocks and discontinuity

NOTE: Because of these properties, historically, the **majority of the CFD** codes is based on the integral form of the governing equations (e.g. Ansys Fluent, OpenFOAM ...)

The **integral form** is essentially the **finite volume** formulation.

# Important tools (for life)



# Eulerian vs Lagrangian approach

## Eulerian description of a plastic duck race

We sit on the banks of a river, watching the flow go by, from the point of view which is fixed in space. We see **how many** plastic ducks pass by.

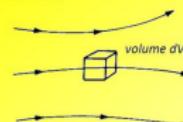
## Lagrangian description of a plastic duck race

We float in the river, so the point of view moves in space together with the flow. We might imagine to follow **each** plastic duck along its way.



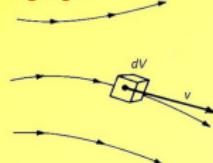
### Difference from the Lagrangian approach:

#### Eulerian



Infinitesimal fluid element  
fixed in space with the fluid  
moving through it

#### Lagrangian



Infinitesimal fluid element  
moving along a streamline  
with the velocity V equal to the  
local flow velocity at each point

Source: (left) <https://www.miathletic.com> (right) <http://slideplayer.com/slide/4670736/>

# The material derivative: a physical interpretation I

In a **Lagrangian** coordinate system, a scalar is represented by:

$$\phi = \phi(t, \mathbf{x}(t))$$

(think about temperature, or chemical concentration etc.), where the position vector is

$$\mathbf{x} = [x, y, z]$$

The velocity is analogously represented by a **vector field**:

$$\mathbf{v} = \mathbf{v}(t, \mathbf{x}(t)) = [u, v, w]$$

Note that the position vector is as well **time-dependent**.

## The material derivative: a physical interpretation II

The **material** (or “total”, “substantial” ... there are many names) derivative with respect to **time** of  $\phi$  is obtained using the **chain rule**:

$$\frac{d}{dt}\phi(t, \mathbf{x}(t)) = \frac{\partial\phi}{\partial t} + \frac{\partial\phi}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial\phi}{\partial y}\frac{\partial y}{\partial t} + \frac{\partial\phi}{\partial z}\frac{\partial z}{\partial t}$$

But we can note the following are **vector quantities**:

$$\left[ \frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z} \right] = \nabla\phi$$

$$\left[ \frac{\partial x}{\partial t}, \frac{\partial y}{\partial t}, \frac{\partial z}{\partial t} \right] = \mathbf{v}$$

Thus we can write the material derivative more compactly using a **scalar product** between the two vectors:

$$\underbrace{\frac{d}{dt}\phi(t, \mathbf{x}(t))}_{\text{Lagrangian (material) derivative}} = \underbrace{\frac{\partial\phi}{\partial t}}_{\text{Eulerian derivative}} + \underbrace{\mathbf{v} \cdot \nabla\phi}_{\text{Convective term}}$$

## Divergence theorem (Gauss theorem)

“The sum of all sources and sinks is equal to the net flux out of a region”:

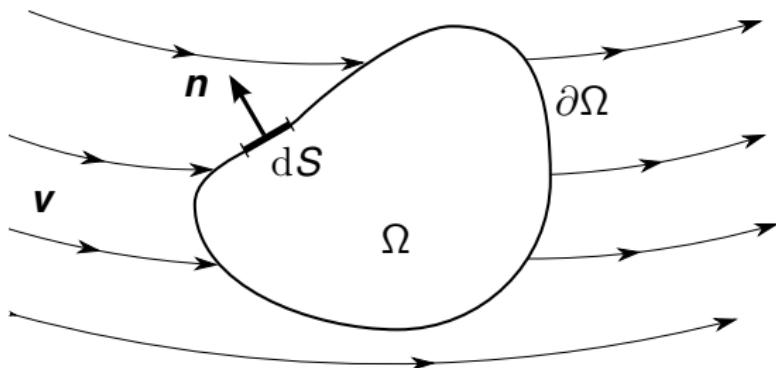
$$\int_{\Omega} (\nabla \cdot \mathbf{F}) dV = \int_{\partial\Omega} (\mathbf{F} \cdot \mathbf{n}) dS \quad (3)$$

In other words, if we want to calculate the **net flux** of any quantity that enter and exit some region of space, i.e. crossing the **surface**, we can compute this desired quantity by checking the **divergence** of that quantity contained in the **volume** of the region.

# The continuity equation

# Derivation: continuity equation

Keep in mind our control volume  $\Omega$ :



# Derivation: continuity equation

We consider the conservation of **mass**:

1. No creation or disappear of mass (no sources or sinks)
2. Single-phase fluids
3. No diffusive flux (e.g., for a fluid at rest, a variation in mass would imply a displacement of fluid)
4. The **density**  $\rho$  is the conserved quantity

Then, by using the conservation law for a scalar (1) on our control volume  $\Omega$  we have the **integral form** of the continuity equation:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho d\Omega + \oint_{\partial\Omega} \rho (\mathbf{v} \cdot \mathbf{n}) dS = 0 \quad (4)$$

NOTE: The positive outwarding convention is used: **inflow** for flow negative flow, **outflow** for positive

# The momentum equation

## Derivation: momentum equation I

It is basically the statement of **Newton's second law**: the variation of momentum is caused by the sum of the net forces on the mass element.

