# OpenFOAM course, part 1: theoretical foundations of finite volume approach

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- To work in CFD, one needs a solid background in both fluid mechanics and numerical analysis; significant errors have been made by people lacking knowledge in one or the other.
- Estimation of numerical errors. A qualitatively incorrect solution of a problem may look reasonable (it may even be a good solution of another problem), the consequences of accepting it may be severe.

Computational Methods for Fluid Dynamics.

*Professor Joel H. Ferziger, Dr. Milovan Perić*

"OpenFOAM is first and foremost a C++ library, used primarily to create executables, known as applications."

OpenFOAM User Guide

# Conservation principles

Conservation laws can be derived by considering a given quantity of matter or *control mass* (CM) and its *extensive* properties, such as mass, momentum and energy.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega_{\mathrm{CM}}} \phi\rho\,\mathrm{d}\Omega = \mathit{zero}(\mathbf{0}) \quad + \text{ sources } + \text{ flows through boundaries}$$

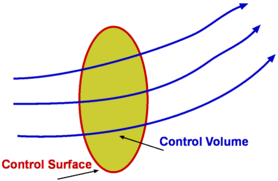
The conservation equation for mass:

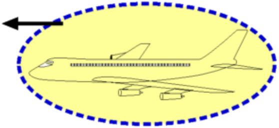
$$\frac{\mathrm{d}m}{\mathrm{d}t} = 0 \; . \tag{1}$$

On the other hand, momentum can be changed by the action of forces and its conservation equation is Newton's second law of motion:

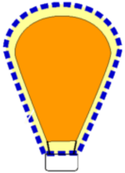
$$\frac{\mathrm{d}(m\vec{v})}{\mathrm{d}t} = \sum \vec{F} \; , \tag{2}$$

where $t$ stands for time, $m$ for mass, $\vec{v}$ for the velocity, and $\vec{f}$ for forces acting on the control mass.



A moving Control Volume around a moving Aeroplane.

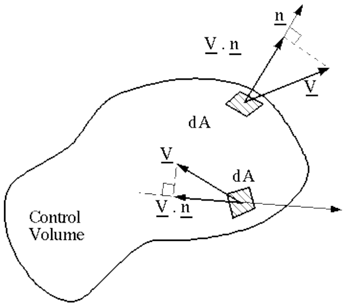


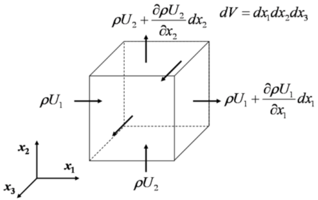
A collapsible Control Volume around a balloon.

CM approach is used to study the dynamics of solid bodies, where the CM (sometimes called the *system*) is easily identified.

In fluid flows, however, it is difficult to follow a parcel of matter. It is more convenient to deal with the flow within a certain spatial region we call a *control volume* (CV), rather than in a parcel of matter which quickly passes through the region of interest. This method of analysis is called the *control volume approach*.

# Closer look to control volume



$\phi$ – conserved intensive property (for mass conservation, $\phi = 1$; for momentum conservation, $\phi = \vec{v}$; for conservation of a scalar, $\phi$ represents the conserved property per unit mass) The corresponding extensive property $\Phi$ can be expressed as:

$$\Phi = \int\limits_{\Omega_{\mathrm{CM}}} \rho\phi \, \mathrm{d}\Omega \, , \tag{3}$$

$\Omega_{\mathrm{CM}}$ stands for volume occupied by the CM
LHS of each conservation equation for a control volume can be written:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega_{\mathrm{CM}}} \rho\phi \, \mathrm{d}\Omega = \frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega_{\mathrm{CV}}} \rho\phi \, \mathrm{d}\Omega + \int\limits_{S_{\mathrm{CV}}} \rho\phi \, (\vec{v} - \vec{v}_{\mathrm{b}}) \cdot \vec{n} \, \mathrm{d}S \, , \tag{4}$$

