Computational Fluid Dynamics
Theory, Numerics, Modelling

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Computational Biomechanics

Summer Term 2017
Fluid phase system

State variables:

\[
\begin{align*}
\text{Density} & \quad \rho \quad \text{(1d)} \\
\text{Velocity} & \quad \vec{u} \quad \text{(3d)} \\
\text{Pressure} & \quad p \quad \text{(1d)} \\
\text{Energy} & \quad e \quad \text{(1d)} \\
\text{Temperature} & \quad T \quad \text{(1d)}
\end{align*}
\]
Fluid phase system

**State variables:**
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- Velocity $\vec{u}$ (3d)
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**Physical laws:**
Fluid phase system

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Physical laws:
- Mass conservation
- Momentum conservation
- Energy conservation

Example for the equations of state:

\[ p = \rho R s T \]

\[ e = c \nu T \]
Fluid phase system

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- Density $\rho$ (1d)
- Velocity $\vec{u}$ (3d)
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**Physical laws:**
- Mass conservation
- Momentum conservation
- Energy conservation
- Equation of state

**Example for the equations of state:**

$$p = \rho R_s T \quad \text{and} \quad e = c_v T$$
Reynolds transport theorem:
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\[
\frac{\partial}{\partial t} \int_{\Omega(t)} f(x, t) \, d\Omega = \int_{\Omega(t)} \left\{ \frac{\partial f}{\partial t}(x, t) + \nabla \cdot (f \, \vec{u}) \right\} \, d\Omega
\]
Mass conservation:

\[ \frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega(t)} f(x, t) \, \mathrm{d}\Omega = \int_{\Omega(t)} \left\{ \frac{\partial f}{\partial t}(x, t) + \nabla \cdot (f \, \vec{u}) \right\} \, \mathrm{d}\Omega \]
Mass conservation:

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

\[
\frac{dm}{dt} = \frac{d}{dt} \int_{\Omega(t)} \rho \, d\Omega
\]

Reynolds transport theorem:

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\frac{d}{dt} \int_{\Omega(t)} f(x, t) \, d\Omega = \int_{\Omega(t)} \left\{ \frac{\partial f}{\partial t}(x, t) + \nabla \cdot (f \, \vec{u}) \right\} \, d\Omega
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Mass conservation:

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Reynolds transport theorem:

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\]

Continuity equation:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0
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Reynolds transport theorem:

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\frac{d}{dt} \int_{\Omega(t)} f(x, t) \, d\Omega = \int_{\Omega(t)} \left\{ \frac{\partial f}{\partial t}(x, t) + \nabla \cdot (f \vec{u}) \right\} \, d\Omega
\]
Momentum conservation:

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

$$\frac{d\vec{p}}{dt} = \frac{d}{dt} \int_{\Omega(t)} \rho \vec{u} \, d\Omega \equiv \int_{\Omega(t)} \left\{ \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) \right\} \, d\Omega =$$

Reynolds transport theorem:

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Force:

$$F = F_\Omega + F_{\partial \Omega}$$

Reynolds transport theorem:

$$\frac{d}{dt} \int_{\Omega(t)} f(x, t) \ d\Omega = \int_{\Omega(t)} \left\{ \frac{\partial f}{\partial t}(x, t) + \nabla \cdot (f \vec{u}) \right\} d\Omega$$
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Force:

$$F = F_{\Omega} + F_{\partial \Omega} = \int_{\Omega(t)} \rho \, \vec{f} \, d\Omega + \int_{\partial \Omega(t)} \sigma \, \vec{n} \, dS$$

Reynolds transport theorem:

$$\frac{d}{dt} \int_{\Omega(t)} f(x, t) \, d\Omega = \int_{\Omega(t)} \left\{ \frac{\partial f}{\partial t} (x, t) + \nabla \cdot (f \vec{u}) \right\} \, d\Omega$$
Energy equation:

\[
\frac{d}{dt} \int_{\Omega(t)} \left\{ \frac{1}{2} \rho |\vec{u}|^2 + \rho e \right\} \, d\Omega
\]
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\[
\frac{d}{dt} \int_{\Omega(t)} \left\{ \frac{1}{2} \rho |\vec{u}|^2 + \rho e \right\} \, d\Omega = \int_{\Omega(t)} \left\{ \right\} \, d\Omega \\
+ \int_{\partial \Omega(t)} \left\{ \right\} \, dS
\]
Energy equation:

\[
\frac{d}{dt} \int_{\Omega(t)} \left\{ \frac{1}{2} \rho |\vec{u}|^2 + \rho e \right\} d\Omega = \int_{\Omega(t)} \left\{ \rho \vec{f} \cdot \vec{u} \right\} d\Omega
\]

\[+ \int_{\partial\Omega(t)} \left\{ (\sigma \vec{n}) \cdot \vec{u} + \kappa \nabla T \cdot \vec{n} \right\} dS
\]

