Computational Fluid Dynamics

Theory, Numerics, Modelling

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Computational Biomechanics

Summer Term 2017

Fluid phase system

State variables:

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- Density ρ (1d)
- Velocity $\vec{u}$ (3d)

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Physical laws:

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- Mass conservation
- Momentum conservation
- Energy conservation

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Physical laws:

- Mass conservation
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- 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:

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

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Mass conservation:

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

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega(t)} \rho \,\mathrm{d}\Omega$$

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Continuity equation:

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

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Force:

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

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Force:

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

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Energy equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega(t)} \left\{ \frac{1}{2} \rho \left| \vec{u} \right|^2 + \rho e \right\} \, \mathrm{d}\Omega$$

Energy equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega(t)} \left\{ \frac{1}{2}\rho \left|\vec{u}\right|^2 + \rho e \right\} \mathrm{d}\Omega = \int\limits_{\Omega(t)} \left\{ \qquad\qquad\qquad \right\} \mathrm{d}\Omega$$

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- volume force: $\int_{\Omega(t)} \rho\, \vec{f}\cdot\vec{u}\,\mathrm{d}\Omega$

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According to:

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According to:

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- heat flux: $\int_{\partial\Omega(t)} \kappa \, \nabla \, T \cdot \vec{n} \, \mathrm{d}S$

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

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

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

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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:

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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

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

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- Viscous stress tensor: (Newtonian fluid)

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

Navier-Stokes equations

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

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

Application to biofluid systems

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   - Fluid-particle interaction
   - Fluid-structure interaction
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Break

5 min

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Navier-Stokes equations

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

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\ \vec{u} = \vec{f} - \frac{1}{\rho}\nabla p + \nu \nabla \cdot \underline{\underline{\tau}} \tag{4}$$

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

Dimensionless Navier-Stokes:

Navier-Stokes momentum equation

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

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

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

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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 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:

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

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

Diffusion term & Reynolds number:

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Dimensionless Navier-Stokes equations

$$\nabla \cdot \vec{v} = 0 \tag{5}$$

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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

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

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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:

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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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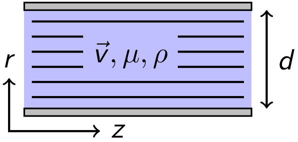
Example: (flow in pipe)



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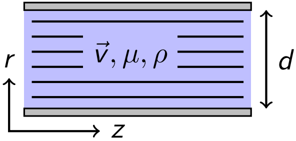
Example: (flow in pipe)

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



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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

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

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Approximation of the dissipation rate (from large scales):

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

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

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

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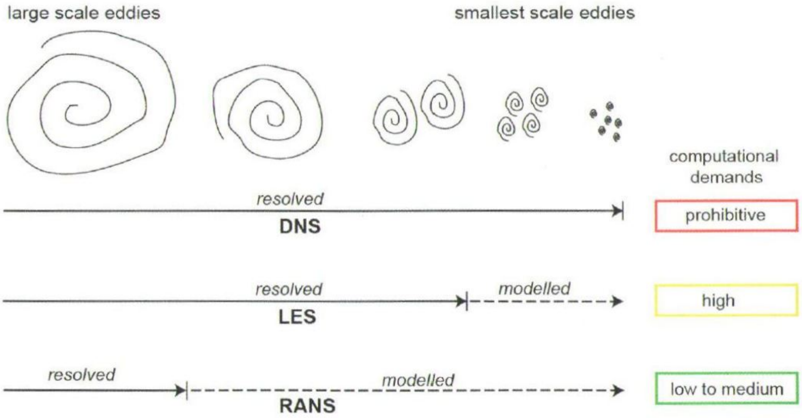
Example: $(L \approx 10^{-3}\mathrm{m}$, $v \approx 0.1\ \frac{\mathrm{m}}{\mathrm{s}}$, $\rho \approx 1060\ \frac{\mathrm{kg}}{\mathrm{m}^3}$, $\mu \approx 3\ \mathrm{mPa} \cdot \mathrm{s})$

$$Re \approx 35$$

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

Simulation approaches:



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- **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: $\langle f(\vec{x},t)\rangle = \lim_{N\to\infty} \sum_{n}^{N} f(\vec{x},t)$
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$$\nabla \cdot \langle \vec{v}'\vec{v}' \rangle = \nabla \cdot \begin{pmatrix} \langle v'_x v'_x\rangle & \langle v'_x v'_y\rangle & \langle v'_x v'_z\rangle \\ \langle v'_y v'_x\rangle & \langle v'_y v'_y\rangle & \langle v'_y v'_z\rangle \\ \langle v'_z v'_x\rangle & \langle v'_z v'_y\rangle & \langle v'_z v'_z\rangle \end{pmatrix}$$

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  - $k = \frac{1}{2} \mathrm{tr} \langle \vec{v}' \vec{v}' \rangle$ (mean of the fluctuating kinetic energy)
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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. ...

