FAKULTA STROJNÍ TUL

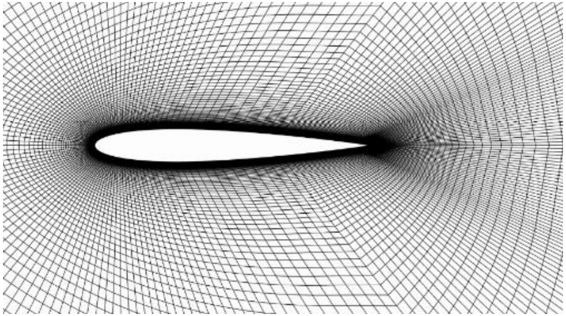
Introduction to Computational Fluid Dynamics (CFD)

Lecture 3, 4

Jan Kracík (jan.kracik@tul.cz)

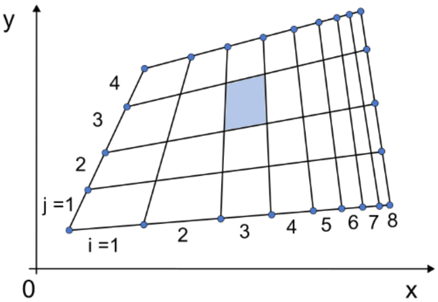
Agenda – Lecture 3, 4

- Computational meshes (topology, density)
- Mesh sensitivity
- Numerical errors
- Boundary conditions (BCs)
- Discretization schemes of convective terms (1st order, 2nd order, …)

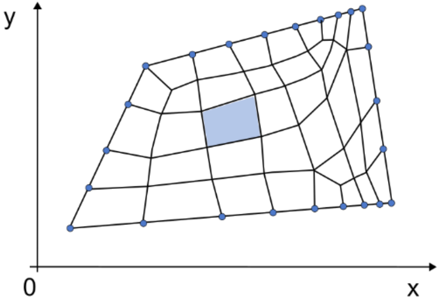


Mesh topology

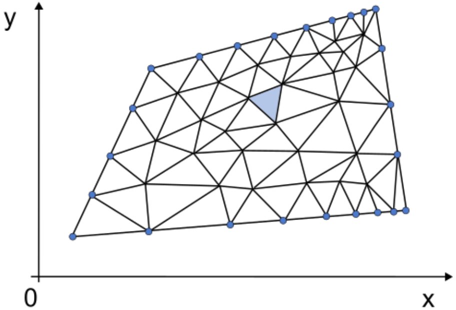
- Most CFD codes use both, **structured** and **unstructured** meshes.



a) Structured quadrilateral 2D mesh (32 cells)



b) Unstructured quadrilateral 2D mesh (38 cells)



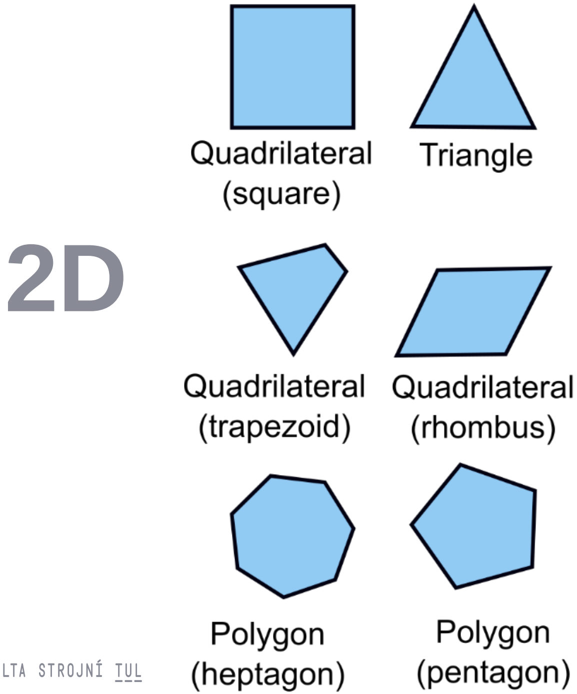
c) Unstructured triangular 2D mesh (76 cells)

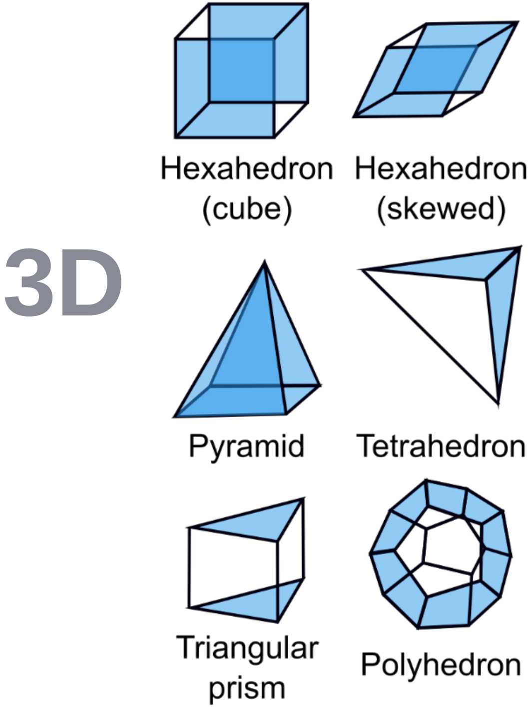
Mesh topology (2)

- Structured meshes consist of planar cells with 4 edges (2D) or volumetric cells with 6 faces (3D).
- Each cell is numbered according to indices (i, j, k).
- We can number intervals (cells) or nodes (not shown here).
- Unstructured meshes consist of cells of various shapes, but typically triangles or quadrilaterals (2D) and tetrahedrons or hexahedrons (3D).
- Unlike structured meshes, one cannot uniquely identify cells by indices for unstructured meshed.
- Instead, cells are numbered in some other way internally in the CFD code.
- A vast number of meshing methodologies exists.