According to:

- volume force: \( \int_{\Omega(t)} \rho \vec{f} \cdot \vec{u} d\Omega \)
Energy equation:

\[
\frac{d}{dt} \int_{\Omega(t)} \left\{ \frac{1}{2} \rho \lvert \vec{u} \rvert^2 + \rho e \right\} \, d\Omega = \int_{\Omega(t)} \left\{ \rho \vec{f} \cdot \vec{u} + \rho \, Q \right\} \, d\Omega \\
+ \int_{\partial\Omega(t)} \left\{ \right\} \, dS
\]

According to:

- volume force: \( \int_{\Omega(t)} \rho \, \vec{f} \cdot \vec{u} \, d\Omega \)
- energy source: \( \int_{\Omega(t)} \rho \, Q \, d\Omega \)
Energy equation:

\[ \frac{d}{dt} \int_{\Omega(t)} \left\{ \frac{1}{2} \rho |\vec{u}|^2 + \rho e \right\} \ d\Omega = \int_{\Omega(t)} \left\{ \rho \vec{f} \cdot \vec{u} + \rho \ Q \right\} \ d\Omega \]

\[ + \int_{\partial \Omega(t)} \left\{ \left( \sigma \ n \right) \cdot \vec{u} \right\} \ dS \]

According to:

- volume force: \( \int_{\Omega(t)} \rho \vec{f} \cdot \vec{u} \ d\Omega \)
- energy source: \( \int_{\Omega(t)} \rho \ Q \ d\Omega \)
- surface force: \( \int_{\partial \Omega(t)} \left( \sigma \ n \right) \cdot \vec{u} \ dS \)
Energy equation:

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

According to:

- volume force: \( \int_{\Omega(t)} \rho \vec{f} \cdot \vec{u} \, d\Omega \)
- energy source: \( \int_{\Omega(t)} \rho Q \, d\Omega \)
- surface force: \( \int_{\partial \Omega(t)} (\sigma \cdot \vec{n}) \cdot \vec{u} \, dS \)
- heat flux: \( \int_{\partial \Omega(t)} \kappa \nabla T \cdot \vec{n} \, dS \)
System equations:

1. mass conservation

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0
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System equations:

1. mass conservation

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0
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2. momentum conservation

\[
\rho \frac{\partial \vec{u}}{\partial t} + (\rho \vec{u} \cdot \nabla) \vec{u} = \rho \vec{f} + \nabla \cdot \sigma
\]
System equations:

1. **mass conservation**

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3. **energy conservation**

\[
\rho \frac{\partial e}{\partial t} = \rho Q + \nabla \cdot (\kappa \nabla T) + \nabla \cdot (\sigma \vec{u}) - (\nabla \cdot \sigma) \vec{u}
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System equations:

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4. equation of state (e.g. ideal gas equation)
The stress tensor \( \sigma \):
The stress tensor $\sigma$:

$$\sigma = -p \cdot \mathbb{1} + \tau$$

with $\tau$ is the viscous stress tensor
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$$\sigma = -p \cdot 1 + \tau$$

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The viscosity term:

- General viscous stress tensor:

$$\tau = F(D(t, x), t)$$
The stress tensor $\sigma$:

$$\sigma = -p \cdot 1 + \tau$$

with $\tau$ is the viscous stress tensor

The viscosity term:

1. General viscous stress tensor:

$$\tau = F(D(t, x), t)$$

2. Strain rate tensor:

$$D := \frac{\partial \epsilon}{\partial t} = \frac{1}{2} \left[ (\nabla \bar{u}) + (\nabla \bar{u})^T \right]$$
Behaviour of the viscous stress tensor:

\[ \tau = F(D(t, x), t) \]
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\]

Time-dependent

Time-independent
Behaviour of the viscous stress tensor:

\[ \tau = F(D(t, x), t) \]

