Introduction to Computational Fluid Dynamics (CFD)

Lecture 3, 4 (Part 2)

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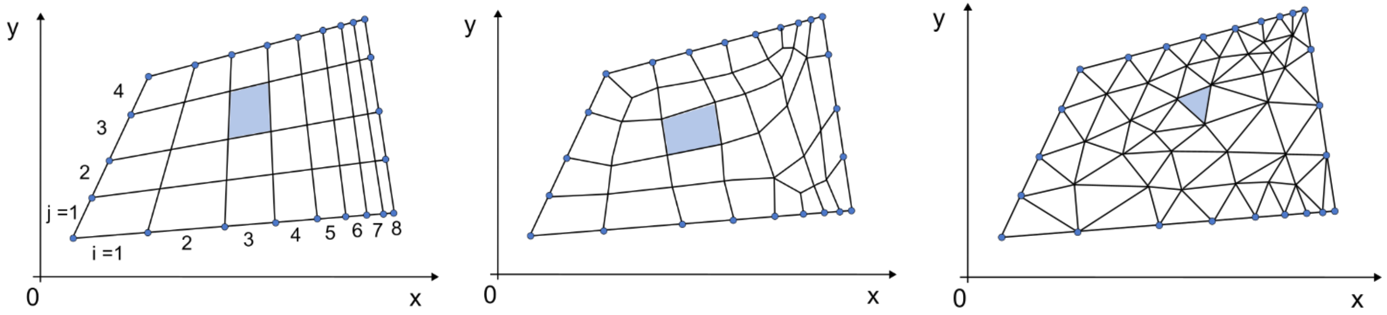
Agenda – Lecture 3

- Computational meshes (topology, density)
- Mesh sensitivity
- Numerical errors

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)

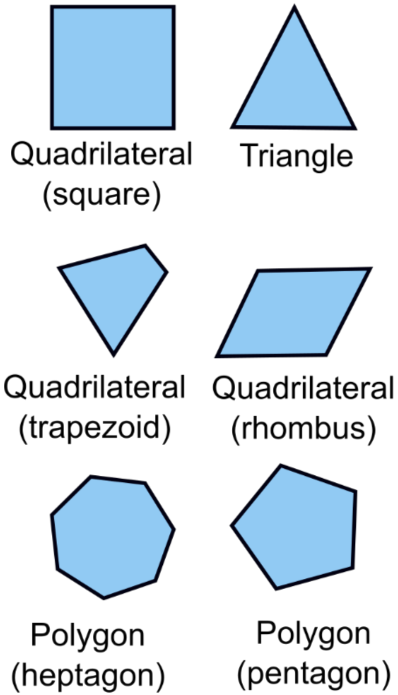
Mesh topology (2)

- 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.

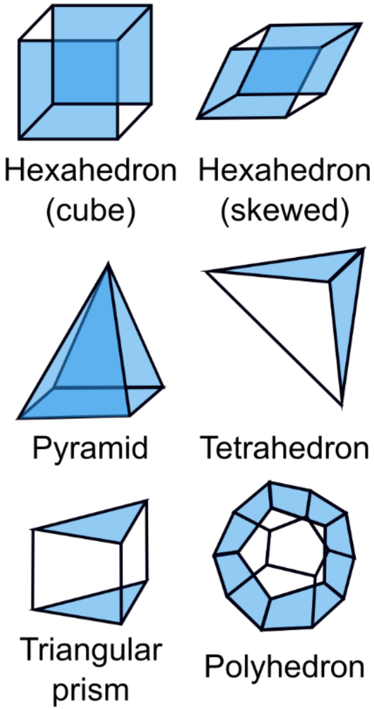
Mesh topology (3)

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

2D



3D



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

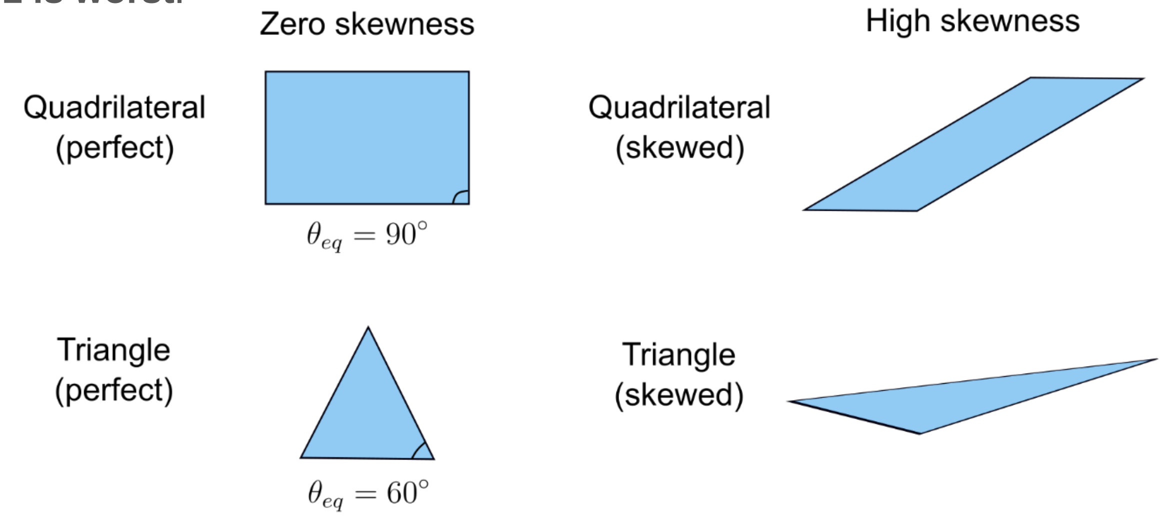
- The quality of the mesh plays a significant role in the accuracy and stability of the numerical simulation.
- Many different metrics exist for assessment mesh quality.
- For example, Equivalent **Skewness** (ES), **Orthogonal Quality** (OQ), **Aspect Ratio** (AR), …
- Regardless of the type of mesh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

Equiangle Skewness

- **Equiangle Skewness** (ES):

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

- 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**.

