Computational Fluid Dynamics 1

Theory, Numerics, Modelling

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Computational Biomechanics

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Fluid phase system

State variables:

- Density ρ (1d)
- Velocity $\vec{u}$ (3d)
- Pressure p (1d)
- Energy e (1d)
- Temperature T (1d)

Physical laws:

- Mass conservation
- Momentum conservation
- Energy conservation
- Equation of state

Example for the equations of state:

$$p = \rho\, R_s\, T \qquad \text{and} \qquad e = c_\nu T$$

Reynolds transport theorem:

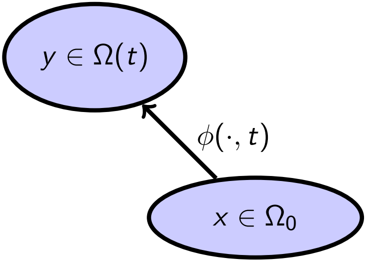
$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega(t)} f(x,t)\,\mathrm{d}\Omega = \int\limits_{\Omega(t)} \left\{ \frac{\partial f}{\partial t}(x,t) + \nabla \cdot (f\,\vec{u}) \right\} \mathrm{d}\Omega$$

For the proof:[1]
For A, Y quadratic matrices, if

$$\frac{\mathrm{d}}{\mathrm{d}t} Y(t) = A(t) \cdot Y(t)$$

holds, so does:

$$\frac{\mathrm{d}}{\mathrm{d}t} \det Y(t) = \mathrm{tr} A(t) \cdot \det Y(t)$$



[1] Skript 1994, Prof. Dr. J. Lorenz, RWTH-Aachen

Mass conservation:

Look at the mass m inside of an arbitrary volume $\Omega(t)$

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega(t)} \rho \, \mathrm{d}\Omega \overset{rtt}{=} \int\limits_{\Omega(t)} \left\{ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \, \vec{u}) \right\} \mathrm{d}\Omega \overset{!}{=} 0$$

Continuity equation:

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

Reynolds transport theorem:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega(t)} f(x,t) \, \mathrm{d}\Omega = \int\limits_{\Omega(t)} \left\{ \frac{\partial f}{\partial t}(x,t) + \nabla \cdot (f \, \vec{u}) \right\} \mathrm{d}\Omega$$

Momentum conservation:

Look at the momentum $\vec{p}$ inside of an arbitrary volume $\Omega(t)$

$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega(t)} \rho\vec{u}\,\mathrm{d}\Omega \overset{rtt}{=} \int\limits_{\Omega(t)} \left\{\frac{\partial\rho\vec{u}}{\partial t} + \nabla\cdot(\rho\,\vec{u}\,\vec{u})\right\}\mathrm{d}\Omega = \vec{F}$$

Force:

$$F = F_{\Omega} + F_{\partial\Omega} = \int\limits_{\Omega(t)} \rho\,\vec{f}\,\mathrm{d}\Omega + \int\limits_{\partial\Omega(t)} \underline{\underline{\sigma}}\,\vec{n}\,\mathrm{d}S$$

Reynolds transport theorem:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega(t)} f(x,t)\,\mathrm{d}\Omega = \int\limits_{\Omega(t)} \left\{\frac{\partial f}{\partial t}(x,t) + \nabla\cdot(f\,\vec{u})\right\}\mathrm{d}\Omega$$

Momentum conservation:

Handling the boundary force:

$$\int_{\partial\Omega(t)} \underline{\underline{\sigma}}\, \vec{n}\, \mathrm{d}S = \int_{\Omega(t)} \nabla \cdot \underline{\underline{\sigma}}\, \mathrm{d}\Omega \quad \text{with} \quad \nabla \cdot \underline{\underline{\sigma}} = \begin{pmatrix} \nabla \cdot \vec{\sigma}_1 \\ \nabla \cdot \vec{\sigma}_2 \\ \nabla \cdot \vec{\sigma}_3 \end{pmatrix}$$

Therefore we get:

$$\int_{\Omega(t)} \left\{ \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho\, \vec{u}\, \vec{u}) \right\} \mathrm{d}\Omega = \int_{\Omega(t)} \left\{ \rho\, \vec{f} + \nabla \cdot \underline{\underline{\sigma}} \right\} \mathrm{d}\Omega$$

Momentum equation:

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho\, \vec{u}\, \vec{u}) = \rho\, \vec{f} + \nabla \cdot \underline{\underline{\sigma}}$$

Momentum equation:

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho\, \vec{u}\, \vec{u}) = \rho\, \vec{f} + \nabla \cdot \underline{\underline{\sigma}}$$

Look on the left side:

$$\begin{aligned} \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho\, \vec{u}\, \vec{u}) &= \rho \frac{\partial \vec{u}}{\partial t} + \vec{u}\, \frac{\partial \rho}{\partial t} + \vec{u} \nabla \cdot (\rho\, \vec{u}) + (\rho\, \vec{u})\ \nabla \cdot \vec{u} \\ &= \rho \frac{\partial \vec{u}}{\partial t} + \vec{u}\, \left\{ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\, \vec{u}) \right\} + (\rho\, \vec{u} \cdot \nabla)\ \vec{u} \\ &= \rho \frac{\partial \vec{u}}{\partial t} + (\rho\, \vec{u} \cdot \nabla)\ \vec{u} \end{aligned}$$