**Time-dependent**  
- increase with time  
  *printer ink, synovial fluid*  

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Behaviour of the viscous stress tensor:

\[ \tau = F(D(t, x), t) \]

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

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Behaviour of the viscous stress tensor:

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**Time-dependent**
- increase with time
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- decrease with time
  - gelatin gels, yogurt

**Time-independent**
- shear thickening
  - corn starch in water
Behaviour of the viscous stress tensor:

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- shear thickening
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- shear thinning
  - *ketchup, blood*
Behaviour of the viscous stress tensor:

\[ \tau = F(D(t,x), t) \]

**Time-dependent**
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**Time-independent**
- shear thickening
  - corn starch in water
- shear thinning
  - ketchup, blood
- generalized newonian fluids
  - water, blood plasma
Behaviour of the viscous stress tensor:

$$\tau = F(D(t,x), t)$$

**Time-dependent**
- increase with time
  - *printer ink, synovial fluid*
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**Time-independent**
- shear thickening
  - *corn starch in water*
- shear thinning
  - *ketchup, blood*
- generalized newonian fluids
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Newtonian fluid:

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

with the dynamic viscosity $\mu$
Incompressible fluid assumption:
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\[ 0 = \frac{d\rho}{dt}(x, t) \]
Incompressible fluid assumption:

\[
0 = \frac{d\rho}{dt}(x, t) = \frac{\partial}{\partial t}\rho(x, t) + \nabla\rho(x, t) \cdot \vec{u}
\]
Incompressible fluid assumption:

\[ 0 = \frac{d\rho}{dt}(x, t) = \frac{\partial}{\partial t} \rho(x, t) + \nabla \rho(x, t) \cdot \vec{u} \]

- Continuity equation:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) \]
Incompressible fluid assumption:

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Continuity equation:

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\]

- It follows: \( \nabla \cdot \vec{u} = 0 \) (divergency free velocity field)
Incompressible fluid assumption:

\[ 0 = \frac{d\rho}{dt}(x, t) = \frac{\partial}{\partial t}\rho(x, t) + \nabla \rho(x, t) \cdot \vec{u} \]

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- It follows: \( \nabla \cdot \vec{u} = 0 \) (divergency free velocity field)

- Viscous stress tensor: (Newtonian fluid)

\[ \tau = \mu \cdot \left[ (\nabla \vec{u}) + (\nabla \vec{u})^T \right] - \left( \frac{2}{3} \mu \nabla \cdot \vec{u} \right) \mathbb{1} \]
Incompressible fluid + isothermal assumption:

From $T = \text{const.}$ with $\frac{d}{dt}\rho = 0$ follows:
Incompressible fluid + isothermal assumption:

From \( T = \text{const.} \) with \( \frac{d}{dt} \rho = 0 \) follows:

1. Pressure is given with \( p \sim \rho \) (equation of state)
Incompressible fluid + isothermal assumption:

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

1. Pressure is given with $p \sim \rho$ (equation of state)
2. Energy is a function of $\rho$ and $\vec{u}$
   $\Rightarrow$ the energy conservation contains no extra information
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For a newtonian fluid we get the Navier-Stokes equations as

**Navier-Stokes equations**

\[
\nabla \cdot \vec{u} = 0 \quad (1)
\]
\[
\rho \frac{\partial \vec{u}}{\partial t} + \rho (\vec{u} \cdot \nabla) \vec{u} = \rho \vec{f} - \nabla p + \mu \nabla \cdot \tau \quad (2)
\]

Note: often, the kinematic viscosity $\nu := \frac{\mu}{\rho}$ is used if $\rho = \text{const}$
Application to biofluid systems
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1. Human air system
   - Fluid-particle interaction
   - Fluid-structure interaction
   - Blood-air barrier
Application to biofluid systems

1. Human air system
   - Fluid-particle interaction
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2. Human blood system
   - Oxygen transportation
   - Fluid-structure interaction
   - Transport of medicine
Application to biofluid systems

1 Human air system
   - Fluid-particle interaction
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   - Oxygen transportation
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3 ...
Break

5 min
System equations:

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\[ \rho \frac{\partial \vec{u}}{\partial t} + (\rho \vec{u} \cdot \nabla) \vec{u} = \rho \vec{f} + \nabla \cdot \sigma \]
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   \[
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4. equation of state (e.g. ideal gas equation)
Incompressible flow/fluid + isothermal assumption:

From $T = \text{const.}$ with $\frac{d}{dt} \rho = 0$ follows:
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For a newtonian fluid we get the Navier-Stokes equations as

\textbf{Navier-Stokes equations}

\begin{align*}
\nabla \cdot \vec{u} &= 0 \\
\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} &= \vec{f} - \frac{1}{\rho} \nabla p + \nu \nabla \cdot \tau
\end{align*}

(3) (4)

Note: often, the kinematic viscosity $\nu := \frac{\mu}{\rho}$ is used
Dimensionless Navier-Stokes: 

**Navier-Stokes momentum equation**

\[
\frac{\partial \tilde{u}}{\partial t} + (\tilde{u} \cdot \nabla) \tilde{u} = \tilde{f} - \frac{1}{\rho} \nabla \tilde{p} + \frac{\mu}{\rho} \nabla \cdot \tau
\]
Dimensionless Navier-Stokes:

**Navier-Stokes momentum equation**

\[
\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \vec{f} - \frac{1}{\rho} \nabla p + \frac{\mu}{\rho} \nabla \cdot \tau
\]

Define characteristic time \( T \), length \( L \) and velocity \( U \) with \( L = U \cdot T \):

\[
\tau = \frac{t}{T}, \quad \vec{v} = \frac{\vec{u}}{U}, \quad \xi = \frac{\vec{x}}{L}
\]
Dimensionless Navier-Stokes:

Navier-Stokes momentum equation

\[
\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \vec{f} - \frac{1}{\rho} \nabla p + \frac{\mu}{\rho} \nabla \cdot \tau
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Define characteristic time \( T \), length \( L \) and velocity \( U \) with \( L = U \cdot T \):

\[
\tau = \frac{t}{T}, \quad \vec{v} = \frac{\vec{u}}{U}, \quad \xi = \frac{\vec{x}}{L}
\]

Dimensionless representation of the momentum equation:

\[
\frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla) \vec{v} = \frac{L}{U^2} \vec{f} - \frac{1}{\rho U^2} \nabla p + \frac{\mu}{\rho UL} \nabla \cdot \tilde{\tau}
\]

dimensionless forcedensity \( \vec{\kappa} := \frac{L}{U^2} \vec{f} \) (look for Froude number)

pressure rescaling \( \tilde{p} := \frac{p}{\rho U^2} \) (NOTE: only for inc. fluid)
Dimensionless Navier-Stokes:

Navier-Stokes momentum equation

\[ \frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \vec{f} - \frac{1}{\rho} \nabla p + \frac{\mu}{\rho} \nabla \cdot \tau \]

Define characteristic time \( T \), length \( L \) and velocity \( U \) with \( L = U \cdot T \):

\[ \tau = \frac{t}{T}, \quad \vec{v} = \frac{\vec{u}}{U}, \quad \xi = \frac{\vec{x}}{L} \]

Dimensionless representation of the momentum equation:

\[ \frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla) \vec{v} = \frac{L}{U^2} \vec{f} - \frac{1}{\rho U^2} \nabla p + \frac{\mu}{\rho U L} \nabla \cdot \vec{\tau} \]

- dimensionless forcedensity \( \vec{\kappa} := \frac{L}{U^2} \vec{f} \) (look for Froude number)
Dimensionless Navier-Stokes:

Navier-Stokes momentum equation

\[
\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = \vec{f} - \frac{1}{\rho} \nabla p + \frac{\mu}{\rho} \nabla \cdot \tau
\]

Define characteristic time \( T \), length \( L \) and velocity \( U \) with \( L = U \cdot T \):

\[
\tau = \frac{t}{T} \quad \vec{v} = \frac{\vec{u}}{U} \quad \vec{\xi} = \frac{\vec{x}}{L}
\]

Dimensionless representation of the momentum equation:

\[
\frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla) \vec{v} = \frac{L}{U^2} \vec{f} - \frac{1}{\rho U^2} \nabla p + \frac{\mu}{\rho U L} \nabla \cdot \vec{\tau}
\]