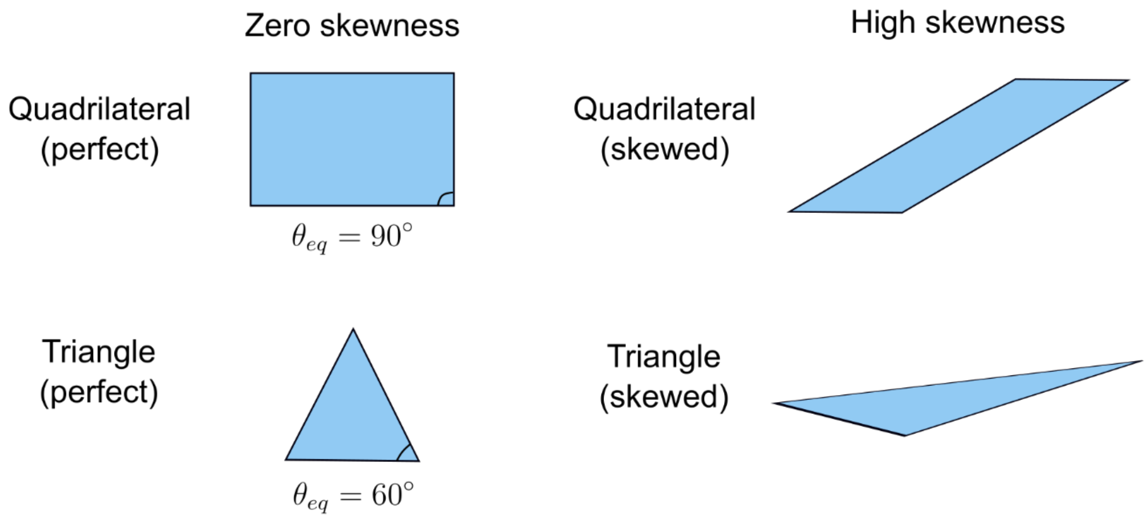


Equiangle Skewness (2)

- 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:

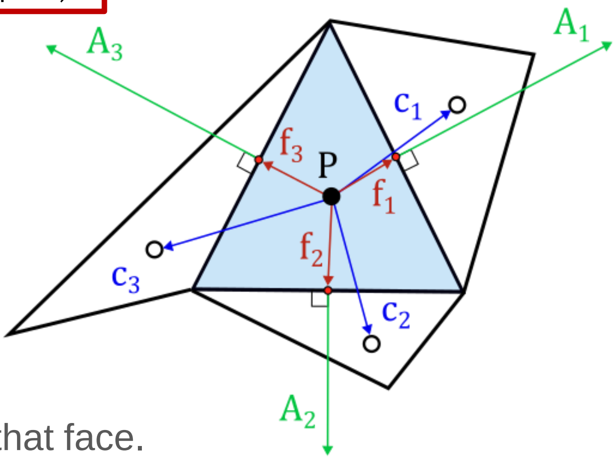
$$\theta_{eq} = \frac{180°(N-2)}{N}$$



Orthogonal Quality

- **Orthogonal Quality** (OQ):

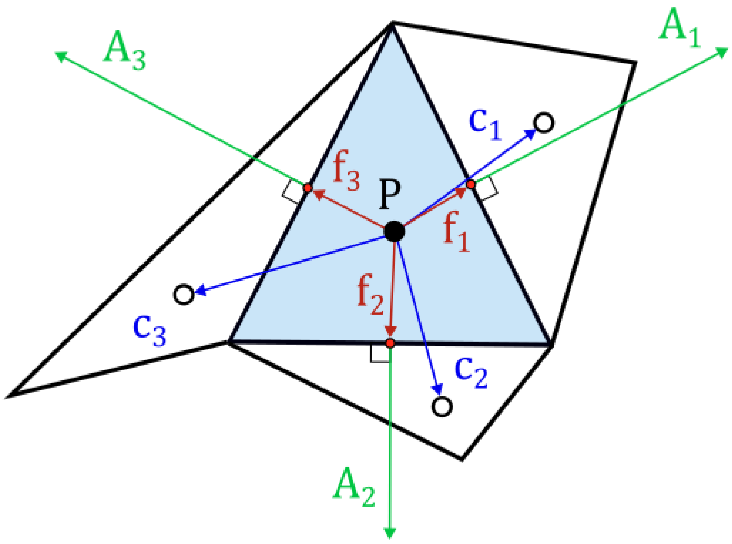
$$OQ = MIN\left(\frac{\vec{A_i}\cdot\vec{f_i}}{|\vec{A_i}||\vec{f_i}|}, \frac{\vec{A_i}\cdot\vec{c_i}}{|\vec{A_i}||\vec{c_i}|}\right)$$



- 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 0.1, with an average value that is significantly higher.

