FACULTY OF MECHANICAL ENGINEERING TUL



Introduction to Computational Fluid Dynamics (CFD)

Lectures 3 and 4 (Part 2)

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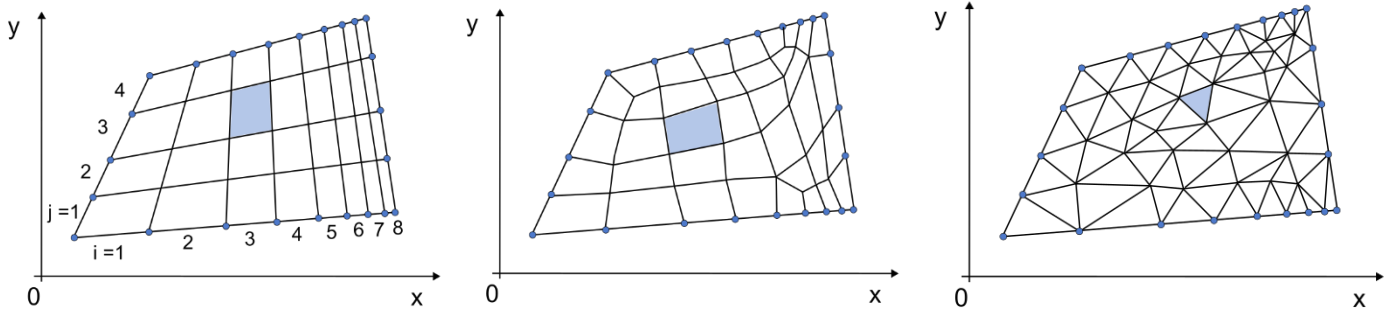
Agenda – Lecture 3

- 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)

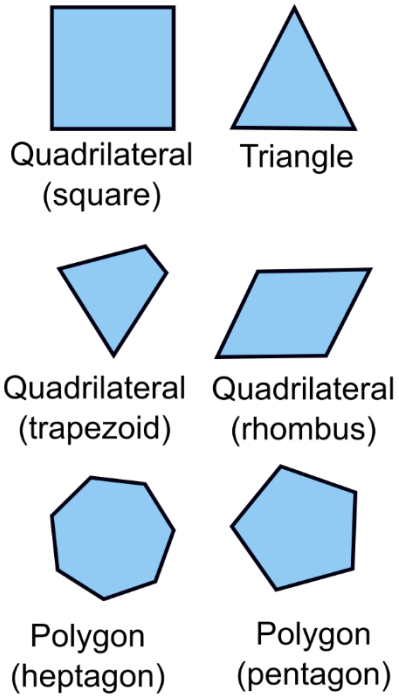
Mesh topology (2)

- Structured meshes consist of planar cells with 4 edges (2D) or volumetric cells with 6 faces (3D).
- Each cell is identified by its indices (i, j, k).
- We can number either the cells or the nodes (not shown here).
- Unstructured meshes consist of cells of various shapes, typically triangles or quadrilaterals (2D) and tetrahedra or hexahedra (3D).
- In unstructured meshes, cells cannot be uniquely identified by indices.
- Instead, the CFD code numbers the cells internally in some other way.
- A vast number of meshing methods exist.

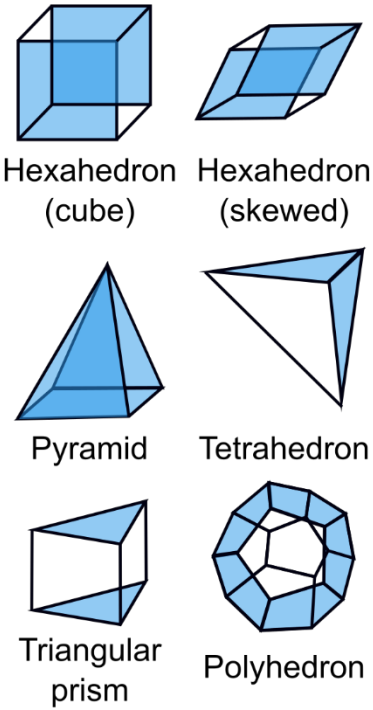
Mesh topology (3)

- Various element shapes are used: hexahedral, tetrahedral, polyhedral, wedge, pyramid, …

2D



3D



Mesh topology (4)