$\Omega_{\mathrm{CV}}$ is the CV volume, $S_{\mathrm{CV}}$ is the surface enclosing CV,
$\vec{n}$ is the unit vector orthogonal to $S_{\mathrm{CV}}$ and directed outwards,
$\vec{v}_{\mathrm{b}}$ is the velocity with which the CV surface is moving.
For fixed CV $\vec{v}_{\mathrm{b}} = \vec{0}$, first derivative on the RHS becomes a local (partial).
The last term is usually called the *convective* (or sometimes, advective) flux of $\phi$ through the CV boundary.

If CV does not change in time $v_b = 0$, $\frac{\partial}{\partial t}\Big|_{CV} = \frac{\partial}{\partial t}$:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega_{\mathrm{CM}}} \rho\phi \,\mathrm{d}\Omega = \int\limits_{\Omega_{\mathrm{CV}}} \frac{\partial}{\partial t}(\rho\phi)\,\mathrm{d}\Omega + \int\limits_{S_{\mathrm{CV}}} \rho\phi\,(\vec{v}, \vec{n})\,\mathrm{d}S \;= \tag{5}$$

*(Homework: Consider "Differentiation under the integral sign" https://en.wikipedia.org/wiki/Differentiation_under_the_integral_sign and describe its connection to differentiation over CM and to Reynolds Transport Theorem.)*

$$= \int\limits_{\Omega_{\mathrm{CV}}} \left[\frac{\partial}{\partial t}(\rho\phi) \;+ \mathrm{div}\,(\rho\phi\vec{v})\right] \mathrm{d}\Omega \tag{6}$$

# Mass Conservation

$$\phi \to 1 \tag{7}$$

$$\frac{\partial}{\partial t}\int_{\Omega} \rho \, \mathrm{d}\Omega + \int_{S} \rho \vec{v} \cdot \vec{n} \, \mathrm{d}S = 0 \, . \tag{8}$$

By applying the Gauss-Ostrogradsky divergence theorem to the convection term, we can transform the surface integral into a volume integral. Allowing the control volume to become infinitesimally small leads to a differential coordinate-free form of the continuity equation:

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\left(\rho \vec{v}\right) = 0 \, . \tag{9}$$

# Momentum Conservation

$$\phi \to \vec{v} \tag{10}$$

$$\frac{\partial}{\partial t}\int_{\Omega}\rho\vec{v}\,\mathrm{d}\Omega + \int_{S}\rho\vec{v}(\vec{v},\vec{n})\,\mathrm{d}S = \sum \vec{F}\,. \tag{11}$$

To express the right hand side in terms of intensive properties, one has to consider the forces which may act on the fluid in a CV:

- body forces (gravity, centrifugal and Coriolis forces, electromagnetic forces, etc.).
- surface forces (pressure, normal and shear stresses, surface tension etc.);

# Momentum Conservation

$$\frac{\partial}{\partial t}\int_{\Omega}\rho\vec{v}\,\mathrm{d}\Omega + \int_{S}\rho\vec{v}(\vec{v},\vec{n})\,\mathrm{d}S = \int_{\Omega}\vec{f}\rho\,\mathrm{d}\Omega + \int_{S}\vec{\sigma}_n\,\mathrm{d}S\ . \qquad (12)$$

$\vec{f}$ – body mass forces per unit of mass, $\sigma_{\vec{n}}$ – surface forces per unit of area. $\sigma_{\vec{n}} = \vec{\sigma}^i n_i$, $\vec{\sigma}^i$ – surface forces per unit of area on $i$-th coordinate plane.