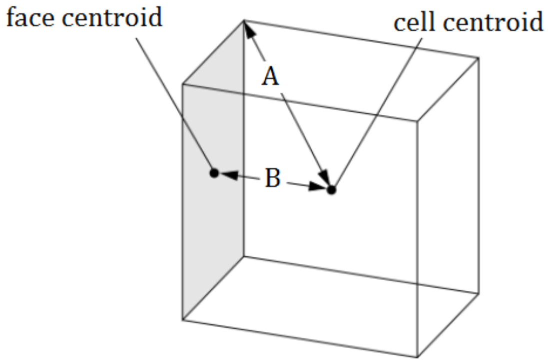


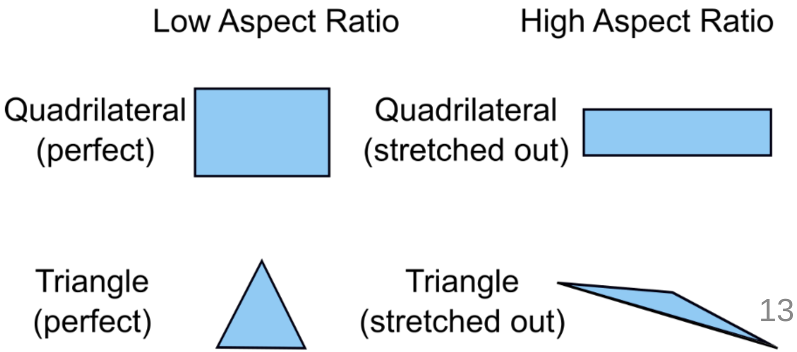
Aspect Ratio

- **Aspect Ratio** (AR): $$AR = \frac{Longest\ Side}{Shortest\ Side} = \frac{A}{B}$$

- 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).**





Mesh quality – Best practices

- Cells with a very large aspect ratio may cause difficulties.

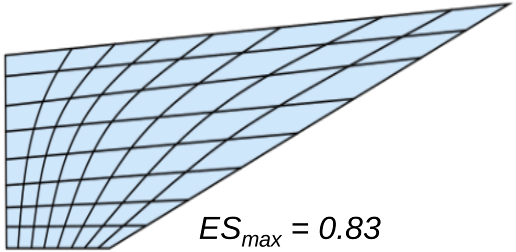
- The cell count can often be minimized by using a structured mesh.

- However, a structured mesh does not have to be always the best choice, depending **on the shape of the domain** (geometry).

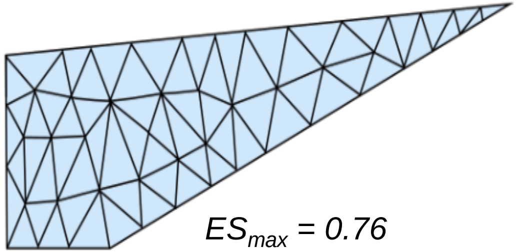
- A high-quality unstructured mesh is always better than a poor-quality structured mesh!

Mesh quality – Best practices

Structured quadrilateral mesh (64 cells)



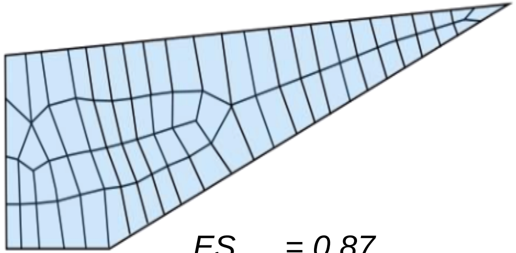
$ES_{max} = 0.83$



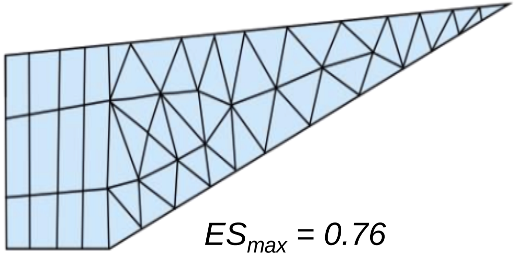
$ES_{max} = 0.76$

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**.

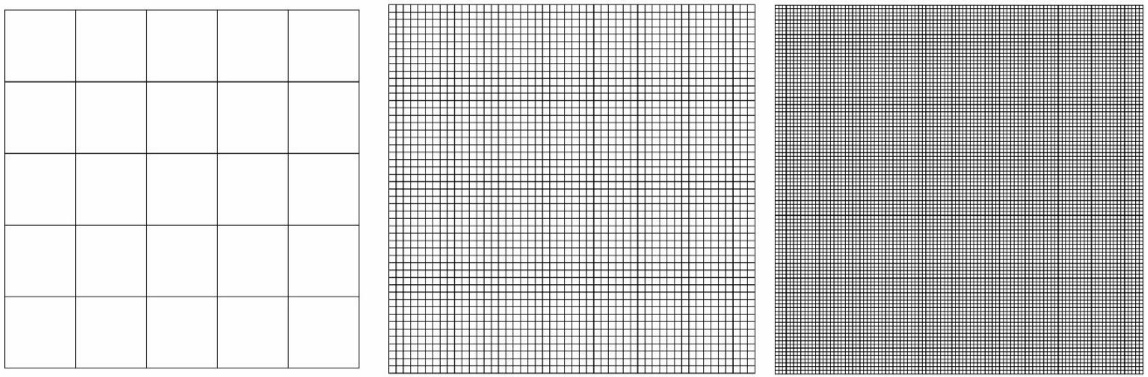
- Among such features belong shear layers, separated regions, shock waves, boundary layers, and mixing zones.

- 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)

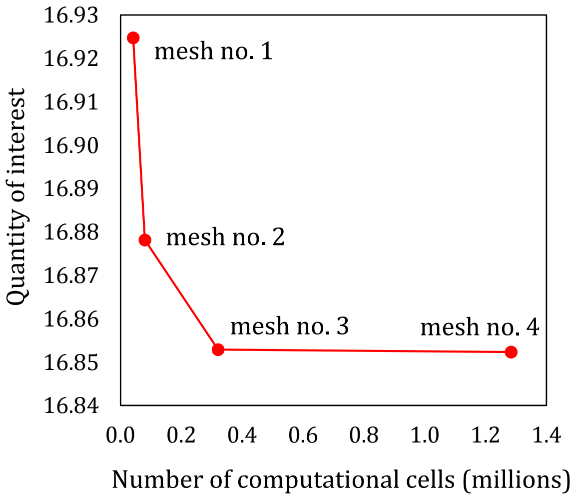
- Flow resolution (1 cell = 1 stored value of pressure, velocity, temperature, etc.)
- Accuracy vs. false diffusion
- Mesh sensitivity study (at least 3 meshes)