We consider the conservation of the **momentum** in the infinitesimal portion of the control volume  $\rho \mathbf{v} d\Omega$ :

1. In the Cartesian coordinate system, the product  $\rho \mathbf{v}$  has **three components**

$$\rho \mathbf{v} = [\rho u, \rho v, \rho w]^T$$

2. The **convective flux tensor**  $\bar{\bar{F}}_C$  have the following three components:

$$x : \rho u \mathbf{v}$$

$$y : \rho v \mathbf{v}$$

$$z : \rho w \mathbf{v}$$

3. No diffusive flux (e.g., for a fluid at rest, a variation in momentum would imply a displacement of fluid)

## Derivation: momentum equation II

We now consider the **forces** acting on the fluid element

- External volume or body forces:** act directly on the mass (e.g. gravitational, buoyancy, Coriolis, centrifugal, electromagnetic)

$$\mathbf{Q}_V = \rho \mathbf{f}_e$$

- Surface forces:** act on the surface of the control volume

- ▶ **Pressure distribution:** isotropic  $-p\bar{\mathbf{I}}$

- ▶ **Normal and shear stresses due to friction:** **viscous stress tensor**  $\bar{\tau}$

Then, by using the conservation law for a vector (2) on our control volume  $\Omega$  we have the **integral form** of the momentum equation:

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega} \rho \mathbf{v} d\Omega + \oint_{\partial\Omega} \rho \mathbf{v} (\mathbf{v} \cdot \mathbf{n}) dS = \\ \int_{\Omega} \rho \mathbf{f}_e d\Omega + \oint_{\partial\Omega} [-p \mathbf{n} + (\bar{\tau} \cdot \mathbf{n})] dS \end{aligned} \quad (5)$$

# The energy equation

## Derivation: energy equation I

It is basically the first law of thermodynamics: the change in time of the **total energy**  $E$  of our control volume is given by the rate of work done by applied forces and by the net heat flux

1. The conserved quantity is the **total energy per unit mass**  $\rho E$ , where  $E = e + |\mathbf{v}|^2/2$ , with  $e$  the internal energy per unit mass
2. Now we do have a **diffusive flux**

$$\mathbf{F}_D = -\gamma \rho \kappa \nabla e$$

which represents the diffusion of heat due to molecular thermal conduction, where  $\gamma = c_p/c_v$  is the ratio of specific heat coefficients.

3. Most commonly we use **Fourier's law**

$$\mathbf{F}_D = -k \nabla T$$

where  $k$  is the **thermal conductivity coefficient**

# Derivation: energy equation II

Other contributions to energy conservation:

## 1. Other heat sources:

- ▶ **rate of volumetric heating** (radiation, chemical ...)  $\dot{q}_h$
- ▶ **rate of work** by body forces  $\mathbf{f}_e$

thus the total **rate** of work by volume sources

$$\mathbf{Q}_V = \rho \mathbf{f}_e \cdot \mathbf{v} + \dot{q}_h$$

## 2. Surface sources: **rate** of work done by pressure, and normal and shear stresses

$$\mathbf{Q}_S = -p \mathbf{v} + \bar{\bar{\tau}} \cdot \mathbf{v}$$

## Derivation: energy equation III

Moreover, we use the relation for total enthalpy

$$H = E + \frac{p}{\rho}$$

Then, by using the conservation law for a scalar (1) on our control volume  $\Omega$  we have the **integral form** of the energy equation:

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega} \rho E d\Omega + \oint_{\partial\Omega} \rho H (\mathbf{v} \cdot \mathbf{n}) dS &= \oint_{\partial\Omega} k (\nabla T \cdot \mathbf{n}) dS + \\ &\quad \int_{\Omega} (\rho \mathbf{f}_e \cdot \mathbf{v} + \dot{q}_h) d\Omega + \oint_{\partial\Omega} (\bar{\tau} \cdot \mathbf{n}) dS \end{aligned} \tag{6}$$

# Comments on viscous stresses I

If we don't consider the viscous stress tensor  $\bar{\tau}$ , we deal with **Euler equations**, or **inviscid** flow:

- ▶ Hyperbolic system
- ▶ Pure convection in inviscid fluid, good approximation in high-speed flow
- ▶ Used to describe shocks, expansion waves
- ▶ Typically, base for development of discretization methods and boundary conditions



Leonhard Euler  
1707–1783

Source: <https://en.wikipedia.org>

# Different “types” of viscosity

## Different “types” of viscosity

The effect of viscosity is to **dissipate the energy** of the system, however it is useful do distinguish between different “types of viscosity” that have different origin:

- ▶ Dynamic viscosity  $\mu$
- ▶ Kinematic viscosity  $\nu$
- ▶ Bulk viscosity  $\lambda$
- ▶ Turbulent viscosity  $\nu_t$
- ▶ Artificial viscosity
- ▶ Numerical viscosity