- Structured meshes usually require fewer cells than unstructured meshes.
- For complex geometries, **unstructured meshes are usually much easier** for the user **to create**.
- Regardless of the mesh type, mesh quality is what matters most 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 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

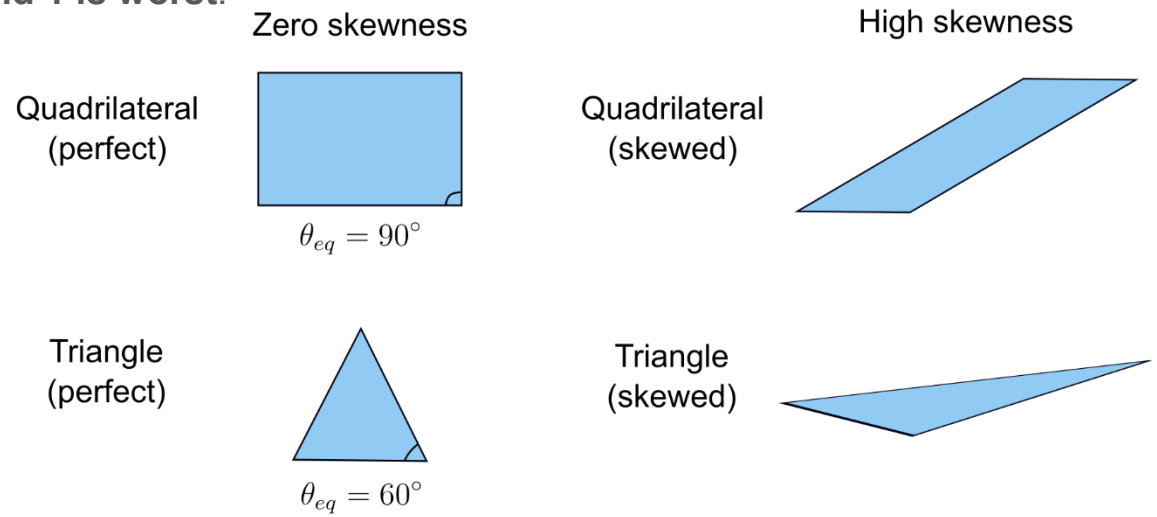
- The quality of the mesh plays a significant role in the accuracy and stability of the numerical simulation.
- Many different metrics exist for assessing mesh quality.
- For example, Equiangle **Skewness** (ES), **Orthogonal Quality** (OQ), **Aspect Ratio** (AR), …
- Regardless of the type of mesh used 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 the 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; for an N-sided polygon, it is defined as:

$$\theta_{eq} = \frac{180°(N-2)}{N}$$

Zero skewness

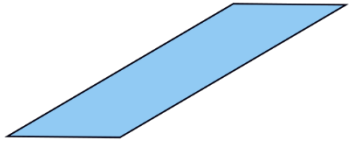
High skewness

Quadrilateral (perfect)

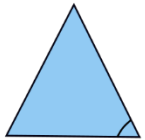


$\theta_{eq} = 90°$

Quadrilateral (skewed)

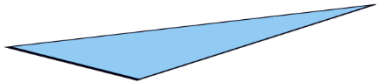


Triangle (perfect)



$\theta_{eq} = 60°$

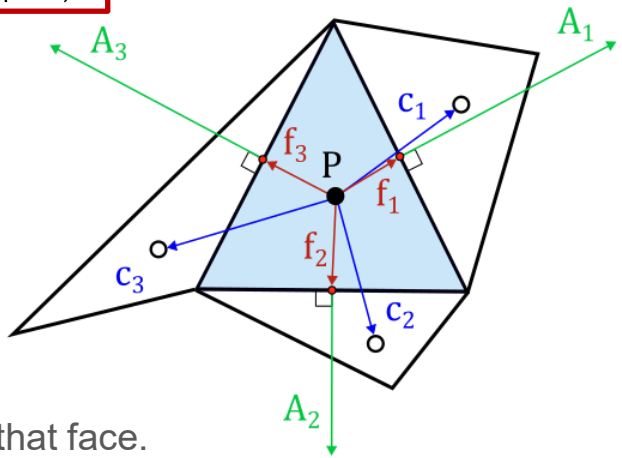
Triangle (skewed)



Orthogonal Quality

- **Orthogonal Quality** (OQ):