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.
- We recognize *2 main types of errors in CFD*:
    - **Acknowledged**
    - **Unacknowledged**

Errors in CFD simulations

Acknowledged

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

Unacknowledged

- Computer programming
- Usage

Errors in CFD simulations

Acknowledged

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

Unacknowledged

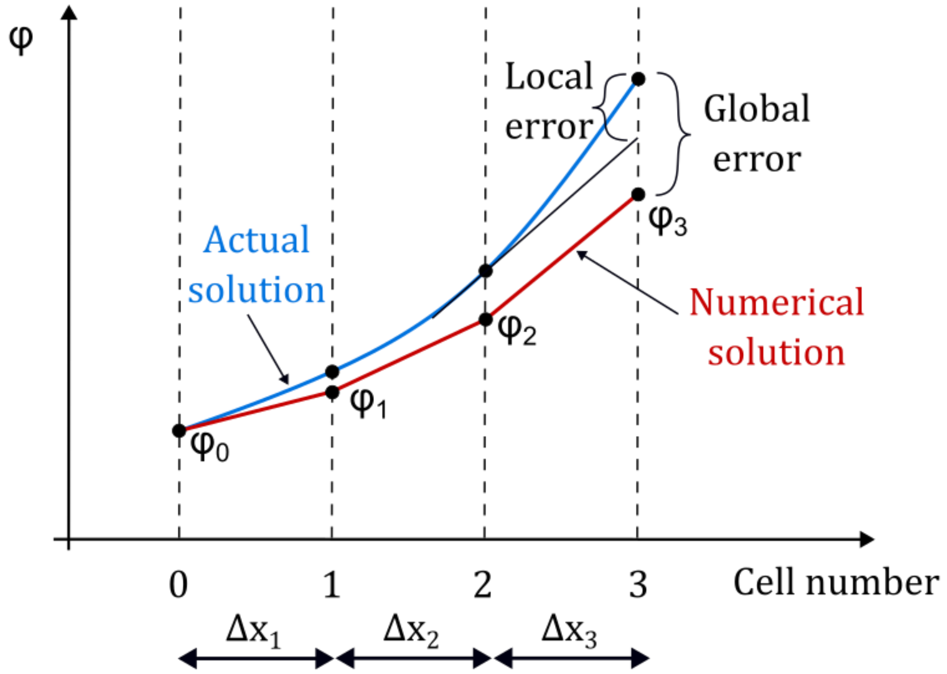
- ❑ [illegible]ng
- ❑ U[illegible]

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 infinite 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**

Round-Off Error (2)

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

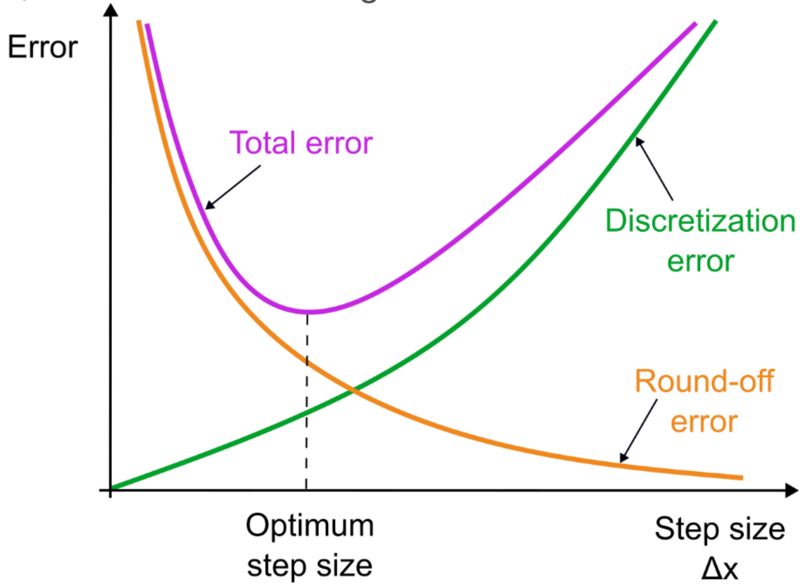
= 1013251 - 1013250

= 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.



Summary – Lecture 3

- **Topology and density** of computational meshes
- The importance of **mesh sensitivity study**
- **Types of errors** in numerical simulations

Agenda – Lecture 4

- Boundary conditions (BCs)
- Discretization schemes of convective terms (1st order, 2nd order, …)

Boundary conditions in CFD simulations

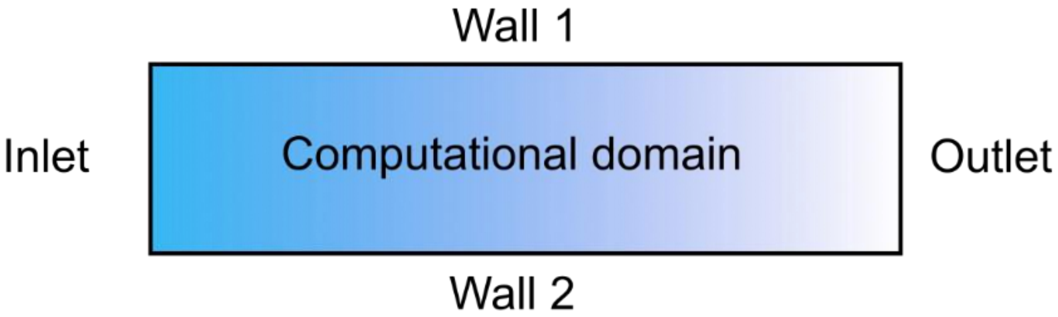
- Appropriate BCs are required to obtain an accurate results!