- dimensionless forcedensity \( \vec{\kappa} := \frac{L}{U^2} \vec{f} \) (look for Froude number)
- pressure rescaling \( \tilde{p} := \frac{p}{\rho U^2} \) (NOTE: only for inc. fluid)
Diffusion term & Reynolds number:

\[ \frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla) \vec{v} = \vec{k} - \nabla \tilde{p} + \frac{\mu}{\rho UL} \nabla \cdot \tilde{\tau} \]
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\frac{\partial \tilde{v}}{\partial \tau} + (\tilde{v} \cdot \nabla) \tilde{v} = \tilde{k} - \nabla \tilde{p} + \frac{\mu}{\rho U L} \nabla \cdot \tilde{\tau}
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Definition of the Reynolds number:

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Re := \frac{\text{inertia forces}}{\text{viscous forces}}
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Dimensionless Navier-Stokes equations

\[
\nabla \cdot \vec{v} = 0 \\
\frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla) \vec{v} = \kappa - \nabla \tilde{p} + \frac{1}{Re} \nabla \cdot \tilde{\tau}
\]
Pressure equation:

\[ \frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla) \vec{v} = \bar{\kappa} - \nabla \bar{p} + \frac{1}{Re} \nabla \cdot \bar{\tau} \]

Divergency free velocity field implies

\[ \nabla \cdot \left( \frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla) \vec{v} \right) = \nabla \cdot \left( \bar{\kappa} - \nabla \bar{p} + \frac{1}{Re} \nabla \cdot \bar{\tau} \right) \]
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with \( \frac{\partial}{\partial \tau} \nabla \cdot \vec{v} = 0 \), we get the Poisson-Pressure equation:

\[ \Delta \tilde{p} = \nabla \cdot \left( \kappa - (\vec{v} \cdot \nabla) \vec{v} + \frac{1}{Re} \nabla \cdot \tilde{\tau} \right) \]
Turbulent flow:

If $Re \ll 1$, the diffusion time scale is much smaller as the time scale for momentum transportation. Velocity field perturbations smooth out quickly. Velocity field tends to be laminar.

If $Re \gg 1$, momentum transportation is the main effect for the fluid flow description. Velocity field perturbations increase quickly. Velocity field tends to be turbulent.

Example: (flow in pipe)

Reynolds number: $Re = \frac{\rho d v}{\mu}$

Observation: Julius Rotta (at 1950)

$Re_{krit} \approx 2300$
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- If $Re << 1$, the diffusion time scale is much smaller as the time scale for momentum transportation
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Kolmogorov scales:

The smallest scales that influences the turbulent flow by dissipation effects.
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**Note:**

To retain energy conservation at the numerical domain, one have to resolve also the dissipative scales in the Navier-Stokes equation!
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Note:
To retain energy conservation at the numerical domain, one have to resolve also the dissipative scales in the Navier-Stokes equation!

The scales are given as: ($\epsilon$ is the average dissipation rate)

length: $\eta = \left(\frac{\mu^3}{\epsilon \rho^3}\right)^{\frac{1}{4}}$

vel: $u_\eta = \left(\frac{\mu}{\rho \epsilon}\right)^{\frac{1}{4}}$

time: $\tau_\eta = \left(\frac{\mu}{\rho \epsilon}\right)^{\frac{1}{2}}$

with

$$Re_\eta = \frac{\eta u_\eta \mu}{\rho} = 1$$
Resolution problem:

Approximation of the dissipation rate (from large scales):

\[ \epsilon \sim \frac{\text{kinetic energy}}{\text{time}} \]
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Therefore we get the relation:

\[ \frac{L}{\eta} = L \cdot \left( \frac{\mu^3}{\varepsilon \rho^3} \right)^{-\frac{1}{4}} \sim L \cdot \left( \frac{U^3 \rho^3}{L \mu^3} \right)^{\frac{1}{4}} \]
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Example: \( (L \approx 10^3 \text{m}, \nu \approx 1 \frac{\text{m}}{\text{s}}, \rho \approx 1.3 \frac{\text{kg}}{\text{m}^3}, \mu \approx 17.1 \mu\text{Pa} \cdot \text{s}) \)

\[ \text{Re} \approx 7.5 \cdot 10^9 \]
\[ \eta \approx 4 \cdot 10^{-5} \text{m} \]
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Example: \( L \approx 10^{-3} \text{m} \), \( \nu \approx 0.1 \frac{\text{m}}{\text{s}} \), \( \rho \approx 1060 \frac{\text{kg}}{\text{m}^3} \), \( \mu \approx 3 \text{ mPa} \cdot \text{s} \)

\[ Re \approx 35 \]

\[ \eta \approx 7 \cdot 10^{-5} \text{m} \]
Simulation approaches:
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- **Direct numerical simulation (DNS):**
  Assumption that the flow inside of a volume element is purely laminar and no dissipation effect occurs. (Note: If this is not true, the energy conservation results in a different flow field.)
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- **Eddy dissipation modelling on small scales:**
  - Reynolds-Averaged Navier Stokes (RANS)
  - Large-Eddy Simulation
  - ...