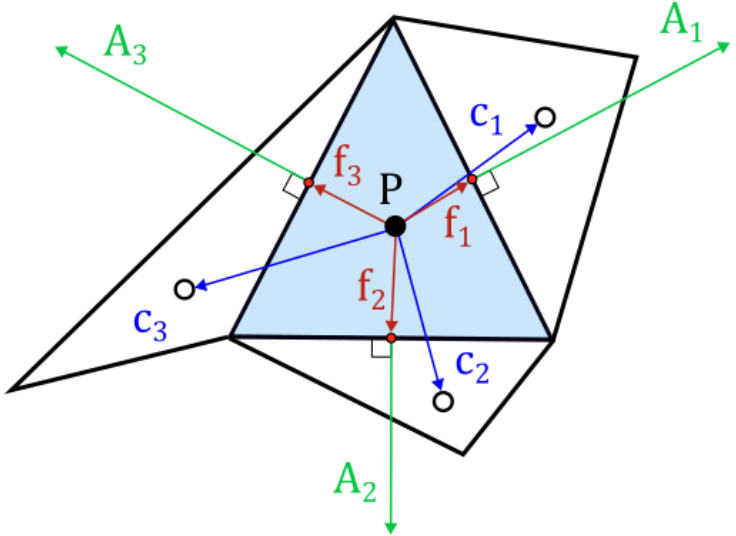
$$OQ = MIN\left(\frac{\overrightarrow{A_i} \cdot \overrightarrow{f_i}}{|\overrightarrow{A_i}||\overrightarrow{f_i}|}, \frac{\overrightarrow{A_i} \cdot \overrightarrow{c_i}}{|\overrightarrow{A_i}||\overrightarrow{c_i}|}\right)$$



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



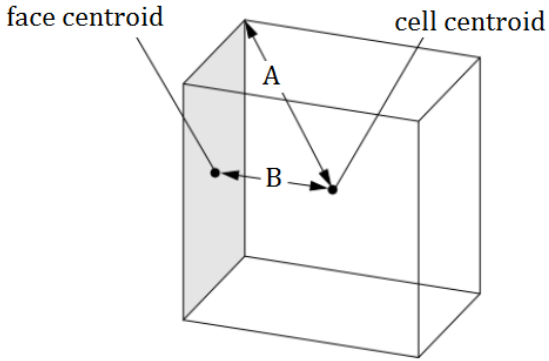
Aspect Ratio

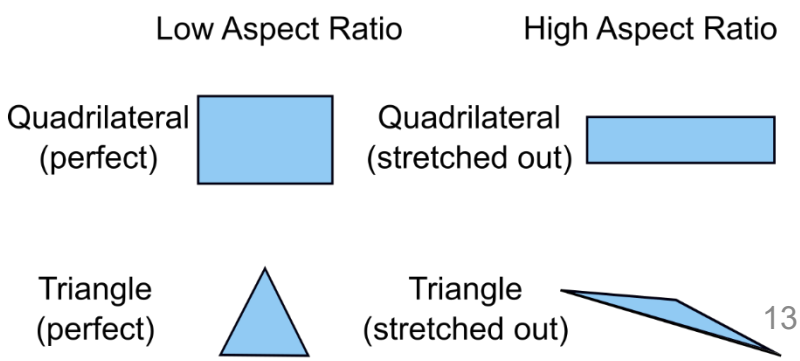
- **Aspect Ratio** (AR):

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

- 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 (a theoretical limit).**



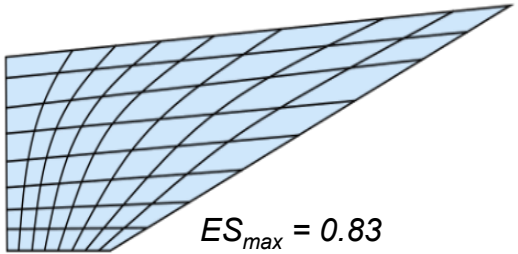


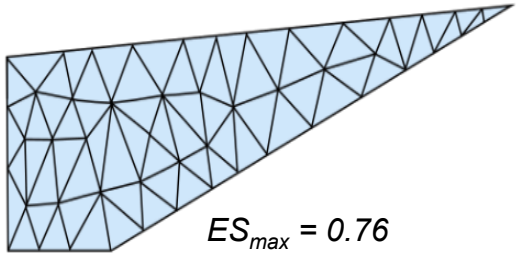
Mesh quality – Best practices

- 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 is not 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