# Dynamic viscosity (Newton's third law)

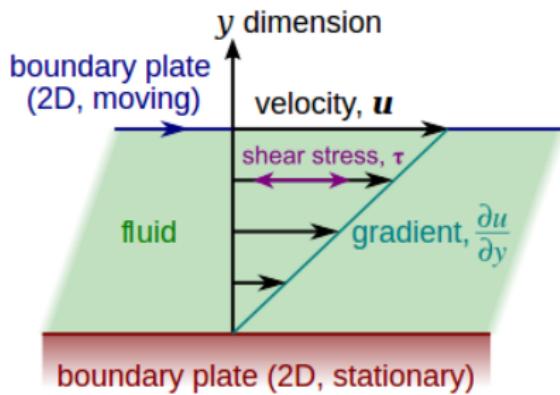
Newton introduced the **dynamic** (or shear) viscosity  $\mu$ :

$$\tau = \frac{F}{A} = \mu \frac{\partial u}{\partial y}$$

where

$$\tau = [\text{Pa}]$$

$$\mu = [\text{Pa} \cdot \text{s}]$$



Note: the flow is **laminar**, and the derivative is taken in the **orthogonal** direction

Source: <https://en.wikipedia.org>

Due to **cohesive forces** within the fluid, the latter exerts an equal and opposite force  $F$  to the shear stress between the fluid layer. This force  $F$  is associated to the **dynamic** viscosity  $\mu$  as  $F = \mu A u / y$ . Note:  $\mu$  is a property of the fluid.

# Kinematic viscosity

The **kinematic** viscosity  $\nu$  is simply defined as:

$$\nu = \frac{\mu}{\rho} = \left[ \frac{m^2}{s} \right]$$

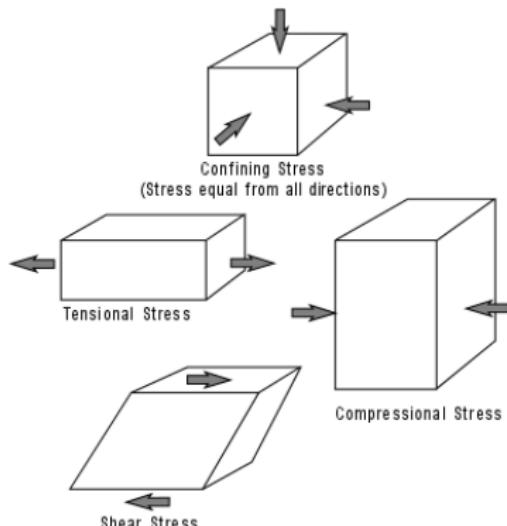
It is often used in defining the **Reynolds** number:

$$Re = \frac{D u \rho}{\mu} = \frac{D u}{\nu} = \frac{\text{Inertial forces}}{\text{Viscous forces}}$$

Where  $D, u$  are characteristic length and velocity, respectively. The kinematic viscosity  $\nu$  is also called "**momentum diffusivity**": it can be interpreted as the capacity of the fluid of **transferring momentum through the shear stress**.

# Bulk viscosity

The **bulk** (or volume, or second) viscosity  $\lambda$  is related to **compressibility effects**. It measures the effect of viscous forces depending on the **rate** of dilatation or compression, when no shear is present.



Compressible  $\Rightarrow \rho = \rho(\mathbf{x}, t)$

Incompressible  $\Rightarrow \rho = \text{constant}$

The bulk viscosity is often neglected for **incompressible fluids**.

Source: <http://www.tulane.edu/~sanelson/eens1110/deform.htm>

## Comments on viscous stresses II

The fluid is considered as **Newtonian**:

- ▶ the shear stress depends on the **velocity gradient**  $\tau_{ij} \sim \mu \partial u_i / \partial x_j$ , where  $\mu$  is the **dynamic viscosity**
- ▶ Stokes introduced the hypothesis for the **bulk viscosity**  
 $\lambda + 2/3\mu = 0$ , where  $\lambda$  is the second viscosity coefficient
- ▶ Coefficients  $\mu$  and  $k$  are **functions of the state** of the fluid: in continuum mechanics, these are determined by **empirical assumptions**



Claude-Louis  
Navier  
1785–1836



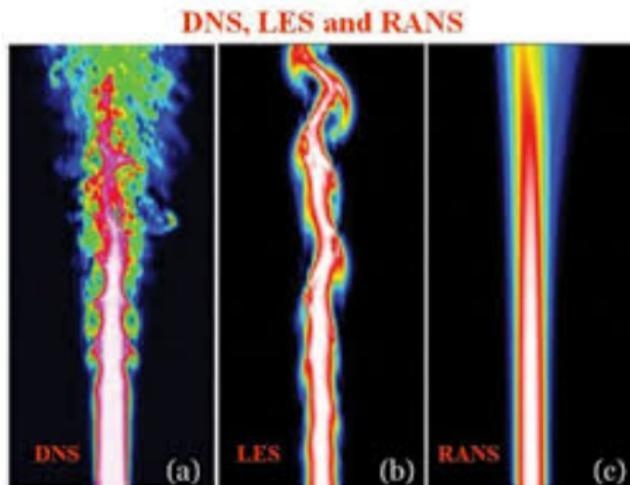
George Stokes  
1819–1903

Source: <https://en.wikipedia.org>

All these are **approximations** used to derive the NS equations. Thus, we need to remember that the NS are a very accurate description of the reality, but still they are a **model** of it