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LES equation:

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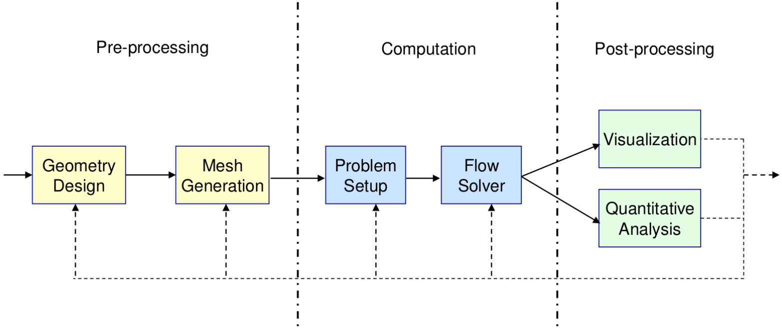
$$\tau^S = \underbrace{\langle \langle \vec{v} \rangle \langle \vec{v} \rangle \rangle - \langle \vec{v} \rangle \langle \vec{v} \rangle}_{L} + \underbrace{\left\langle \langle \vec{v} \rangle \vec{v}' \right\rangle - \left\langle \vec{v}' \langle \vec{v} \rangle \right\rangle}_{C} + \underbrace{\left\langle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

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

Break

5 min

Application



Geometry

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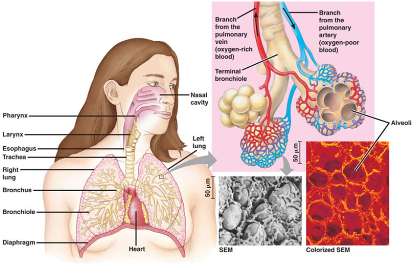

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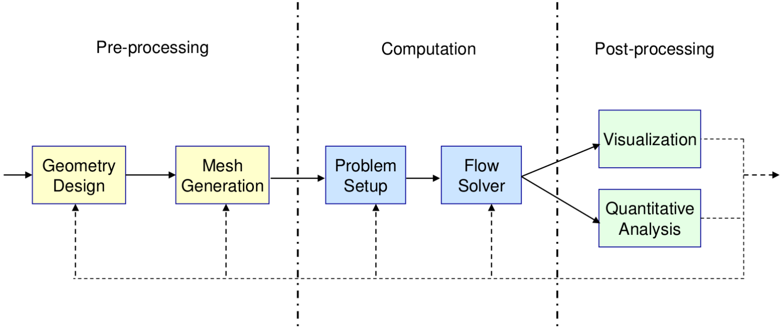
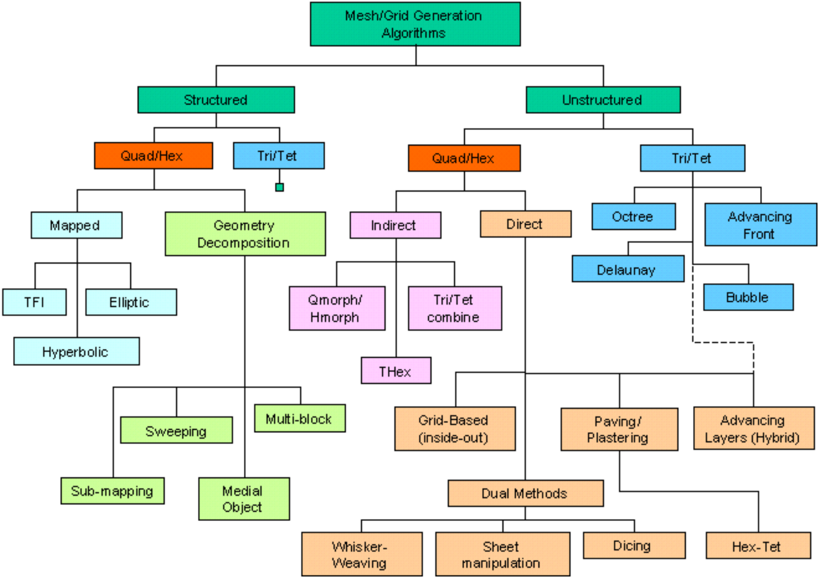