\[ v = \langle v \rangle + v' \quad \text{and} \quad p = \langle p \rangle + p' \]

with the mean value \( \langle \cdot \rangle \) of \( \cdot \) and the fluctuating part \( \cdot' \).
RANS:

- Special cases: temporal or spatial averaging
- In general: \( \langle f(\vec{x}, t) \rangle = \lim_{N \to \infty} \sum_{n}^N f(\vec{x}, t) \)
- Fluctuating part: \( \langle f' \rangle = 0 \)
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Correlation property:

$$\nabla \cdot \langle \vec{v}' \vec{v}' \rangle = \nabla \cdot \begin{pmatrix}
\langle v'_x v'_x \rangle & \langle v'_x v'_y \rangle & \langle v'_x v'_z \rangle \\
\langle v'_y v'_x \rangle & \langle v'_y v'_y \rangle & \langle v'_y v'_z \rangle \\
\langle v'_z v'_x \rangle & \langle v'_z v'_y \rangle & \langle v'_z v'_z \rangle 
\end{pmatrix}$$
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- Zero equation models $\nu_T = \xi^2 |\partial_\perp \langle v \rangle|$ (mixing length $\xi$)
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- One equation models (example: Spalart and Allmaras)

$$\frac{\partial \nu_T}{\partial t} + \langle \vec{v} \rangle \nabla \nu_T = \nabla \left( \frac{\nu_T}{\sigma_T} \nabla \nu_T \right) + S_\nu$$

- Two equation models ($k-\epsilon$, $k-\omega$, SST)

  - $k = \frac{1}{2} \text{tr} \langle \vec{v}' \vec{v}' \rangle$ (mean of the fluctuating kinetic energy)
  - Dissipation rate $\epsilon$
  - Eddy frequency $\omega$

  1. $k-\epsilon$: good on free flow fields with no walls
  2. $k-\omega$: near wall approximation is good
  3. SST brings the advantage of both together
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Large-Eddy simulations (LES):

spatial averaging method

\[ \langle \vec{v}(\vec{x}, t) \rangle := \int_V \vec{v}(\vec{x}', t) \cdot G(\vec{x}, \vec{x}', \Delta) \, dV' \]

with

1. step-function

\[ G := \begin{cases} \frac{1}{\Delta^3}, & \text{if } |\vec{x} - \vec{x}'| < \Delta/2 \\ 0, & \text{else} \end{cases} \]

2. gauss-filter

\[ G := A(\Delta) \exp \left\{ \frac{-\beta |\vec{x} - \vec{x}'|}{\Delta^2} \right\} \]

3. ...
Large-Eddy simulations (LES):

**LES equation:**

\[
\nabla \cdot \langle \vec{v} \rangle = 0
\]

\[
\frac{\partial \langle \vec{v} \rangle}{\partial t} + (\langle \vec{v} \rangle \cdot \nabla) \langle \vec{v} \rangle = \vec{f} - \nabla \langle p \rangle + \frac{1}{Re} \nabla \cdot \langle \tilde{\tau} \rangle - \nabla \cdot \tau^S
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with \( \tau^S := \langle \vec{v} \vec{v} \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle \).
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\]

with \( \tau^S := \langle \vec{v} \vec{v} \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle \). Detailed look:

\[
\tau^S = \left[ \langle \langle \vec{v} \rangle \langle \vec{v} \rangle \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle \right]_L + \left[ \langle \langle \vec{v} \rangle \vec{v}' \rangle - \langle \vec{v}' \langle \vec{v} \rangle \rangle \right]_C + \left[ \langle \vec{v}' \vec{v}' \rangle \right]_{\tau^{SR}}
\]

- **Leonard-strain**: creation of small eddys through large eddys
- **Cross-stress**: interaction of the different scales
- **Subgrid-scale Reynolds stress tensor**
Break