# Turbulent viscosity

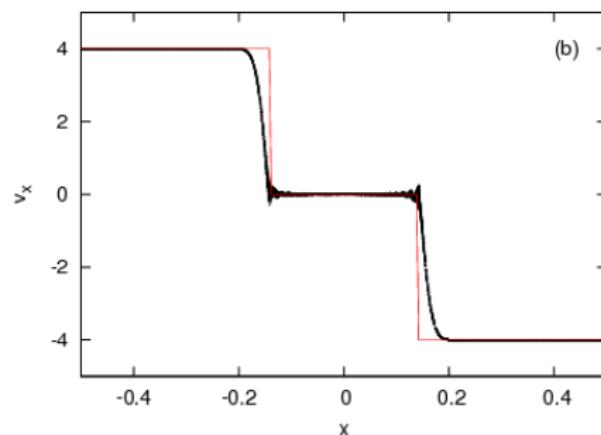
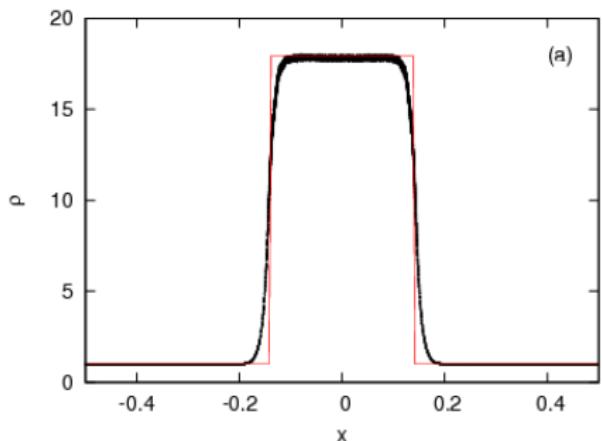
When **modelling the turbulence**, we choose to approximate the effect of **dissipation of energy** of the flow. We basically calculate an additional **turbulent viscosity**  $\nu_t$



Source: <http://www.uttei.enea.it/>

# Artificial viscosity

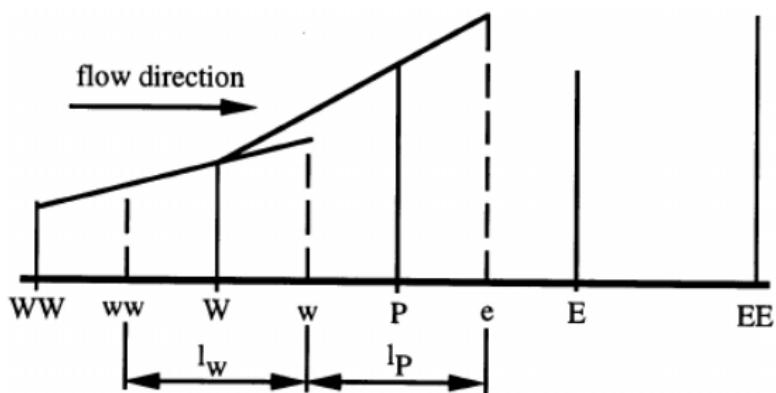
In capturing of high-gradients and discontinuities (shocks), sometimes **artificial viscosity** is added **locally** in order to dissipate the non-physical oscillations of the numerical solution.



Source: <http://inspirehep.net/record/886603/plots>

# Numerical viscosity

This is **(un)wanted** viscosity due to the used **discretization** (numerical scheme and mesh). For example, the **up-wind** approximation for the derivative adds a certain amount of **numerical viscosity** (remember the linear advection example in 1D)



# Discretization techniques

If not considering analytical methods, which are only viable for few simplified problems, we can say that almost all numerical strategies follow the **same workflow**:

**1.** Discretization of space:

- ▶ Finite Difference (FD)
- ▶ Finite Volumes (FV)
- ▶ Finite Elements (FE)
- ▶ Spectral methods, hybrid, Boundary Element Method (BEM) .....

**2.** Advancement in time:

- ▶ Typically, some kind of Finite Difference method (implicit/explicit methods ...)

**3.** We get a **system of equations**:  $\mathbf{A} \mathbf{x} = \mathbf{b}$ , that we input in the computer

# Forms of the governing equations I: integral form

We derived the governing system of equations in the **integral form**, since it is naturally suited for Finite Volume discretizations:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho d\Omega + \oint_{\partial\Omega} \rho (\mathbf{v} \cdot \mathbf{n}) dS = 0 \quad (\text{Continuity eq})$$

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega} \rho \mathbf{v} d\Omega + \oint_{\partial\Omega} \rho \mathbf{v} (\mathbf{v} \cdot \mathbf{n}) dS = \\ \int_{\Omega} \rho \mathbf{f}_e d\Omega + \oint_{\partial\Omega} [-\rho \mathbf{n} + (\bar{\tau} \cdot \mathbf{n})] dS \end{aligned} \quad (\text{Momentum eq})$$

$$\frac{\partial}{\partial t} \int_{\Omega} \rho E d\Omega + \dots \quad (\text{Energy eq})$$

However it is possible to derive the **differential form** of the equations, using some tools of calculus...