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

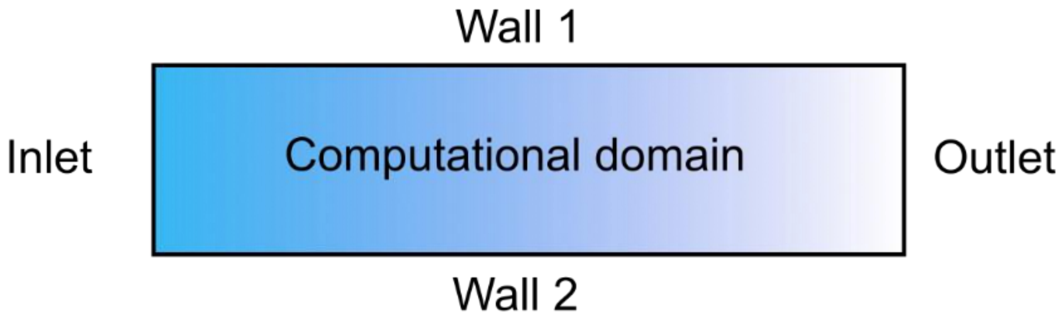


Wall boundary conditions

- One of 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, …)

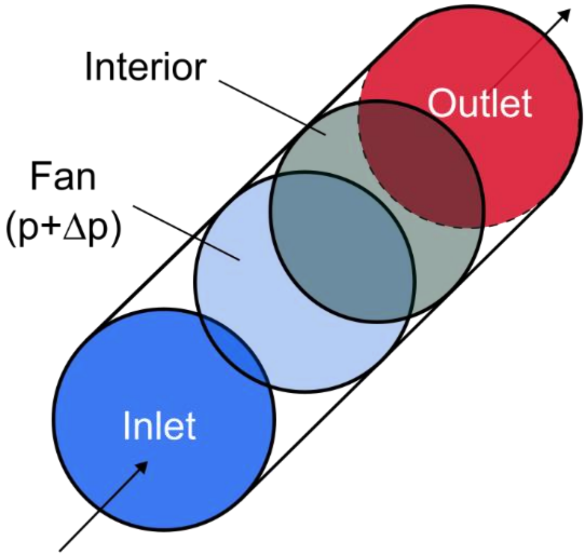
- If the energy equation or other scalar equations (turbulence) are being solved, their parameters must also be specified.

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.

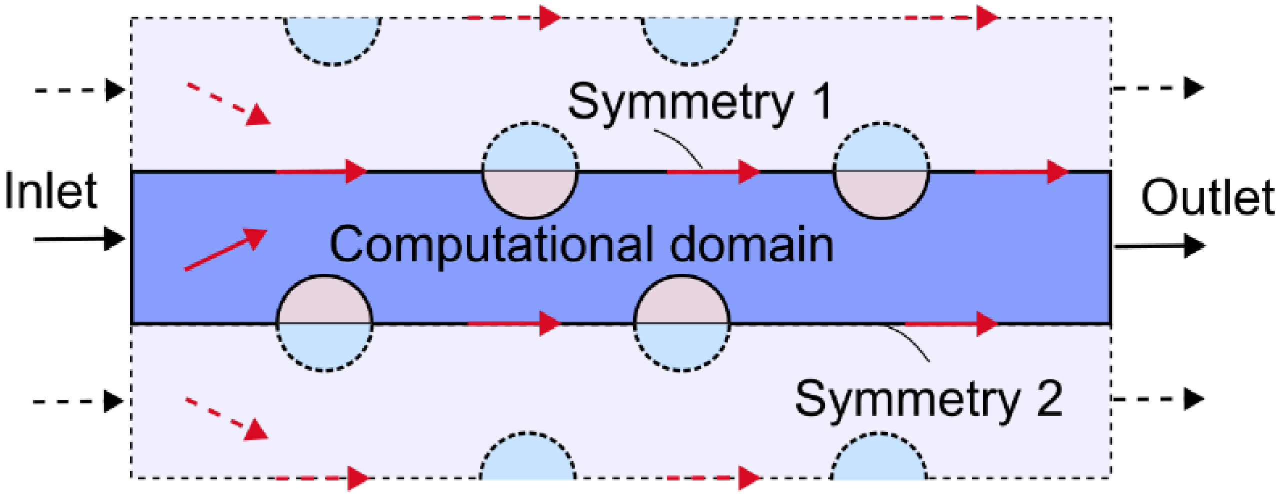
- They enforce some kind of periodicity or symmetry of the domain.

Classification of Symmetry/Periodic BCs:

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

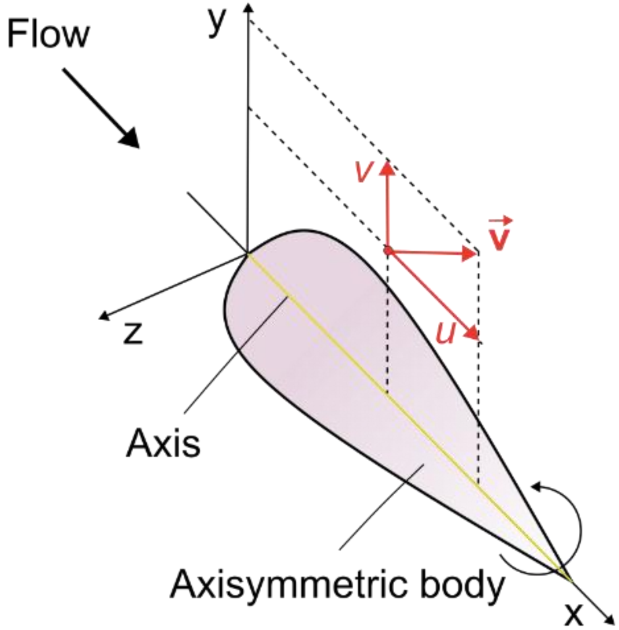
Symmetry boundary conditions

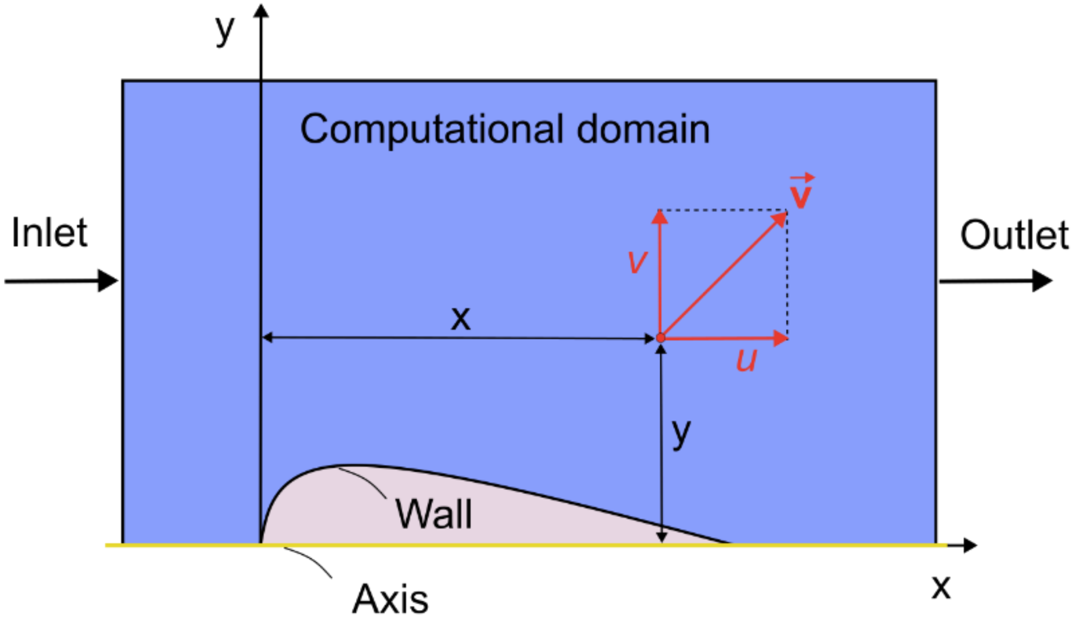
Symmetry *(plane symmetric)*



Symmetry boundary conditions (2)

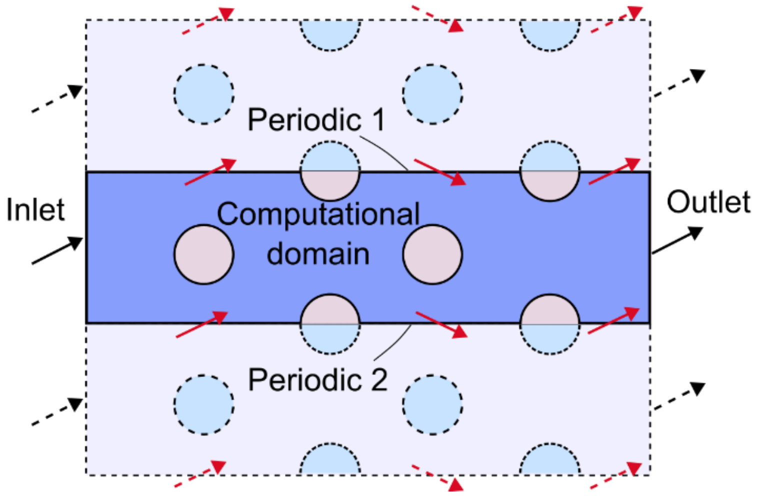
Axis *(axisymmetric)*



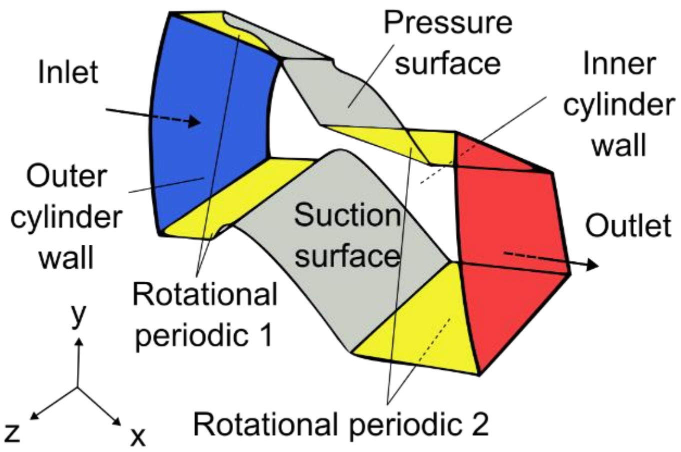


Periodic boundary conditions

Translational periodic

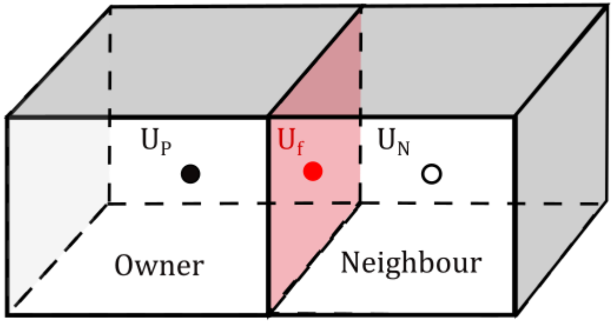


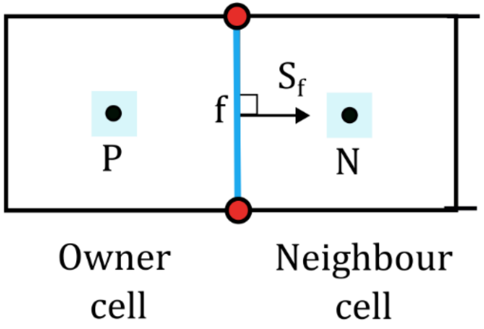
Rotational periodic



Discretization schemes for convective terms

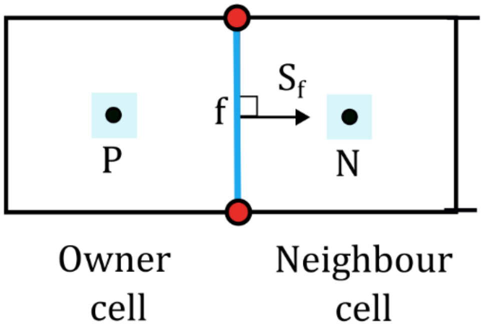
- Also known as **interpolation schemes**.
- **Values are usually stored at cell centroids**.
- For fluxes (gradients), **we need values at cell faces**.
- There are several options how to determine the cell face values.





