Computational Fluid Dynamics 2

Turbulence effects and Particle transport

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Computational Biomechanics

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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)

Incompressible fluid / flow assumption:

Incompressible flow:

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

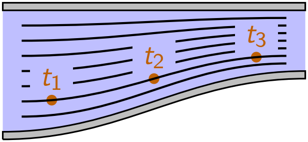
Incompressible fluid:

$$\frac{\partial\rho}{\partial t}(x,t) = \nabla\rho(x,t) = 0$$

- Continuity equation:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\,\vec{u}) = \overbrace{\underbrace{\frac{\partial\rho}{\partial t}}_{0,\,fluid\ ass.} + \underbrace{\nabla\rho\cdot\vec{u}}_{0,\,fluid\ ass.}}^{0,\,flow\ ass.} + \rho\nabla\cdot\vec{u} = \rho\nabla\cdot\vec{u} = 0$$

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



Incompressible flow/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

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

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\ \vec{u} = \vec{f}\ - \frac{1}{\rho}\nabla p\ + \nu \nabla \cdot \underline{\underline{\tau}} \tag{2}$$

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

Dimensionless Navier-Stokes:

Navier-Stokes momentum equation

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

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

$$\tau = \frac{t}{T} \qquad \vec{v} = \frac{\vec{u}}{U} \qquad \vec{\xi} = \frac{\vec{x}}{L}$$

Dimensionless representation of the momentum equation:

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

- 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)

Diffusion term & Reynolds number:

$$\frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla)\ \vec{v} = \vec{\kappa}\ - \nabla \tilde{p}\ + \frac{\mu}{\rho U L} \nabla \cdot \underline{\underline{\tilde{\tau}}}$$

Definition of the Reynolds number:

$$Re := \frac{inertia\ forces}{viscous\ forces} = \frac{\rho U L}{\mu}$$

- inertia force: $F_{in} = \frac{\rho L^3 \cdot U}{T}$ (momentum transfer)
- viscous force: $F_{vis} = \mu L^2 \cdot \frac{U}{L}$ (*"velocity diffusion"*)

Dimensionless Navier-Stokes equations

$$\nabla \cdot \vec{v} = 0 \tag{3}$$

$$\frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla)\ \vec{v} = \vec{\kappa}\ - \nabla \tilde{p}\ + \frac{1}{Re} \nabla \cdot \underline{\underline{\tilde{\tau}}} \tag{4}$$

Pressure equation:

$$\frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla)\ \vec{v} = \vec{\kappa}\ - \nabla \tilde{p}\ + \frac{1}{Re} \nabla \cdot \underline{\underline{\tilde{\tau}}}$$

Divergency free velocity field implies

$$\nabla \cdot \left(\frac{\partial \vec{v}}{\partial \tau} + (\vec{v} \cdot \nabla)\ \vec{v} \right) = \nabla \cdot \left(\vec{\kappa}\ - \nabla \tilde{p}\ + \frac{1}{Re} \nabla \cdot \underline{\underline{\tilde{\tau}}} \right)$$

with $\frac{\partial}{\partial \tau} \nabla \cdot \vec{v} = 0$, we get the Poissin-Pressure equation:

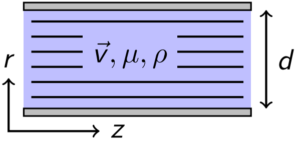
$$\Delta \tilde{p} = \nabla \cdot \left(\vec{\kappa}\ - (\vec{v} \cdot \nabla)\ \vec{v}\ + \frac{1}{Re} \nabla \cdot \underline{\underline{\tilde{\tau}}} \right)$$

Turbulent flow:

- If $Re << 1$, 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 $Re >> 1$, momentum transportation is the main effect for the fluid flow description
  - velocity field perturbations increase quickly
  - velocity field tends to be turbulent

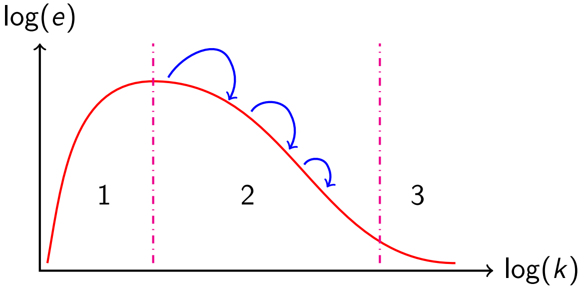
Example: (flow in pipe)

- Reynolds number: $Re = \frac{\rho\, d\, v_z}{\mu}$
- Observation: Julius Rotta (at 1950) $Re_{krit.} \approx 2300$



Energy cascade:

1. energy injection range (small viscous effects)
2. inertial subrange
3. dissipation range (large viscous effects)



visualization after the model of Lewis Fry Richardson

$e :=$ energy, $k :=$ wave number

Kolmogorov scales:

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

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: (ϵ is the average dissipation rate)

$$\textit{length}: \ \eta = \left(\frac{\mu^3}{\epsilon\,\rho^3}\right)^{\frac{1}{4}} \quad \textit{vel}: \ u_\eta = \left(\frac{\mu}{\rho}\,\epsilon\right)^{\frac{1}{4}} \quad \textit{time}: \ \tau_\eta = \left(\frac{\mu}{\rho\,\epsilon}\right)^{\frac{1}{2}}$$

with

$$Re_\eta = \frac{\eta\,u_\eta\,\mu}{\rho} = 1$$

Resolution problem:

Approximation of the dissipation rate (from large scales):

$$\epsilon \sim \frac{\textit{kinetic energy}}{\textit{time}} \sim \frac{U^2}{T} = \frac{U^3}{L}$$

Therefore we get the relation:

$$\frac{L}{\eta} = L \cdot \left(\frac{\mu^3}{\epsilon\, \rho^3} \right)^{-\frac{1}{4}} \sim L \cdot \left(\frac{U^3\, \rho^3}{L\, \mu^3} \right)^{\frac{1}{4}} = Re^{\frac{3}{4}}$$

Example: $(L \approx 10^3 \mathrm{m}\ ,\ v \approx 1\ \frac{\mathrm{m}}{\mathrm{s}},\ \rho \approx 1.3\ \frac{\mathrm{kg}}{\mathrm{m}^3},\ \mu \approx 17.1\ \mu\mathrm{Pa}\cdot\mathrm{s})$

$$Re \approx 7.5 \cdot 10^9$$

$$\eta \approx 4 \cdot 10^{-5}\, \mathrm{m}$$

Resolution problem:

Approximation of the dissipation rate (from large scales):

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Therefore we get the relation:

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Example: $(L \approx 10^{-3}\mathrm{m}\ ,\ v \approx 0.1\ \frac{\mathrm{m}}{\mathrm{s}},\ \rho \approx 1060\ \frac{\mathrm{kg}}{\mathrm{m}^3},\ \mu \approx 3\ \mathrm{mPa}\cdot\mathrm{s})$

$$Re \approx 35$$

$$\eta \approx 7 \cdot 10^{-5}\,\mathrm{m}$$

Simulation approaches:

- **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.)

- **Eddy dissipation modelling on small scales:**
  - Reynolds-Averaged Navier Stokes (RANS)
  - Large-Eddy Simulation
  - ...

$$v = \langle v \rangle + v' \qquad \text{and} \qquad p = \langle p \rangle + p'$$

with the mean value $\langle \cdot \rangle$ of $\cdot$ and the fluctuating part $\cdot'$.

RANS:

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

Reynolds equations:

$$\nabla \cdot \langle \vec{v} \rangle = 0$$

$$\frac{\partial \langle \vec{v} \rangle}{\partial t} + (\langle \vec{v} \rangle \cdot \nabla)\ \langle \vec{v} \rangle = \vec{f} - \nabla \langle p \rangle + \frac{1}{Re} \nabla \cdot \langle \underline{\underline{\tilde{\tau}}} \rangle - \underbrace{\left\langle \left(\vec{v}' \cdot \nabla \right)\ \vec{v}' \right\rangle}_{\textit{correlation property}}$$

$$\nabla \cdot \langle \vec{v}' \vec{v}' \rangle = \nabla \cdot \begin{pmatrix} \langle v'_x v'_x \rangle & \langle v'_x v'_y \rangle & \langle v'_x v'_z \rangle \\ \langle v'_y v'_x \rangle & \langle v'_y v'_y \rangle & \langle v'_y v'_z \rangle \\ \langle v'_z v'_x \rangle & \langle v'_z v'_y \rangle & \langle v'_z v'_z \rangle \end{pmatrix}$$

RANS models:

- Zero equation models $\nu_T = \xi^2 \ |\partial_\perp \langle v \rangle|$ (mixing length ξ)

- 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)
  - $k = \frac{1}{2} \mathrm{tr} \langle \vec{v}' \vec{v}' \rangle$ (mean of the fluctuating kinetic energy)
  - dissipation rate ϵ
  - eddy frequency ω

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 booth together

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

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

2. gauss-filter

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

3. ...

Large-Eddy simulations (LES):

LES equation:

$$\nabla \cdot \langle \vec{v} \rangle = 0$$

$$\frac{\partial \langle \vec{v} \rangle}{\partial t} + (\langle \vec{v} \rangle \cdot \nabla)\ \langle \vec{v} \rangle = \vec{f}\ - \nabla \langle p \rangle\ + \frac{1}{Re} \nabla \cdot \langle \underline{\underline{\tilde{T}}} \rangle - \nabla \cdot \tau^S$$

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

$$\tau^S = \underbrace{\langle \langle \vec{v} \rangle \langle \vec{v} \rangle \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle}_{L} + \underbrace{\left\langle \langle \vec{v} \rangle \vec{v}' \right\rangle - \left\langle \vec{v}' \langle \vec{v} \rangle \right\rangle}_{C} + \underbrace{\left\langle \vec{v}' \vec{v}' \right\rangle}_{\tau^{SR}}$$

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