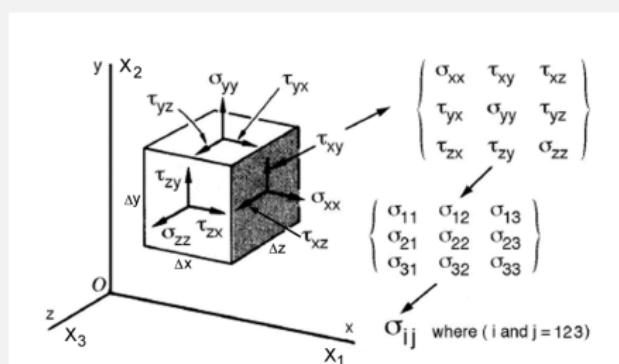
# Some important tools from calculus

# Important tools I

## Tensors

A tensor is a **generalization** of the concept of vector. Examples for tensors of different order are:

- ▶ **Order 0:** scalar values, e.g. the pressure, temperature etc.
- ▶ **Order 1:** vector fields, e.g. velocity  $\mathbf{v} = [u, v, w]^\top$
- ▶ **Order 2:** e.g. elasticity tensor, stress tensor:  $\tau_{ij} = \begin{bmatrix} \tau_{11} & \tau_{12} & \tau_{13} \\ \tau_{21} & \tau_{22} & \tau_{23} \\ \tau_{31} & \tau_{32} & \tau_{33} \end{bmatrix}$



Source:

<http://www.esm.rkriz.net/classes/ESM4714/methods/EEG.html>

# Important tools III

## Gradient

It is a **generalization of the concept of derivative** for functions with multiple variables. It is a **vector valued** function. Physically, it gives the **tangent to the slope of a function**. It “**rises by one**” the order of the object (tensor):

$$\text{From scalar to vector: } \nabla p = \text{grad}(p) = \left[ \frac{\partial p}{\partial x}, \frac{\partial p}{\partial y}, \frac{\partial p}{\partial z} \right]^T$$

$$\text{From vector to tensor: } \nabla \mathbf{v} = \text{grad}(\mathbf{v}) = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial v}{\partial x} & \frac{\partial w}{\partial x} \\ \frac{\partial u}{\partial y} & \frac{\partial v}{\partial y} & \frac{\partial w}{\partial y} \\ \frac{\partial u}{\partial z} & \frac{\partial v}{\partial z} & \frac{\partial w}{\partial z} \end{bmatrix}$$

# Important tools II

## Divergence

It is a **vector** operation. Physically, gives us information on the “**volume concentration**” of flux. This operator “**lowers by one**” the order of the object (tensor):

$$\text{From vector to scalar: } \nabla \cdot \mathbf{v} = \text{div}(\mathbf{v}) = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$$

$$\text{From tensor to vector: } \nabla \cdot \boldsymbol{\tau}_{ij} = \text{div}(\boldsymbol{\tau}_{ij}) = \begin{bmatrix} \frac{\partial \tau_{11}}{\partial x} + \frac{\partial \tau_{21}}{\partial y} + \frac{\partial \tau_{31}}{\partial z} \\ \frac{\partial \tau_{12}}{\partial x} + \frac{\partial \tau_{22}}{\partial y} + \frac{\partial \tau_{32}}{\partial z} \\ \frac{\partial \tau_{13}}{\partial x} + \frac{\partial \tau_{23}}{\partial y} + \frac{\partial \tau_{33}}{\partial z} \end{bmatrix}$$

## Forms of the governing equations II: differential form

However, we can obtain the **differential form**, for using other discretizations methods.

We apply the divergence theorem (3) to surface integrals, and Leibniz integral rule for time derivative, and we get the **differential, conservative form**:

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

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = \rho \mathbf{f}_e - \nabla p + \nabla \cdot \bar{\tau} \quad (8)$$

$$+ \text{Energy equation differential} \quad (9)$$

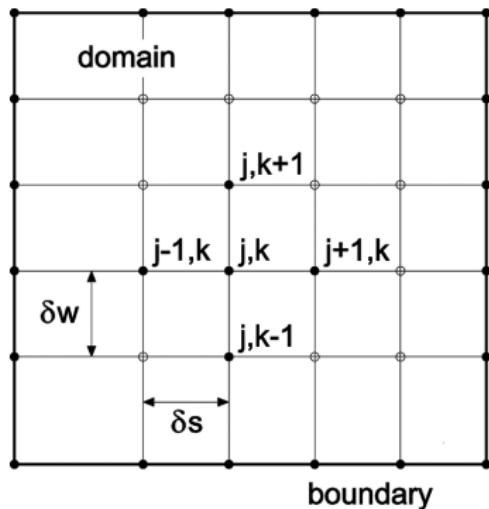
The symbol  $\mathbf{v} \otimes \mathbf{v}$  or just simply  $\mathbf{v}\mathbf{v}^T$  (*without the dot*) stays for **outer (or dyadic)**

**product:**  $\mathbf{v} \otimes \mathbf{v} = \mathbf{v}\mathbf{v}^T = \begin{bmatrix} uu & uv & uw \\ vu & vv & vw \\ wu & wv & ww \end{bmatrix}$