5 min
Application

Pre-processing

Geometry Design → Mesh Generation → Problem Setup → Flow Solver

Computation

Visualization → Quantitative Analysis

Post-processing
Geometry

- Not as easy
Geometry

- Not as easy
- complicated
Geometry

- Not as easy
- complicated
- often simplified
Geometry

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Application
Mesh

Mesh quality determined by:

- area
- aspect ratio
- diagonal ratio
- edge ratio
- skewness
- orthogonal quality
- stretch
- taper
- volume
Mesh - Orthogonal Quality

\[ OQ = \min_i \left\{ \frac{A_i \hat{f}_i}{|\hat{A}_i||\hat{f}_i|}, \frac{A_i \hat{c}_i}{|\hat{A}_i||\hat{c}_i|} \right\}, \quad (7) \]

- \( A_i \): face normal vector
- \( \hat{f}_i \): vector from the centroid of the cell to the centroid of that face
- \( \hat{c}_i \): vector from the centroid of the cell to the adjacent cell
Mesh - Orthogonal Quality

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(7)

$A_i$ face normal vector

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Mesh

Boundary layer mesh for flows with high Reynold’s number, strong gradients exist within the boundary layer close to a solid wall (with a no-slip boundary condition)
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Mesh

Inflation layer examples:
Mesh

Hints for mesh generation

- minimize mesh complexity
  - use structured mesh when appropriate
  - use quad / hex elements when appropriate
  - use tri / tet elements for complex geometries
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  - do not use too many (or too few) elements
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- minimize number of mesh elements
  - do not use too many (or too few) elements
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- maximize solution accuracy
  - concentrate mesh elements in critical regions (e.g. boundary layers, wakes, shocks)
  - align quad / hex meshes with flow direction
  - avoid poor quality elements (e.g. twisted, skewed)
Application
Problem Definition - Boundary conditions

Choosing appropriate boundary conditions:
- nature of flow – incompressible / compressible ...
- physical models – turbulence, species transport ...
- position of boundary
- what is known
- convergence of solution may (strongly) depend on choice of boundary conditions
Problem Definition - Numerical solver

two basic solver approaches:

- pressure-based solver
  - originally developed for low-speed flows
  - pressure determined from pressure or pressure-correction equation (obtained from manipulating continuity and momentum equations)

- density-based solver
  - originally developed for high-speed flows
  - density determined from continuity equation
  - pressure determined from equation of state

similar discretization method is used for both pressure-based and density-based solvers.
linearization and solving of the discrete equations is different for two approaches.
Application
Calculation - Convergence of the iterative numerical scheme

at convergence:
- all discretized conservation equations are satisfied in all cells to a specified tolerance
- solution no longer changes significantly with more iterations
- overall mass, momentum, energy and scalar balances are obtained
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  - generally decrease in residuals by $10^{-3}$ indicates basic global convergence - major flow features have been established
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- checking for property conservation
  - overall heat and mass balances should be within 0.1% of net flux through domain
Convergence difficulties

- numerical instabilities can arise due to:
  - ill-posed problem (no physical solution)
  - poor quality mesh
  - inappropriate boundary conditions
  - inappropriate solver settings
  - inappropriate initial conditions
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- numerical instabilities can arise due to:
  - ill-posed problem (no physical solution)
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- trouble-shooting
  - ensure problem is physically realizable
  - compute an initial solution with a first-order discretization scheme
  - decrease under-relaxation for equations having convergence problems (segregated)
  - reduce CFL number (unsteady flow)
  - re-mesh or refine mesh regions with high aspect ratio or highly skewed cells
Application
Post Processing

- qualitative analysis (visualization):
  - displaying the mesh
  - contours of flow fields (e.g. pressure, velocity, temperature, concentrations ... )
  - contours of derived field quantities
  - velocity vectors
  - animation (using keyframes or frame-by-frame)

- quantitative analysis:
  - XY plots (e.g. pressure, velocity, temperature vs position)
  - forces and moments on surfaces
  - surface and volume integrals
  - Flow solvers may contain a complete post-processing environment
  - generally not necessary to use external post-processing software
Verification & Validation

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  A representation of a physical system or process intended to enhance our ability to understand, predict, or control its behaviour.
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Essentially, one implements a model into a computer code and then uses the code to perform a CFD simulation which yields values used in the engineering analysis.
Verification & Validation - Level 1
Verification & Validation - Level 2