Discretization schemes for convective terms (2)

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



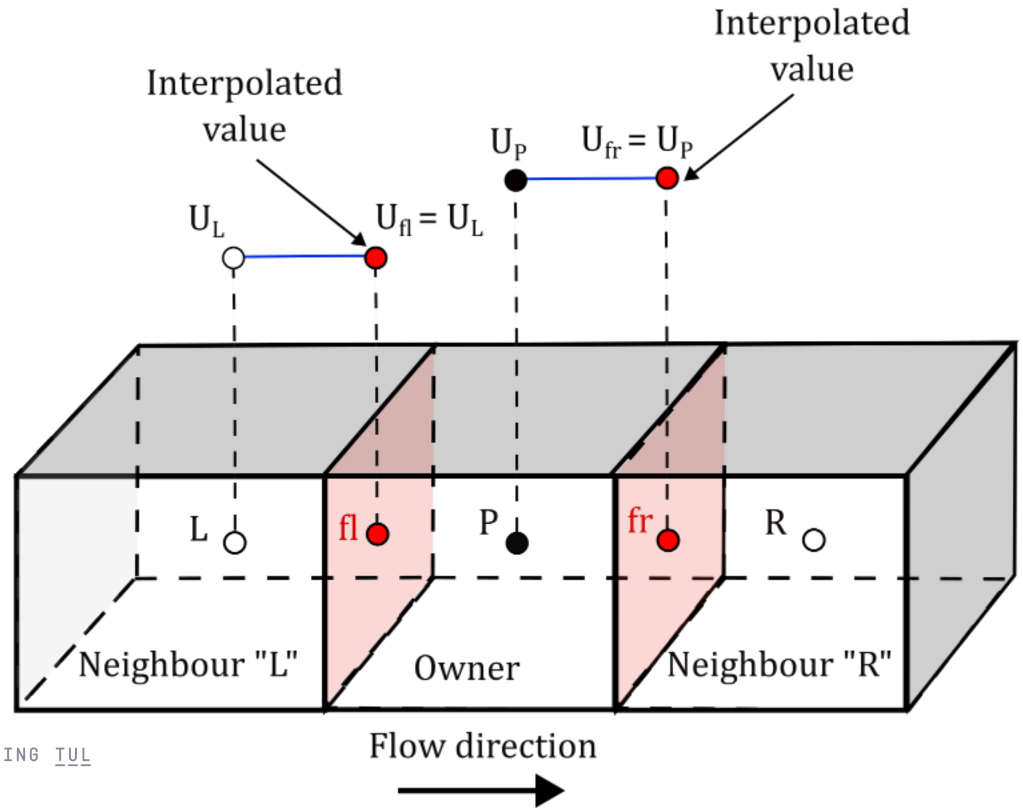
Most often used schemes for convective terms:

- 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.

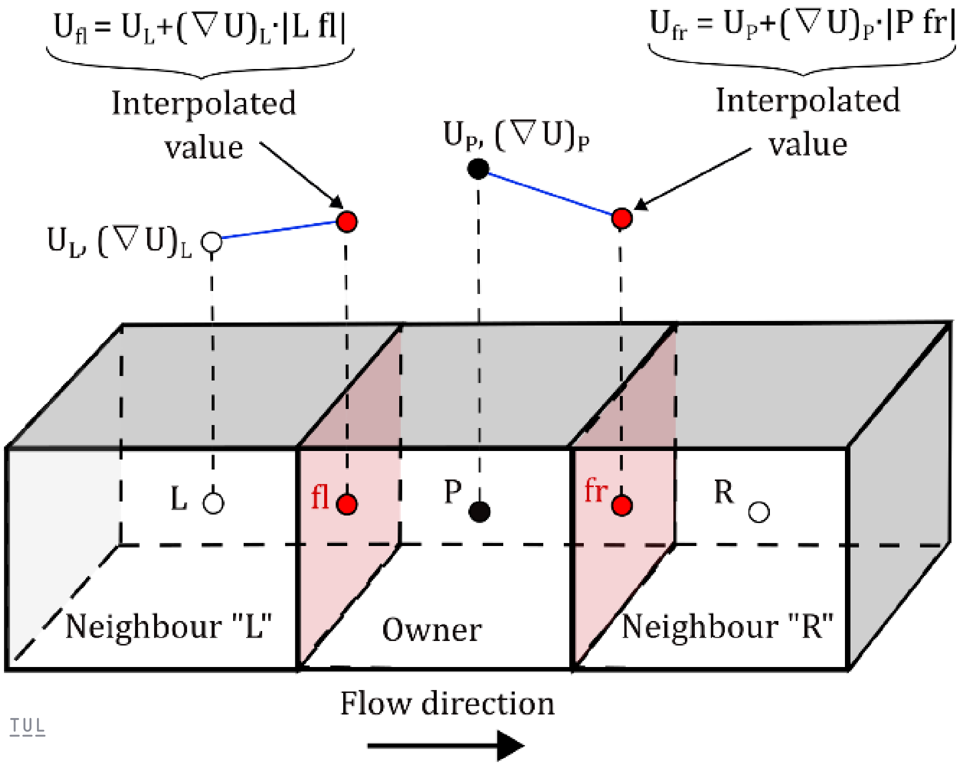
First-Order Upwind Scheme (2)



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**.