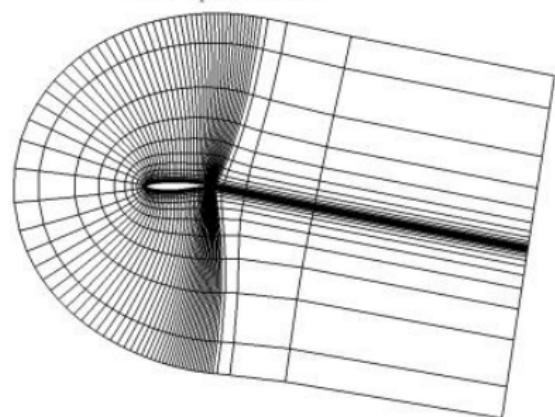
# Space discretization: Finite differences

# Finite difference (FD) method I

- ▶ Historically the first used for partial differential equations (used by Euler, 1768)
- ▶ Uses the **differential form** of the equations (7)–(9)
- ▶ Typically uses a regular **structured grids**: either regular (left), or curvilinear (right) grid:



Example C-Grid



Source: (left) "Comparison Between a Meshless Method and the Finite Difference Method for Solving the Reynolds Equation in Finite Bearings" (right) <http://www.innovative-cfd.com/cfd-grid.html>

# Finite difference (FD) method II

The FD is the method used in the 1D examples in Python we saw by Lorena A. Barba:

- ▶ Unknowns are placed at the **nodes** of the grid
- ▶ At each node of the grid, we approximate the derivatives in the PDE
- ▶ We can use Taylor expansions, or polynomial forms

# Finite difference (FD) method III

## Advantages:

- ▶ Relatively easy implementation
- ▶ Good results and efficiency on simple geometries
- ▶ Several high-order schemes available

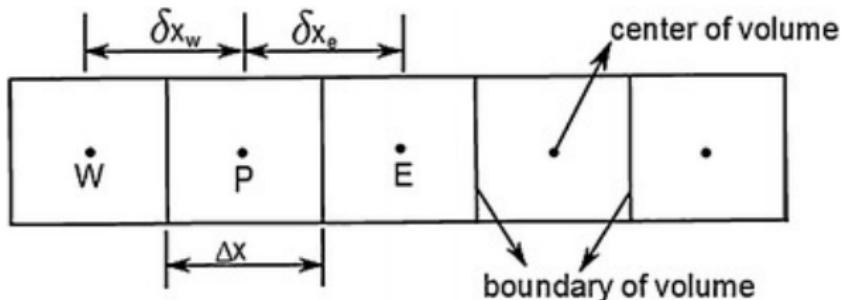
## Disadvantages:

- ▶ Generally limited to **structured** meshes
- ▶ Conservation property is **not guaranteed** in general
- ▶ For non uniform grids, a **coordinate transformation to the “computational space”** has to be considered and discretized consistently (Jacobian of coordinate transformation, from the chain rule)

# Space discretization: Finite volumes

# Finite Volume (FV) method I

- ▶ First used in CFD in 1972
- ▶ The space is divided into **arbitrary polyhedral** control volumes (CV): these are the elements of the mesh
- ▶ On **each control volume** we enforce the governing equations
- ▶ Thus, the **conservation** property holds both on each control volume **locally**, and **globally**: if we sum up the contributions of the different CVs, **telescopically** all the fluxes cancel out, and we recover the conservation equation over the **whole domain**



# Conservation property

## Meaning of “conservation property”:

We derived the Navier Stokes equations by using the **conservation laws** of mass, momentum and energy. The Finite Volume numerical method naturally **respects these laws**. Thus, in absence of sources or sinks, the amount of a conserved quantity leaving a closed volume is equal to the amount entering that volume. Essentially, the Finite Volume method **respects the physics**.



Source: <http://www.mne.psu.edu>

# Finite Volume (FV) method II

- ▶ Uses directly the **integral form** of the equations (4)–(6) as we have derived them:

$$\frac{\partial}{\partial t} \int_{\Omega} \mathbf{W} d\Omega + \oint_{\partial\Omega} (\mathbf{F}_C - \mathbf{F}_V) d\mathcal{S} = \int_{\Omega} \mathbf{Q} d\Omega$$

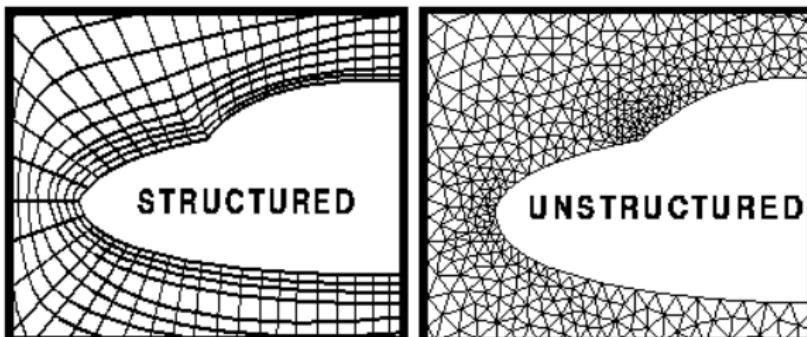
$$\mathbf{W} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} \quad \mathbf{F}_C = \begin{bmatrix} \rho \mathbf{V} \\ \rho u \mathbf{V} + n_x p \\ \rho v \mathbf{V} + n_y p \\ \rho w \mathbf{V} + n_z p \\ \rho H \mathbf{V} \end{bmatrix} \quad \mathbf{F}_V = \begin{bmatrix} 0 \\ \tau_{1j} \cdot \mathbf{n} \\ \tau_{2j} \cdot \mathbf{n} \\ \tau_{3j} \cdot \mathbf{n} \\ \Theta_{En} \cdot \mathbf{n} \end{bmatrix} \quad (10)$$

where  $\mathbf{V} = \mathbf{v} \cdot \mathbf{n}$  is the “contravariant velocity”