Mesh topology (3)

- Elements of a various shape are used: hexaheral, tetrahedral, polyhedral, wedge, pyramids, …





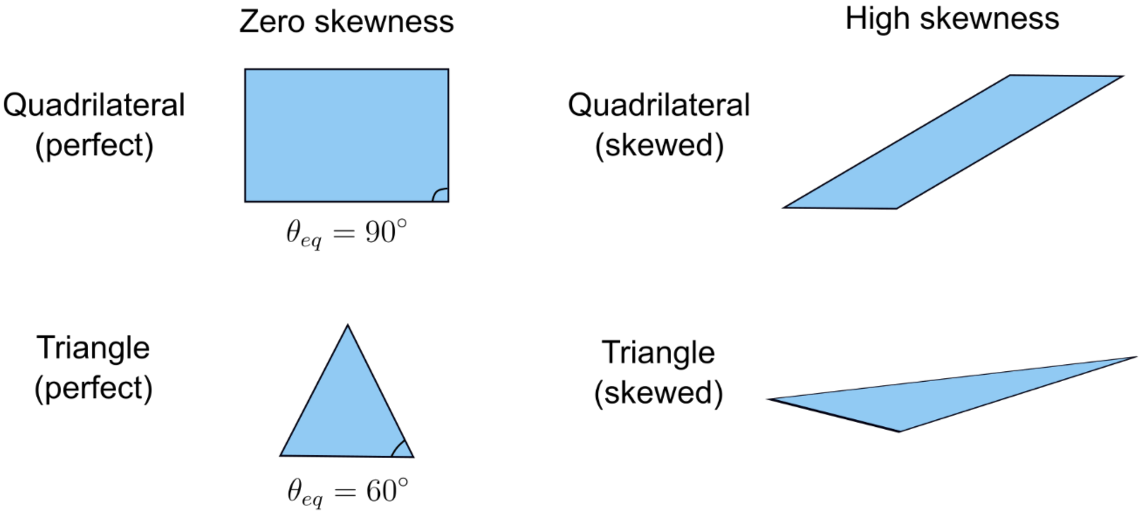
Mesh topology (4)

- Fewer cells are usually generated for structured meshes than for unstructured meshes.
- For complex geometries, unstructured meshes are usually much easier for the user to create.
- Regardless of the type of mesh you use, it is the quality of the mesh that is most important for reliable and meaningful CFD simulations.
- Cells must not be highly skewed or deformed, as this could lead to convergence difficulties and inaccuracies in the simulation.
- Additionally, abrupt changes in cell size across the domain must also be avoided, so the mesh should be as smooth and regular as possible (errors, stability).
- No holes, no overlapping cells, no negative volumes !!!

Mesh quality

- The quality of the mesh plays a significant role in the accuracy and stability of the numerical simulation.
- Many different metrics exist for assessment mesh quality.
- For example, Equivalent **Skewness** (ES), **Orthogonal Quality** (OQ), **Aspect Ratio** (AR), …
- Regardless of the type of mesh used in your domain, checking the quality of your mesh is essential.

Equiangle Skewness

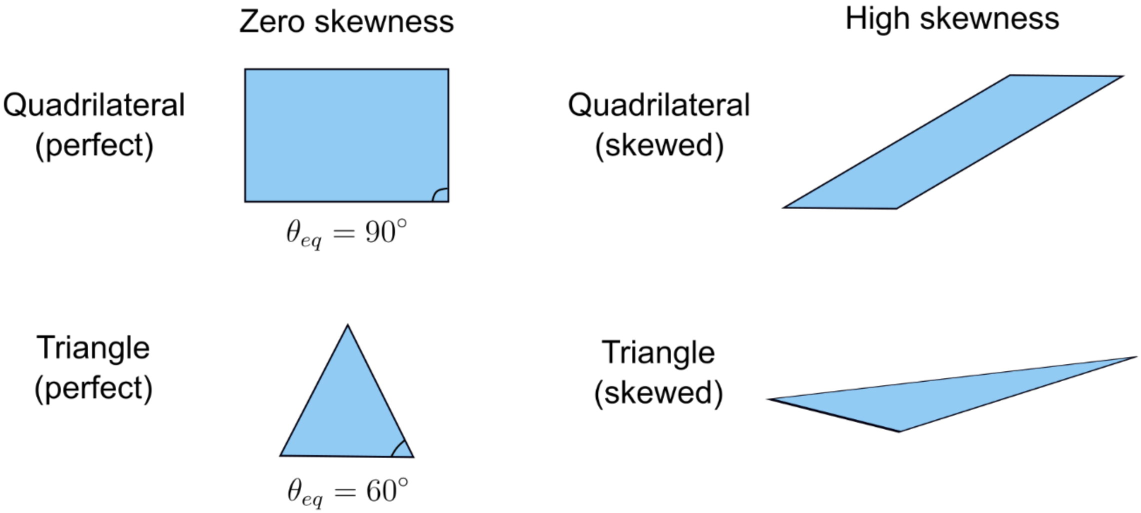


- **Equiangle Skewness** (ES):

$$\boxed{ES = MAX\left(\frac{\Theta_{max} - \Theta_{eq}}{180° - \Theta_{eq}}, \frac{\Theta_{eq} - \Theta_{min}}{\Theta_{eq}}\right)}$$

- Θ_{min} and Θ_{max} are minimum and maximum angles in degrees between any two edges of the cell ($0 < ES < 1$), where **0 is best** and **1 is worst**.