Reminder continuity equation:

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

Energy equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)} \left\{\frac{1}{2}\rho\,|\vec{u}|^2 + \rho e\right\}\,\mathrm{d}\Omega = \int_{\Omega(t)} \left\{\rho\vec{f}\cdot\vec{u} + \rho\;Q\right\}\,\mathrm{d}\Omega + \int_{\partial\Omega(t)} \left\{\,\left(\underline{\underline{\sigma}}\;\vec{n}\right)\cdot\vec{u} + \kappa\,\nabla\;T\cdot\vec{n}\right\}\,\mathrm{d}S$$

According to:

- volume force: $\int_{\Omega(t)} \rho\;\vec{f}\cdot\vec{u}\,\mathrm{d}\Omega$
- energy source: $\int_{\Omega(t)} \rho\;Q\;\mathrm{d}\Omega$
- surface force: $\int_{\partial\Omega(t)} \left(\underline{\underline{\sigma}}\;\vec{n}\right)\cdot\vec{u}\,\mathrm{d}S$
- heat flux: $\int_{\partial\Omega(t)} \kappa\;\nabla\;T\cdot\vec{n}\,\mathrm{d}S$

System equations:

1. mass conservation

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

2. momentum conservation

$$\rho \frac{\partial \vec{u}}{\partial t} + (\rho \, \vec{u} \cdot \nabla) \; \vec{u} = \rho \, \vec{f} \; + \nabla \cdot \underline{\underline{\sigma}}$$

3. energy conservation

$$\rho \frac{\partial e}{\partial t} = \rho \; Q + \nabla \cdot (\kappa \; \nabla \; T\,) + \nabla \cdot \left(\underline{\underline{\sigma}} \; \vec{u}\right) - \left(\nabla \cdot \underline{\underline{\sigma}}\right) \vec{u}$$

4. equation of state (e.g. ideal gas equation)

The stress tensor $\underline{\underline{\sigma}}$:

$$\underline{\underline{\sigma}} = -p \cdot \mathbb{1} + \underline{\underline{\tau}} \qquad \text{with } \underline{\underline{\tau}} \text{ is the viscous stress tensor}$$

The viscosity term:

1. General viscous stress tensor:

$$\underline{\underline{\tau}} = F(D(t,x),t)$$

2. Strain rate tensor:

$$D := \frac{\partial \underline{\underline{\epsilon}}}{\partial t} = \frac{1}{2}\left[(\nabla\ \vec{u}) + (\nabla\ \vec{u})^T\right]$$

Behaviour of the viscous stress tensor:

$$\underline{\underline{\tau}} = F(D(t,x),t)$$

Time-dependent

- increase with time
  printer ink, synovial fluid
- decrease with time
  gelatin gels, yogurt

Time-independent

- shear thickening
  corn starch in water
- shear thinning
  ketchup, blood
- generalized newonian fluids
  water, blood plasma

Newtonian fluid:

$$\underline{\underline{\tau}} = \mu \cdot \left[(\nabla \ \vec{u}) + (\nabla \ \vec{u})^T \right] - \left(\frac{2}{3} \mu \nabla \cdot \vec{u} \right) \mathbb{1}$$

with the dynamic viscosity μ

Incompressible fluid assumption:

$$0 = \frac{\mathrm{d}\rho}{\mathrm{d}t}(x,t) = \frac{\partial}{\partial t}\rho(x,t) + \nabla\rho(x,t)\cdot\vec{u}$$

- Continuity equation:

$$\begin{aligned}\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\,\vec{u}\,) &= \frac{\partial\rho}{\partial t} + \nabla\rho\cdot\vec{u} + \rho\nabla\cdot\vec{u} \\ &= \rho\nabla\cdot\vec{u} = 0\end{aligned}$$

- It follows: $\nabla\cdot\vec{u} = 0$ (divergency free velocity field)
- Viscous stress tensor: (Newtonian fluid)

$$\underline{\underline{\tau}} = \mu\cdot\left[(\nabla\ \vec{u}) + (\nabla\ \vec{u})^T\right] - \cancel{\left(\frac{2}{3}\mu\nabla\cdot\vec{u}\right)}\,\mathbb{1}$$

Incompressible fluid + isothermal assumption:

From $T = const.$ with $\frac{\mathrm{d}}{\mathrm{d}t}\rho = 0$ follows:

1. Pressure is given with $p \sim \rho$ (equation of state)
2. Energy is a function of ρ and $\vec{u}$
   $\Rightarrow$ the energy conservation contains no extra information

For a newtonian fluid we get the Navier-Stokes equations as

Navier-Stokes equations

$$\nabla \cdot \vec{u} = 0 \tag{1}$$

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho \left(\vec{u} \cdot \nabla \right) \vec{u} = \rho \vec{f} - \nabla p + \mu \nabla \cdot \underline{\underline{\tau}} \tag{2}$$

Note: often, the kinematic viscosity $\nu := \frac{\mu}{\rho}$ is used if $\rho = const$

Application to biofluid systems

1. Human air system
    - Fluid-particle interaction
    - Fluid-structure interaction
    - Blood-air barrier
2. Human blood system
    - Oxygen transportation
    - Fluid-structure interaction
    - Transport of medicine
3. ...