# Mesh types: structured vs unstructured

There are mainly **two** types of grids:

- ▶ **Structured** (left): each grid point is uniquely identified by indexes  $i, j, k$ ; elements are quadrilaterals (2D), or hexahedrons (3D), can be **curvilinear**
- ▶ **Unstructured** (right): no particular ordering of the grid points; elements are a mixture of quadrilaterals and triangles (2D), or tetrahedrons, hexahedrons, prisms, pyramids, polyhedral ...

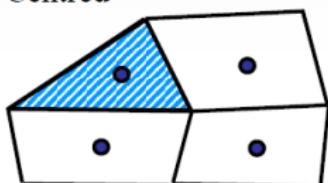


Source: <https://ntl.bts.gov/DOCS/ch5.html>

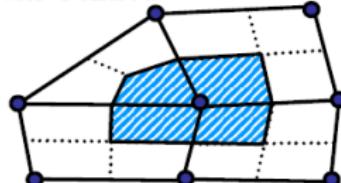
# Finite Volume (FV) method III

- ▶ **Two** classical types depending on the *location of the unknowns*: **cell-centred** and **vertex-centred** (also called *dual-control volume*)

Cell-Centred



Vertex-Centred



Source: <https://www.cfd-online.com>

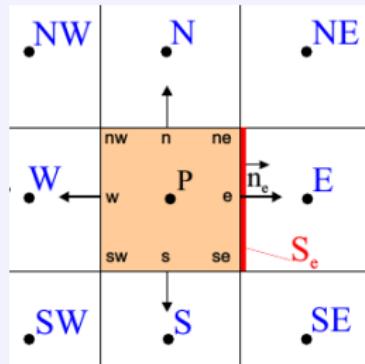
- ▶ **Volume integrals:** the classical FV is developed for 1st and 2nd order accuracy, although higher order approximations are available (using neighbouring nodes)
- ▶ **Surface integrals**, i.e. the **fluxes** crossing the individual faces of the control volume, are then approximated using **several schemes** with **varying accuracy, stability, efficiency**

# Finite volumes: approximation of integrals

# Volume integrals

# Approximation of volume integrals

$$\int_{\Omega} Q d\Omega = \bar{Q} \text{Vol}(\Omega) \approx Q_p \text{Vol}(\Omega)$$



Source: "Introduction to numerical simulation of fluid flows"

- Where  $Q$  is the **mean value** and  $Q_p$  the value of  $Q$  at the **control volume center**. This approximation is exact if  $Q$  is either **constant or linear** within the CV; otherwise is of **second order**
- Higher order** approximation requires the values of  $Q$  at **more locations** than just the center of the control volume: we need also to compute the solution at the locations  $w, nw, n, ne, e, se, s, sw$  (see Figure above)

# Surface integrals

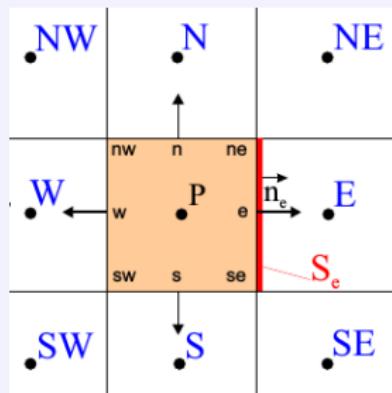
# Approximation of surface integrals

$$\int_{\partial\Omega} F dS = \sum_k \int_{S_k} F dS$$

where  $\partial\Omega = \cup S_k$ .

For each face  $S_k$  we approximate

$$\int_{S_k} F dS = \bar{F} \text{Area}(S_k) \approx F_p \text{Area}(S_k)$$



Source: "Introduction to numerical simulation of fluid flows"

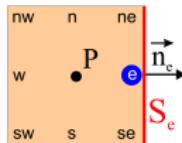
As for volume integrals, we need to find some **point values**  $F_p$  for approximating the mean value  $\bar{F}$

# Approximation of surface integrals

**Supposing that we know** the values at various points  $ne$ ,  $e$ ,  $se$  of the **east face**  $S_e$ :

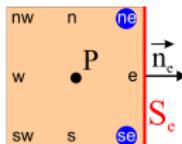
- ▶ Midpoint rule,  $\mathcal{O}(\Delta x^2)$ :

$$\int_{S_e} F dS = \bar{F}_e \text{Area}(S_e) \approx F_e \text{Area}(S_e)$$



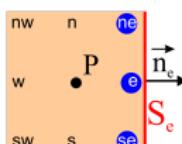
- ▶ Trapezoidal rule,  $\mathcal{O}(\Delta x^2)$ :

$$\int_{S_e} F dS = \bar{F}_e \text{Area}(S_e) \approx \left( \frac{F_{ne} + F_{se}}{2} \right) \text{Area}(S_e)$$