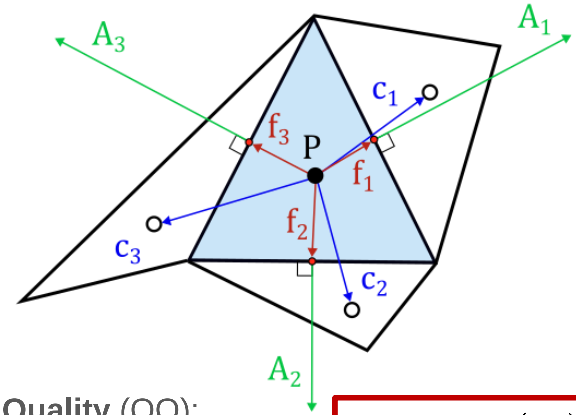
Equiangle Skewness (2)



- ○ the maximum skewness for a tetrahedral mesh should be kept below 0.95.
- ○ Θ_{eq} is the angle between any two edges of an ideal equilateral cell with the same number of edges defined for N-sided polygon as:

$$\theta_{eq} = \frac{180°(N-2)}{N}$$

Orthogonal Quality

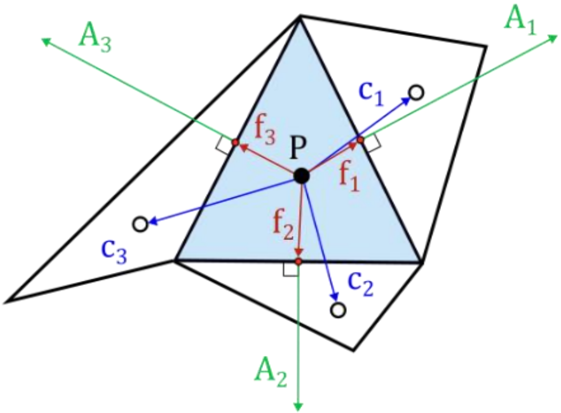


- **Orthogonal Quality** (OQ):

$$OQ = MIN\left(\frac{\overrightarrow{A_i}\cdot\overrightarrow{f_i}}{|\overrightarrow{A_i}||\overrightarrow{f_i}|},\frac{\overrightarrow{A_i}\cdot\overrightarrow{c_i}}{|\overrightarrow{A_i}||\overrightarrow{c_i}|}\right)$$

- A_i is the area vector of a face.
- f_i is a vector from the centroid of the cell to the centroid of that face.
- c_i is a vector from the centroid of the cell to the centroid of the adjacent cell that shares that face.

Orthogonal Quality (2)



- $0 < OQ < 1$, where **0 is worst** and **1 is best** .
- The minimum orthogonal quality for all types of cells should be more than 0.01, with an average value that is significantly higher.

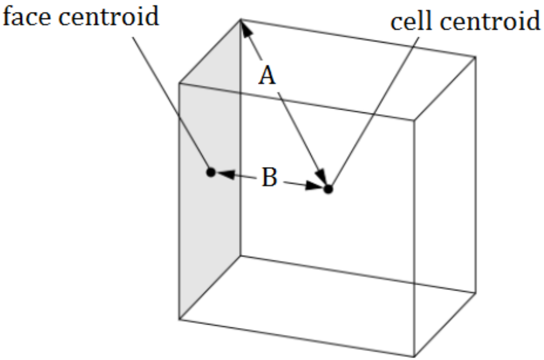
Aspect Ratio (1)

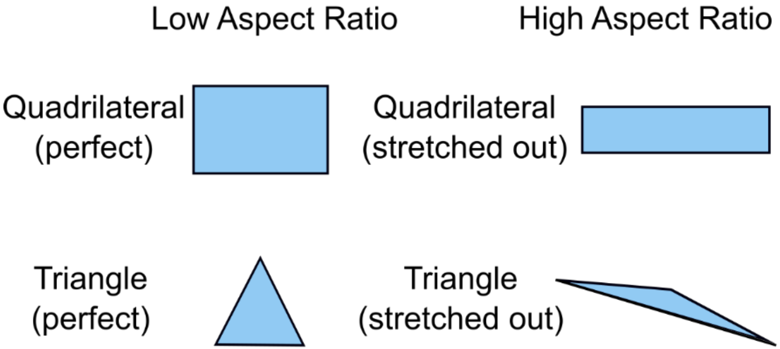
○ **Aspect Ratio** (AR):

$$\boxed{AR = \frac{Longest\ Side}{Shortest\ Side} = \frac{A}{B}}$$

○ AR is computed as the ratio of the maximum value to the minimum value of any of the following distances: normal distances between the cell centroid and face centroids, distances between the cell centroid and nodes, or faces enclosing the 3D element.

○ 1 or 1.41 < AR < ∞, where **1 (1.41) is best and ∞ is worst (not possible).**




Low Aspect Ratio

High Aspect Ratio

Quadrilateral (perfect)

Quadrilateral (stretched out)

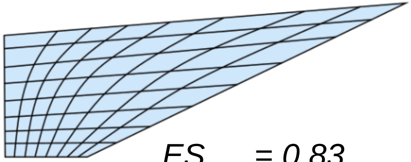
Triangle (perfect)

Triangle (stretched out)

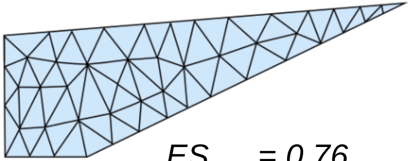
Mesh quality – Best practices

- Cells with a very large aspect ratio may cause difficulties.
- The cell count can often be minimized by using a structured mesh.
- However, a structured mesh does not have to be always the best choice, depending on **the shape of the domain** (geometry).
- A high-quality unstructured mesh is always better than a poor-quality structured mesh!