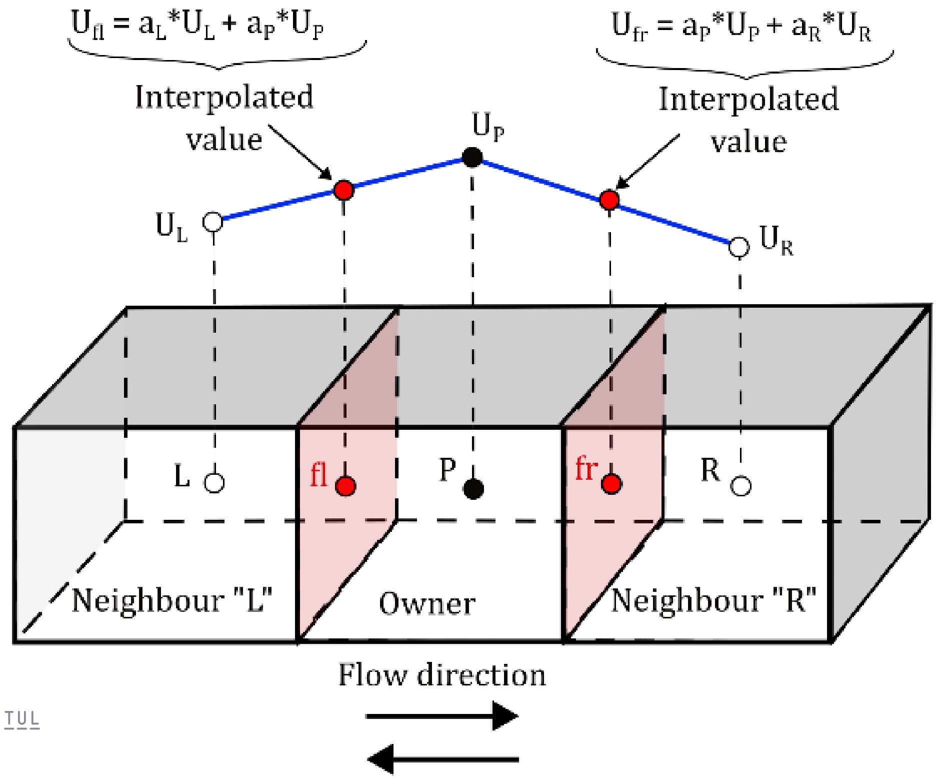
Second-Order Upwind Scheme (2)



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).

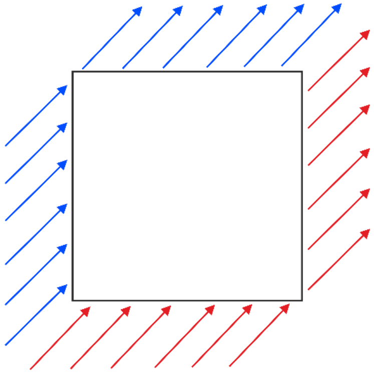
Central-Differencing Scheme (2)



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.

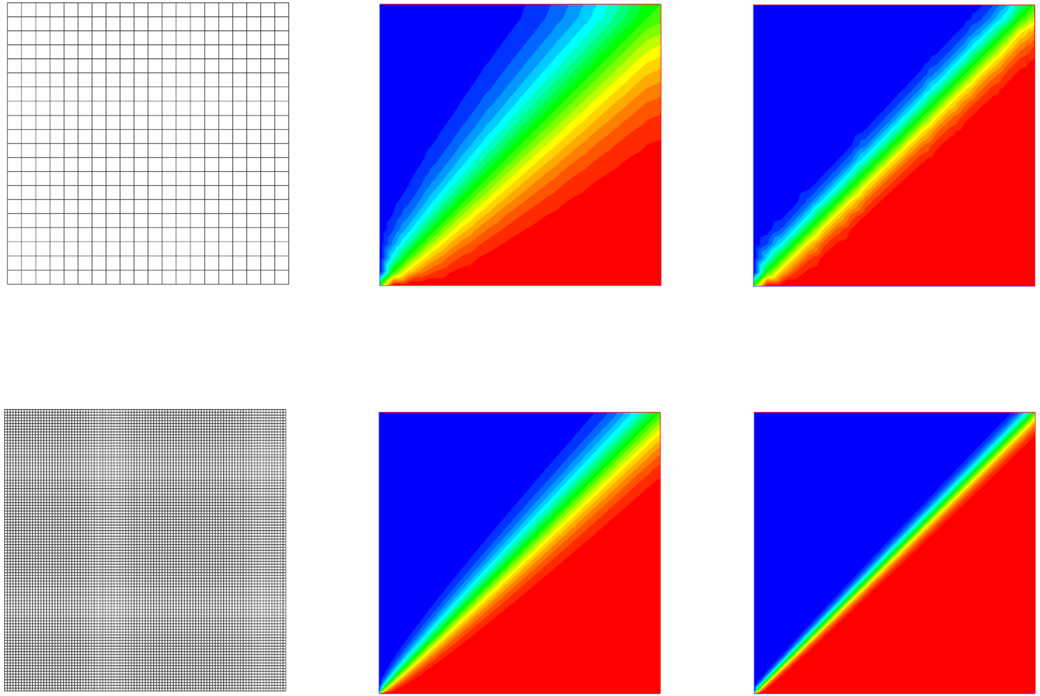


Accuracy and False Diffusion (2)

1st Order Upwind | 2nd Order Upwind

Coarse — 20 x 20 (400 cells)

Fine — 100 x 100 (10000 cells)



Summary – Lecture 4

- **Boundary conditions**
- **Discretization (interpolation) schemes of convective terms**

Thank you.