- ▶ Simpson rule,  $\mathcal{O}(\Delta x^4)$ :

$$\int_{S_e} F dS = \bar{F}_e \text{Area}(S_e) \approx \left( \frac{F_{ne} + 4F_e + F_{se}}{6} \right) \text{Area}(S_e)$$



Source: "Introduction to numerical simulation of fluid flows"

# Two kinds of approximation

## Two kinds of approximation

Conceptually, in FV there are **two types of approximations** made, *both* for volume and for surface integrals:

- ▶ **Approximation I:** we actually don't know how to compute the mean value  $\bar{Q}$ , we have to **approximate by some quadrature** formula, i.e. using *point values*  $Q_p$
- ▶ **Interpolation II:** we usually don't know the point values  $Q_w, Q_{nw}, Q_n, Q_{ne}$  etc, but they have to be **interpolated** from the (known) nodal values  $Q_p$  from the **centres of the cells** (this cell and the neighbours)

$$\int_{\Omega} Q d\Omega = \bar{Q} \text{Vol}(\Omega) \stackrel{\text{I+II}}{\approx} Q_p \text{Vol}(\Omega)$$

# Approximation of surface integrals

- ▶ **Surface integrals:** we can use different “treatments” for convective and viscous fluxes. However, the real “bestiary” is for the **convective fluxes**.
- ▶ We just name some flux approximation schemes in CFD, as are typical choices that the user has to face:
  - ▶ **Centered schemes:** based on central difference formulae; more efficient but has stability issues
  - ▶ **Upwind schemes:** based on the physical properties of the Euler equations; more computation required (needed “limiters” to eliminate spurious oscillations) but more stable and capable to capture discontinuities. We name: flux-vector splitting, flux-difference splitting, total variation diminishing ...

# Finite Volume (FV) method V

## Advantages:

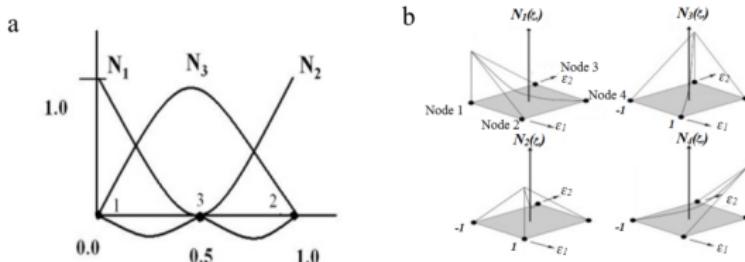
- ▶ Directly apply the integral spatial discretization in the **physical space** (no coordinate transformation to a computational space, unlike FD and typically FEM)
- ▶ Flexible for complex geometries: both structured and un-structured meshes
- ▶ Mass, momentum and energy are **conserved** by definition

## Disadvantages:

- ▶ Historically, less developed mathematical framework (i.e. compared to FEM)
- ▶ More difficult to attain high-order accuracy (compared to FD and FEM), specially for unstructured meshes

# Space discretization: Finite elements

# Finite Element (FEM) method I



- ▶ First used in 1956
- ▶ Historically for structure analysis, but since the '90 also in CFD
- ▶ Typically, we employ an unstructured mesh
- ▶ Choice of **weight** and **shape** functions  
→ an **integral formulation** equivalent to the differential form is solved!
- ▶ Usually **combined** with FV (boundary, viscous fluxes)

# Finite Element (FEM) method II

## Advantages:

- ▶ Integral formulation: valid for shocks and discontinuities
- ▶ Flexible for complex geometries
- ▶ Straightforward high-order
- ▶ Very rigorous mathematical foundation

## Disadvantages:

- ▶ Higher computational effort
- ▶ Conservation not always guaranteed

# Finite Element (FEM) method III

NOTE: For the one-dimensional case, it can be shown that the FD, FV and FEM are **mathematically equivalent!**

# Time discretization

As mentioned, in CFD, **different** discretizations are employed for space and time (“method of lines”).

We only mention some important time schemes in CFD, as are typical choices that the user has to face:

1. Advancement in time, typically, some kind of Finite Difference method
2. **Explicit methods:** in general, more efficient since all the equation is put on the Right Hand Side and no matrix need to be solved, **but less stable** (Multistage methods (Runge-Kutta), local time stepping, **multigrid...**)
3. **Implicit methods:** in general, higher computational cost due to matrix inversion, but **more stable** and significantly larger time steps can be used (dual time stepping, iterative solvers, preconditioning ...)

# Considerations on accuracy

# Considerations on accuracy I

Three types of **systematic** errors:

1. **Model error:** difference between the real problem and the chosen model equations
2. **Discretization error:** difference between the exact solution of the model equations and the exact solution of the discretized system
3. **Convergence error:** difference between the exact solution of the discretized system and the solution obtained iteratively

Some are dominant on the others, depending on the problem, and sometimes they can even compensate (e.g. have a more accurate solution on a coarser mesh)!