Structured quadrilateral mesh (64 cells)



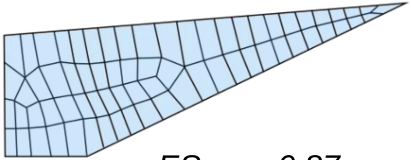
$ES_{max} = 0.83$



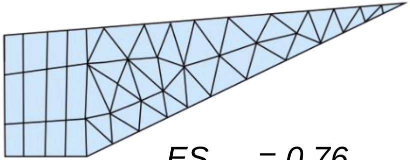
$ES_{max} = 0.76$

Unstructured triangular mesh (70 cells)

Unstructured quadrilateral mesh (67 cells)



$ES_{max} = 0.87$



$ES_{max} = 0.76$

Hybrid (unstructured and structured) mesh (62 cells)

Mesh density

- Since a real continuous domain is defined as discrete, the degree to which the **important features of the flow are resolved depends on the density and distribution of mesh elements**.

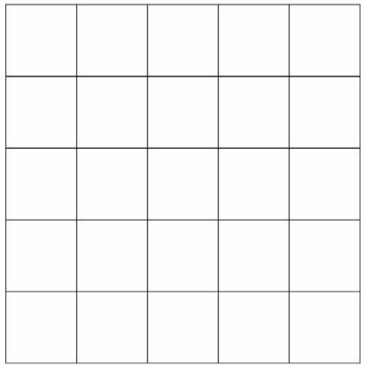
- Among such features belong shear layers, separated regions, shock waves, boundary layers, and mixing zones.

- Poor resolution in critical regions can dramatically affect results!

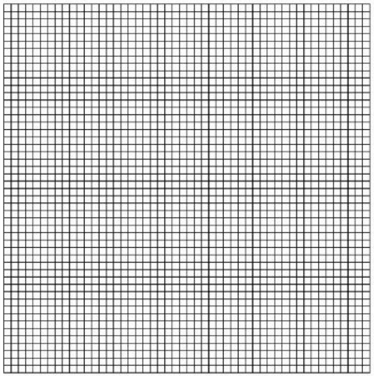
- **Resolution of the boundary layer** plays a significant role in the accuracy of the computed wall shear stress and heat transfer coefficient.

Mesh density (2)

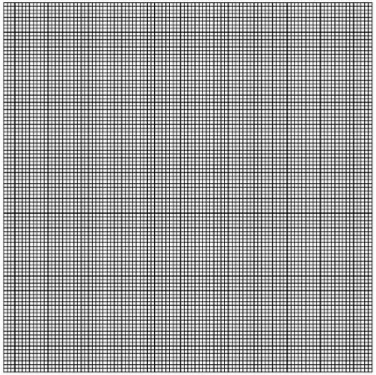
- Flow resolution (1 cell = 1 stored value of pressure, velocity, temperature, etc.)
- Accuracy vs. false diffusion
- Mesh sensitivity study (at least 3 meshes)



a) Coarse mesh
(5x5), 25 cells



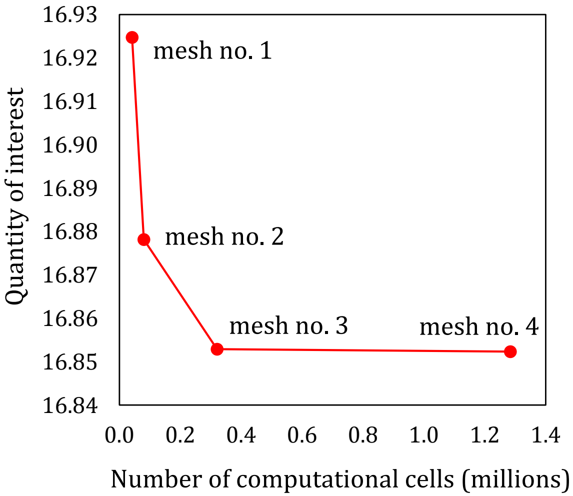
b) **Medium** mesh
(50x50), 2,500 cells



c) **Fine** mesh
(100x100), 10,000 cells

Mesh sensitivity study

- Influence of mesh density should be always investigated!
- We always look for a trade-off between accuracy and computational cost.
- Mesh sensitivity study is related to **the domain discretization error**.



Mesh 1 – 40,000 cells	“Coarse”
Mesh 2 – 80,000 cells	“Medium”
Mesh 3 – 320,000 cells	“Fine”
Mesh 4 – 1,200,000 cells	“Very fine”

Errors in CFD simulations

○ CFD simulation results always differ from its true or exact values.

○ This difference is **the error of the solution**.

○ The total error is always a sum of the following errors.

Classification of errors:

☐ Physical modeling
☐ Geometry modelling
☐ Geometry discretization
☐ Equation discretization
☐ Round-off (computer)
☐ Iterative convergence

Acknowledged

☐ Computer programming
☐ Usage

Unacknowledged

Errors in CFD simulations (2)

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Acknowledged

- ☐ Co [illegible] ro [illegible] g
- ☐ Usa [illegible]

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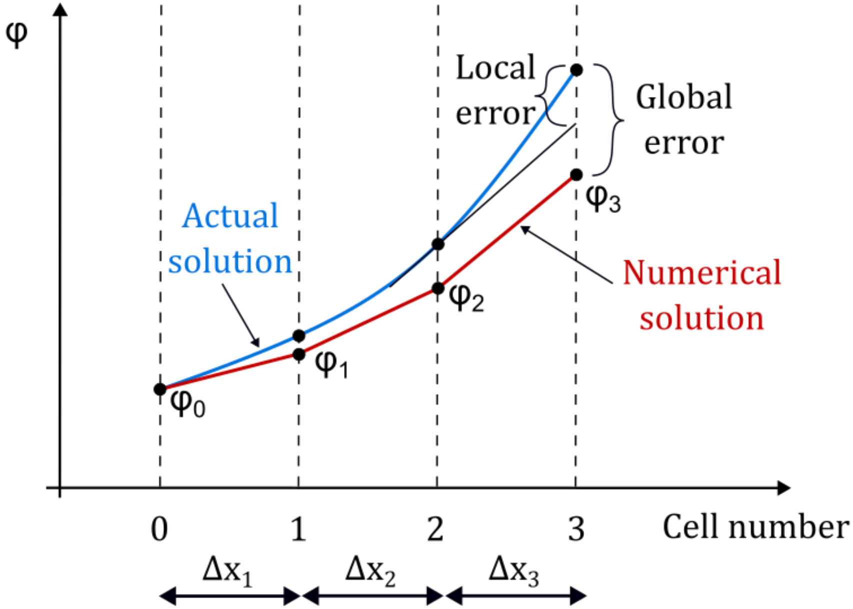
Discretization Error

- ○ The discretization error can be related to the domain, equations, and time domain.