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$$\int_{\Omega}\left(\frac{\partial}{\partial t}(\rho\vec{v})+\nabla_{i}(\rho\vec{v}v^{i})\right)\,\mathrm{d}\Omega=\int_{\Omega}\left(\vec{f}\rho+\nabla_{i}\vec{\sigma}^{i}\right)\,\mathrm{d}\Omega\ . \tag{14}$$

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$$\int_\Omega \left(\frac{\partial}{\partial t}(\rho\vec{v}) + \nabla_i(\rho\vec{v}v^i)\right)\,\mathrm{d}\Omega = \int_\Omega \left(\vec{f}\rho + \nabla_i\vec{\sigma}^i\right)\,\mathrm{d}\Omega\,. \qquad (14)$$

$$\frac{\partial}{\partial t}(\rho\vec{v}) + \nabla_i(\rho\vec{v}v^i) = \vec{f}\rho + \nabla_i\vec{\sigma}^i. \qquad (15)$$

# Scalar Conservation

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla_i(\rho\phi v^i) = \sum F_\phi \tag{16}$$

$F_\phi$ – sources and fluxes through boundaries
Diffusive transport is always present (even in stagnant fluids), and it is usually described by a gradient approximation, e.g. *Fourier's law* for heat diffusion and *Fick's law* for mass diffusion:

$$f_\phi^{\mathrm{d}} = \int_S \Gamma \,\mathrm{grad}\,\phi \cdot \vec{n}\,\mathrm{d}S \ , \tag{17}$$

where $\Gamma$ is the diffusivity for the quantity $\phi$.

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Fluid is a substance that continually deforms (flows) under an applied shear stress.
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In viscous compressible fluid (second viscosity assumed to be 0):

$$\sigma^{ik} = -\left(p + \frac{2}{3}\mu \operatorname{div} \vec{v}\right) g^{ik} + 2\mu e^{ik} \tag{21}$$

# Difference between solids and fluids

An ideal elastic solid will deform under load and, once the load is removed, will return to its original state. Some solids are plastic. These deform under the action of a sufficient load and deformation continues as long as a load is applied, providing the material does not rupture. Deformation ceases when the load is removed, but the plastic solid does not return to its original state.

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$$E = \mu\frac{3\lambda + 2\mu}{\lambda + \mu}, \quad \sigma = \frac{\lambda}{2(\lambda + \mu)} \tag{23}$$

# Differentianl equations of continuum media: *divergence* form

$$\frac{\partial \rho}{\partial t} + \nabla_i(\rho v^i) = 0 \tag{24}$$

$$\frac{\partial}{\partial t}(\rho v^k) + \nabla_i(\rho v^k v^i) = \nabla_i \sigma^{ik} + \rho f^k \tag{25}$$

$$\frac{\partial}{\partial t}(\rho \phi) + \nabla_i(\rho \phi v^i) = \sum f_\phi \tag{26}$$

Such a form is somtimes also called *conservation* form since as we will see in FV mehod integral quantities are conserved after space discretisation (decomposition to finite volumes).
So this form of equations is essential for OpenFOAM

## *Divergence* form of differentianl equations in tensor notation

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\,(\rho \vec{v}) = 0$$
$$\frac{\partial}{\partial t}(\rho \vec{v}) + \mathrm{div}\,(\rho \vec{v}\vec{v}) = \mathrm{div}\,\sigma + \rho \vec{f}$$
$$\frac{\partial}{\partial t}(\rho \phi) + \mathrm{div}\,(\rho \phi \vec{v}) = \sum f_\phi$$

$$\vec{v}\vec{v} \text{ means } \vec{v} \otimes \vec{v} = [v_i v_k] = \begin{bmatrix} v_1 v_1 & v_1 v_2 & v_1 v_3 \\ v_2 v_1 & v_2 v_2 & v_2 v_3 \\ v_3 v_1 & v_3 v_2 & v_3 v_3 \end{bmatrix}$$

$\mathrm{div}\,(\rho \vec{v}\vec{v})$ means $\mathrm{div}\,(\rho v^k \vec{v}) e_k$ ; $\mathrm{div}\,(\sigma)$ means $\nabla_i p^{ik} e_k$

Do you think that engeneers who uses OpenFOAM and commercial packages for years always understand it? **You're wrong!**