Mesh


Mesh/Grid Generation Algorithms
Structured
Unstructured
Quad/Hex
Tri/Tet
Quad/Hex
Tri/Tet
Mapped
Geometry Decomposition
Indirect
Direct
Octree
Advancing Front
Delaunay
Bubble
TFI
Elliptic
Hyperbolic
Qmorph/ Hmorph
Tri/Tet combine
THex
Sweeping
Multi-block
Sub-mapping
Medial Object
Grid-Based (inside-out)
Paving/ Plastering
Advancing Layers (Hybrid)
Dual Methods
Whisker-Weaving
Sheet manipulation
Dicing
Hex-Tet

Mesh

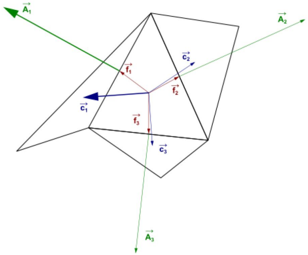
Mesh quality determined by:

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

Mesh - Orthogonal Quality

$$OQ = \min_i \left\{ \frac{A_i \dot{f_i}}{|\vec{A_i}||\vec{f_i}|}, \frac{A_i \dot{c_i}}{|\vec{A_i}||\vec{c_i}|} \right\}, \quad (7)$$

A_i face normal vector
f_i vector from the centroid of the cell to the centroid of that face
c_i vector from the centroid of the cell to the adjacent cell



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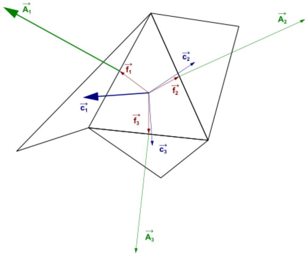

Unacceptable	Bad	Acceptable	Good	Very good	Excellent
0-0.001	0.001-0.14	0.15-0.20	0.20-0.69	0.70-0.95	0.95-1.00

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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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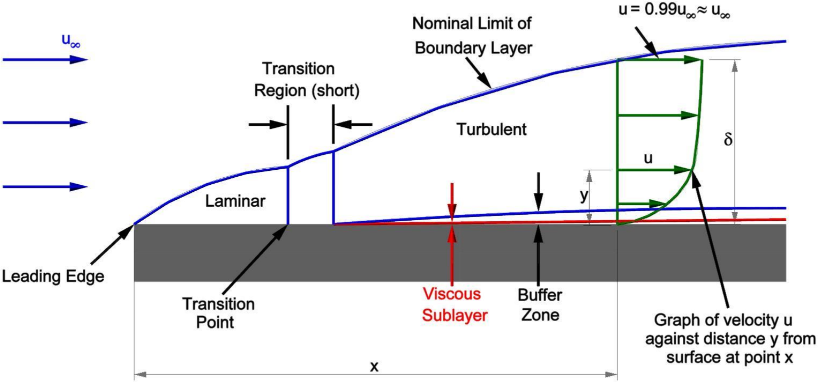
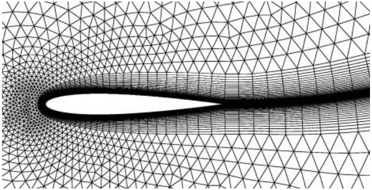
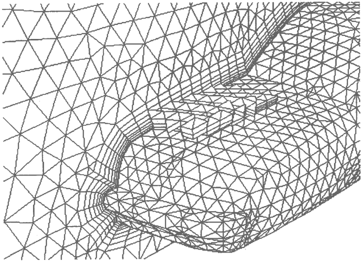


Mesh

Inflation layer examples:





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Hints for mesh generation

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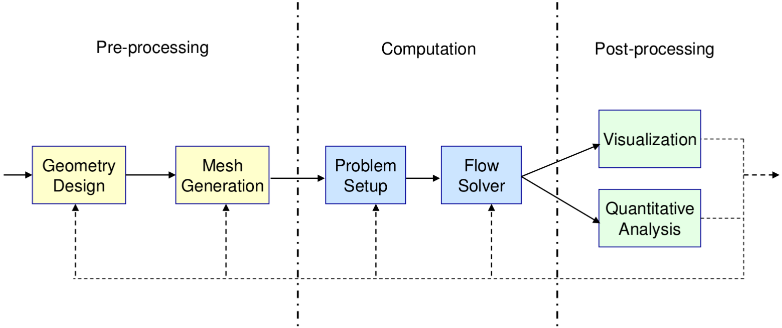
- maximize solution accuracy
  - concentrate mesh elements in critical regions (e.g. boundary layers, wakes, shocks)
  - align quad / hex meshes with flow direction
  - avoid poor quality elements (e.g. twisted, skewed)

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

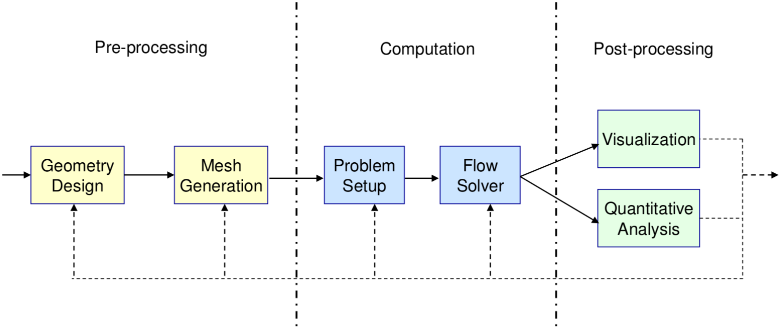
Problem Definition- Numerical solver

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



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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
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- numerical instabilities can arise due to :
  - ill-posed problem (no physical solution)
  - poor quality mesh
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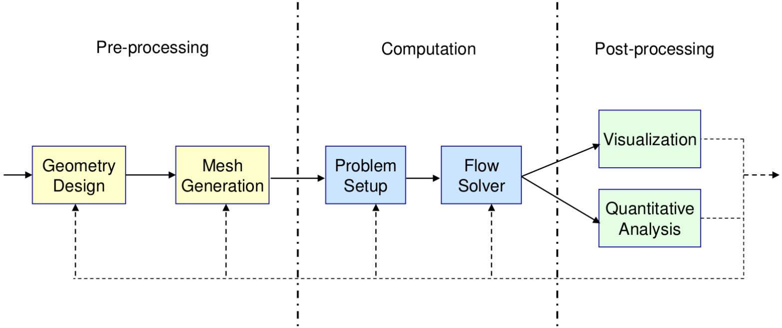
  - inappropriate solver settings
  - inappropriate initial conditions
- trouble-shooting
  - ensure problem is physically realizable
  - compute an initial solution with a first-order discretization scheme
  - decrease under-relaxation for equations having convergence problems (segregated)
  - reduce 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

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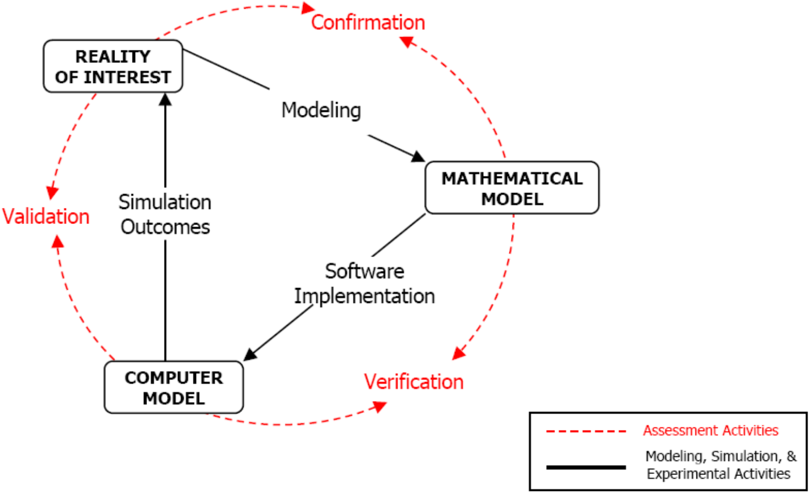
Essentially, one implements a model into a computer code and then uses the code to perform a CFD simulation which yields values used in the engineering analysis.

Verification & Validation - Level 1



Verification & Validation - Level 2