Discretization error:

- ☐ Local error
- ☐ Global error

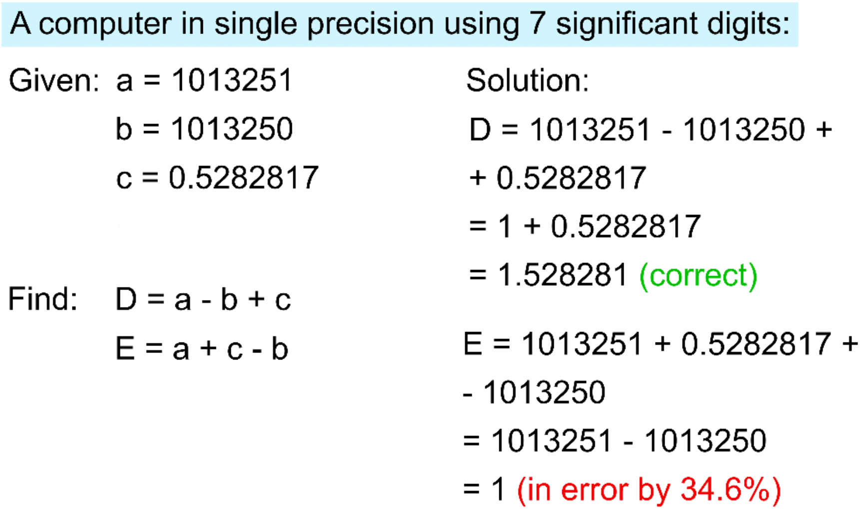


Round-Off Error

- This type of error would not exist if we had a computer that could retain an infinte number of digits for all numbers.
- In that case, the numerical and the exact solution would be the same if we did not consider any other types of error.

Round-off error:

- ❑ Single-precision error
- ❑ Double-precision error



A computer in single precision using 7 significant digits:

Given: a = 1013251
b = 1013250
c = 0.5282817

Find: D = a - b + c
E = a + c - b

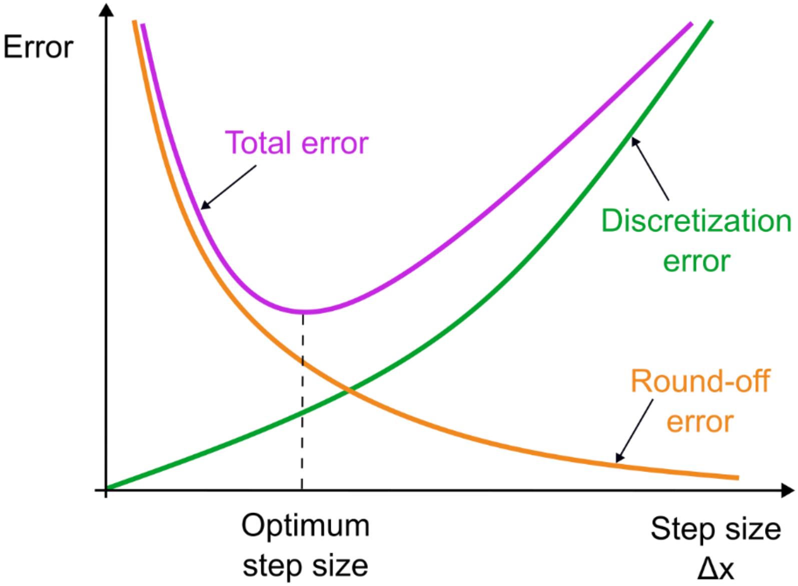
Solution:
D = 1013251 - 1013250 +
+ 0.5282817
= 1 + 0.5282817
= 1.528281 (correct)

E = 1013251 + 0.5282817 +
- 1013250
= 1013251 - 1013250
= 1 (in error by 34.6%)

Controling the total error

- Disregarding all other types of error and considering only the 2 aforementioned types, we can combine them to get an optimum step size (Time step for transient problems).

- By doing so, we get a total error, as shown in the diagram below.



Boundary conditions in CFD simulations

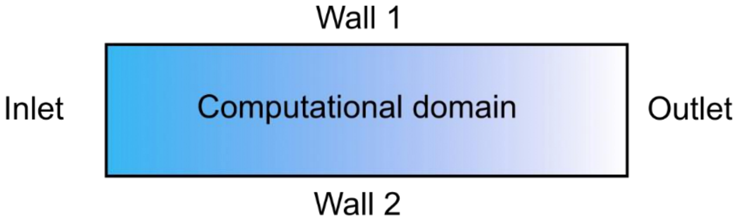
- Appropriate BCs are required to obtain an accurate results!

General BCs:

- ☐ Dirichlet BC (a value is specified)
- ☐ Neumann BC (a gradient is specified)
- ☐ Combined and special BC

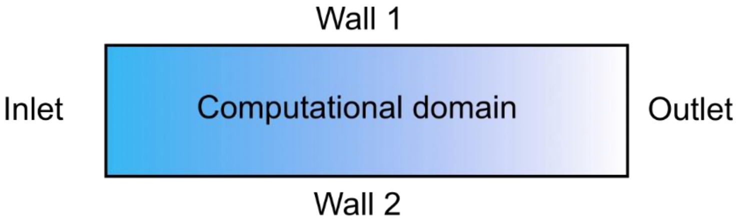
Specific types of BCs:

- ☐ Wall BCs
- ☐ Inflow/Outflow BCs
- ☐ Internal BCs
- ☐ Other (miscellaneous) BCs



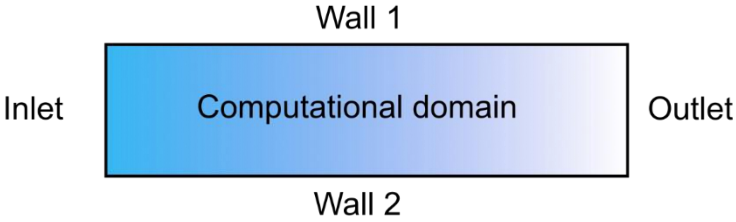
Wall boundary conditions

- The simplest BCs.
- Fluid cannot pass through a wall, therefore the normal component of velocity is set to zero (relative to the wall).
- If the no-slip condition is used, the tangential component of velocity is also set to zero.
- If the energy equation is being solved, either wall temperature or wall heat flux must be defined (but not both).
- BCs for other transport equations must also be specified (e.g. turbulence).



Wall boundary conditions (2)

- We can also specify a zero-shear-stress along free surfaces to simulate an “inviscid“ wall.
- By using this, we can simulate a free surface of a swimming pool.
- But we suppress the waves on the free surface and associated pressure fluctuations.
- For turbulent flows, wall roughness may be specified by means of wall functions (the law-of-the-wall).



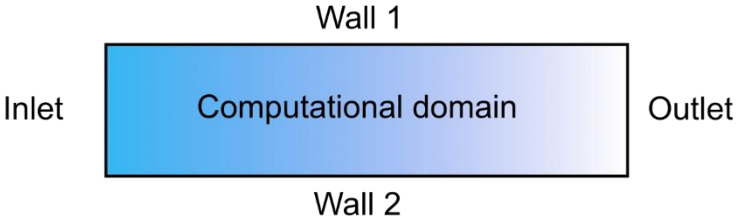
Inflow/Outflow boundary conditions

- The boundaries through which a fluid enters (Inflow) or leaves (Outflow) the computational domain.

Classification of Inflow/Outflow BCs:

- ☐ Velocity-specified BCs (velocity inlet, mass flow inlet, …)
- ☐ Pressure-specified BCs (pressure inlet, pressure outlet, …)
- ☐ Not specified BCs (outflow, …)

- If the energy equation or other scalar equations (turbulence) are being solved, their parameters must also be specified.

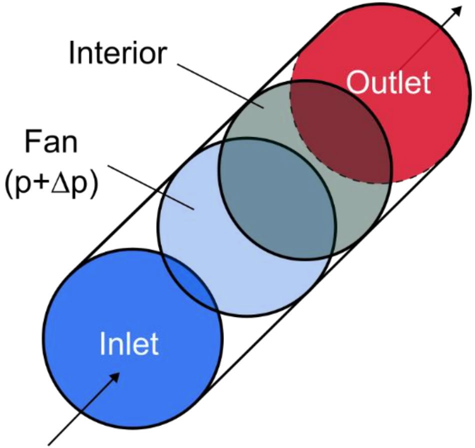


Internal boundary conditions

- DO NOT define a boundary of the computational domain.
- They are specified INSIDE the domain.

Classification of Internal BCs:

- ☐ Interior BCs (a flow crosses through the domain)
- ☐ Fan BCs (induce a pressure rise/drop across the domain)



Symmetry and periodic boundary conditions

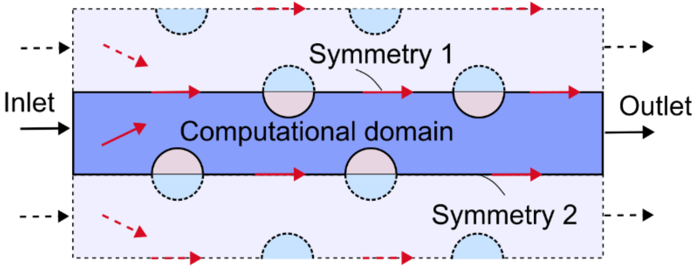
- They are neither walls nor inlets or outlets of the computational domain.

- They enforce some kind of periodicity or symmetry of the domain.

Classification of Symmetry/Periodic BCs:

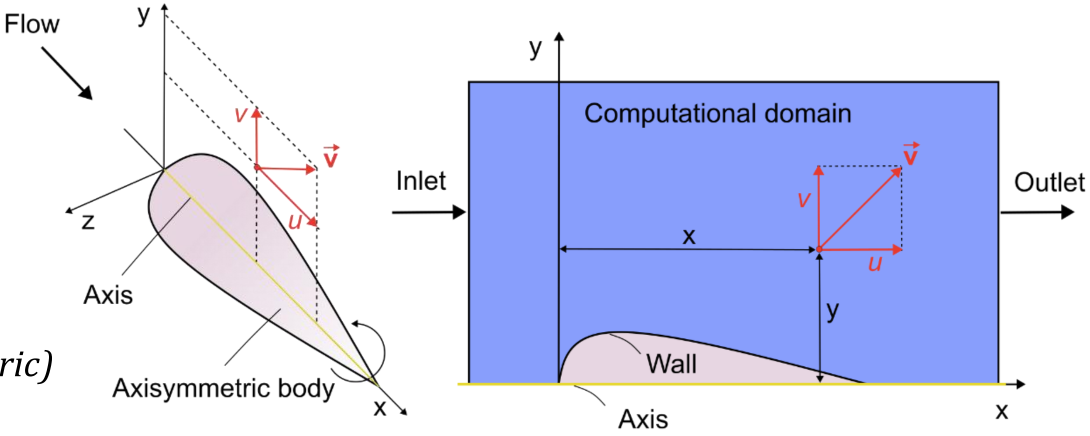
- ☐ Periodic BCs (translational or rotational)
- ☐ Symmetry BCs (a symmetry plane or axis for axisymmetric flows)

Symmetry boundary conditions



Symmetry

(plane symmetric)

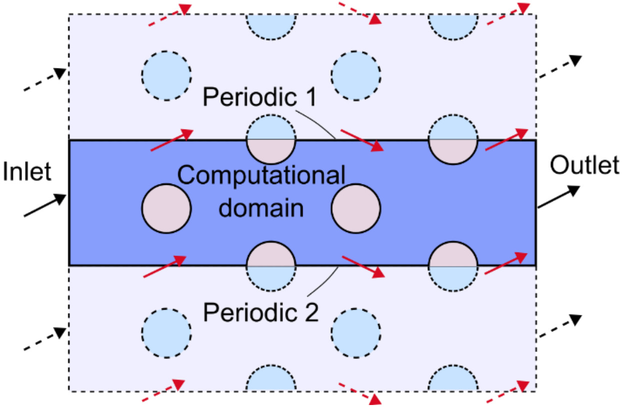


Axis

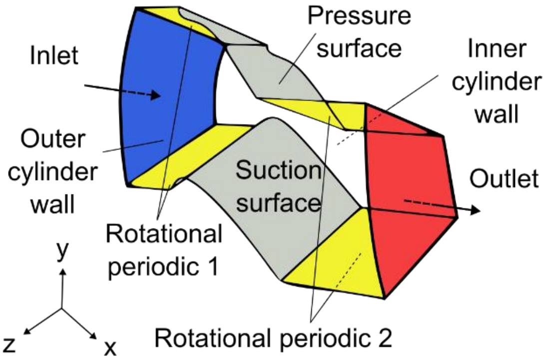
(axisymmetric)

Periodic boundary conditions

Translational periodic

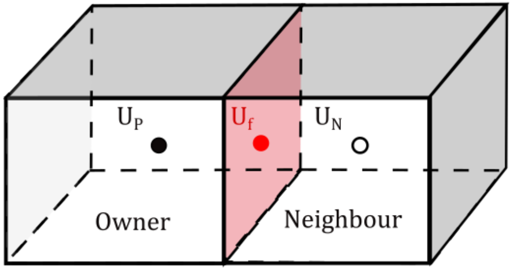


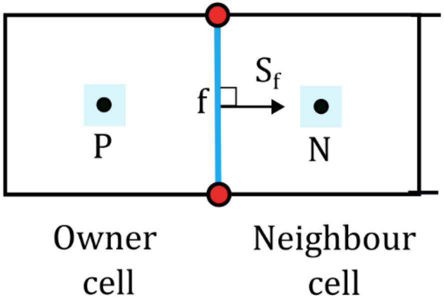
Rotational periodic



Discretization schemes for convective terms

- Also known as interpolation schemes.
- Values are usually stored at cell centroids.
- For fluxes (gradients), we need values at cell faces.
- There are several options how to determine the cell face values.





Discretization schemes for convective terms (2)

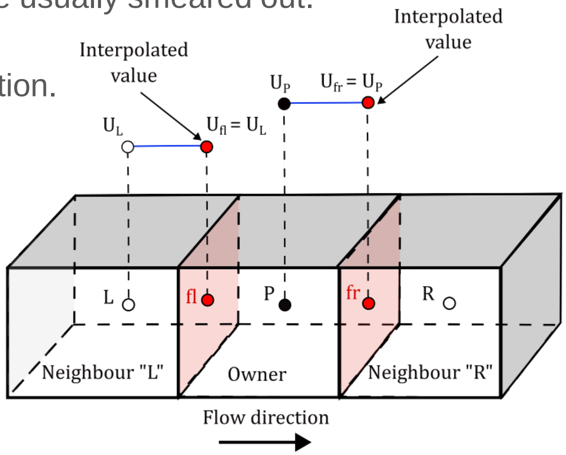
- Face values of U (Uf) are found by using an appropriate scheme.
- Assumption about variation of U between 2 cell centers.

Most often used schemes for convective terms:

- ☐ First-Order Upwind
- ☐ Second-Order Upwind
- ☐ Central Differencing (linear interpolation)
- ☐ QUICK (Quadratic Upstream Interpolation for Convective Kinematics)

First-Order Upwind Scheme

- The simplest numerical scheme.
- Value of U at the face is the same as the value at the cell centre UPSTREAM the face (DIRECTION-DEPENDENT !)
- Easy to implement and results in very stable calculations.
- Very diffusive, gradients in the flow field are usually smeared out.
- Best scheme for the beginning of a calculation.



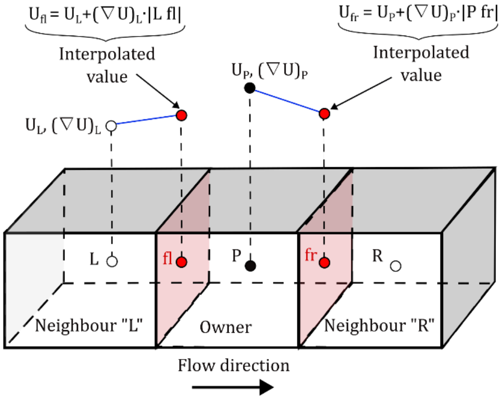
Second-Order Upwind Scheme

- Value of U at the face from the cell centroid value and its gradient upstream the face.

- More accurate than First-Order Upwind (also DIRECTION-DEPENDENT !).

- In regions with strong gradients can results in face values that are outside of the range of cell values (limiters may be applied).

- Popular scheme for its trade-off between accuracy and stability.



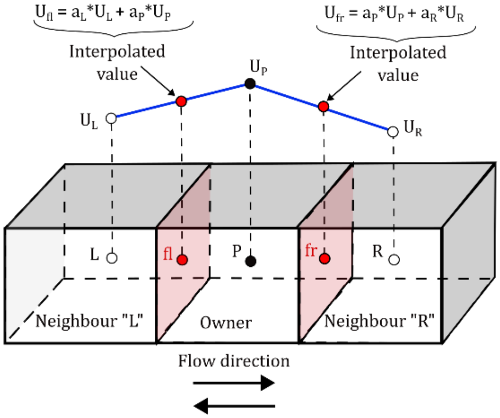
Central-Differencing Scheme

- Value of U at the face by linear interpolation between the cell upstream and downstream.

- More accurate than First-Order Upwind.

- May lead to oscillations in the solution (divergence) if the local Peclet number is larger than 2.

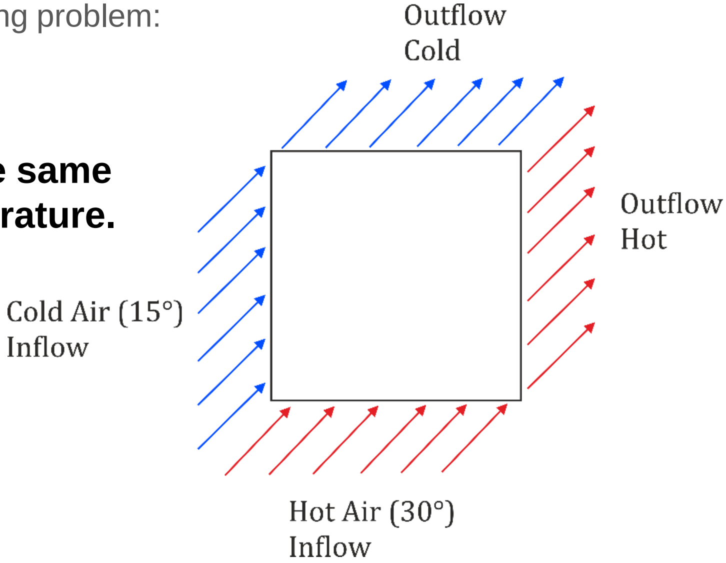
- Possible to switch to First-Order Upwind in cells where Peclet number is greater than 2 (hybrid scheme).



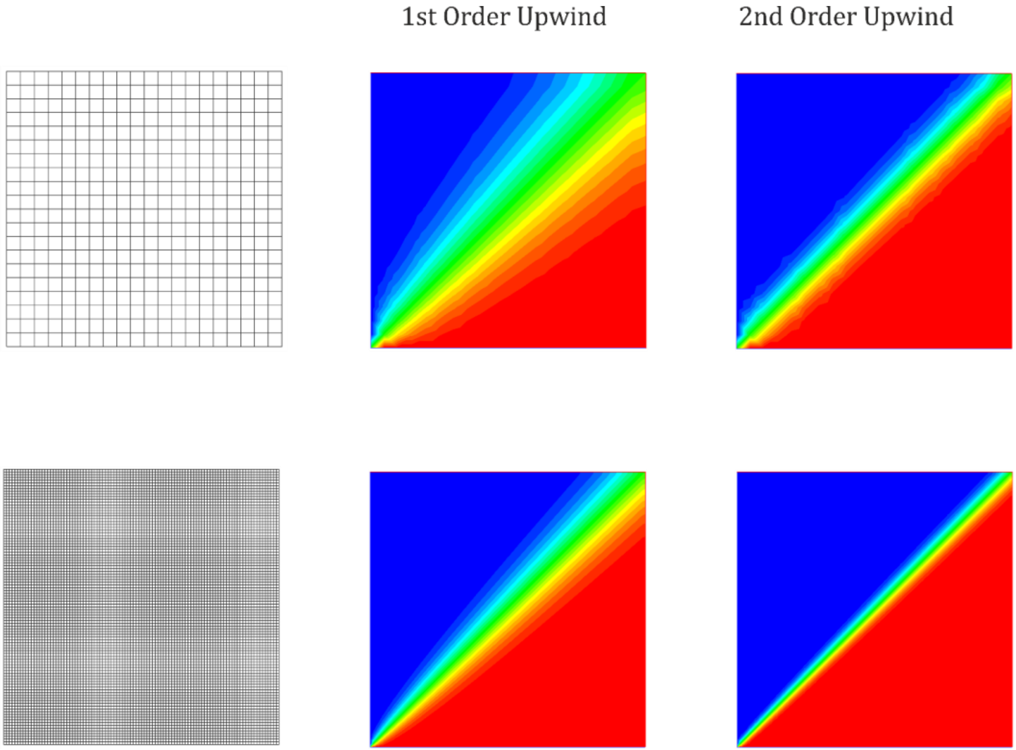
Accuracy and False Diffusion

- We always try to find a trade-off between accuracy and computational time costs.
- Sometimes a less accurate solution can show us important trends in a short time.
- A less accurate solution is often used as a starting point for a more accurate solution.
- As an example, consider the following problem:

2 parallel streams moving at the same velocity but at a different temperature.



Accuracy and False Diffusion (2)



Coarse 20 x 20 (400 cells)

Fine 100 x 100 (10000 cells)

Summary

- Mesh topology and density play a crucial role
- Mesh sensitivity study (discretization error)
- Numerical errors in the final solution
- Boundary conditions
- Discretization schemes of convective terms (accuracy vs. time cost)

Thank You!