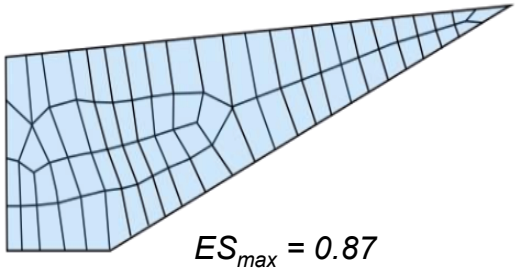
Structured quadrilateral mesh (64 cells)

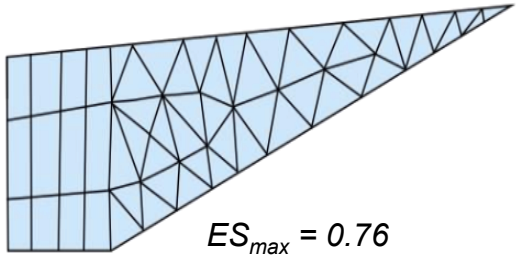




Unstructured triangular mesh (70 cells)

Unstructured quadrilateral mesh (67 cells)





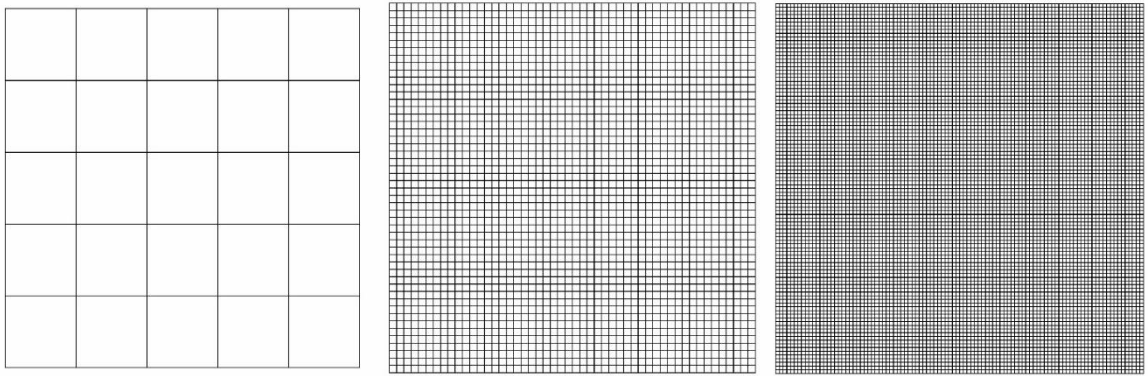
Hybrid (unstructured and structured) mesh (62 cells)

Mesh density

- Since a continuous domain is represented by a discrete mesh, the degree to which the **important features of the flow are resolved depends on the density and distribution of mesh elements**.
- Such features include 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)



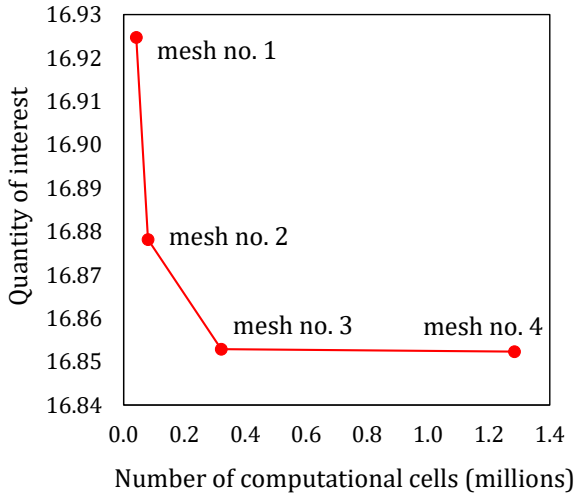
a) **Coarse** mesh (5x5), 25 cells

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

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

Mesh sensitivity study

- The influence of mesh density should **always be investigated!**
- We always look for **a trade-off between accuracy and computational cost**.
- A mesh sensitivity study addresses **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 the true (exact) values.
- This difference is **the error of the solution**.
- The total error is the sum of the following errors.
- We distinguish *two main types of errors in CFD*:

  - **Acknowledged**
  - **Unacknowledged**

Errors in CFD simulations

Acknowledged

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

Unacknowledged

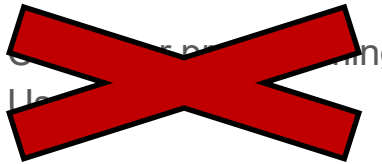
- ❑ Computer programming
- ❑ Usage

Errors in CFD simulations

Acknowledged

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

Unacknowledged

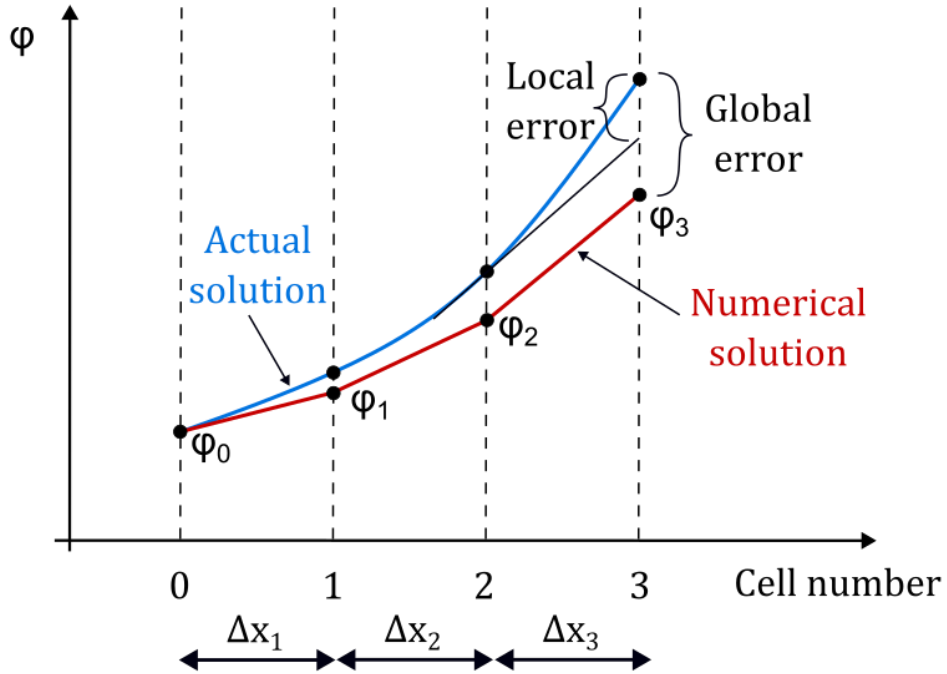


Discretization Error

- The discretization error can be associated with the spatial domain, the equations and time.

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 exact solutions would be identical (neglecting all 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:

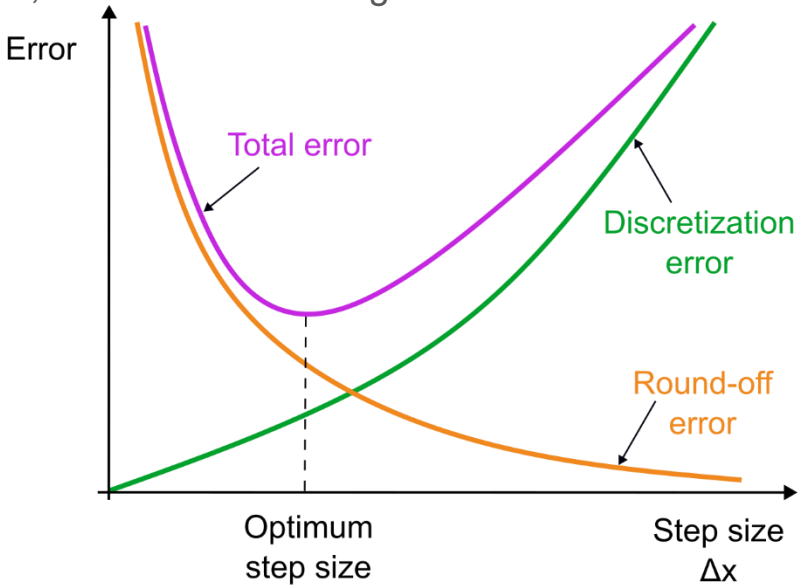
D = 1013251 - 1013250 +
+ 0.5282817
= 1 + 0.5282817
= 1.528281 (correct)

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

Controlling the total error

- Neglecting all other types of error and considering only the two above, we can find the optimum step size (time step for transient problems).

- The total error is the sum of both, as shown in the diagram below.



Summary – Lecture 3

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

Agenda – Lecture 4

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

Boundary conditions in CFD simulations

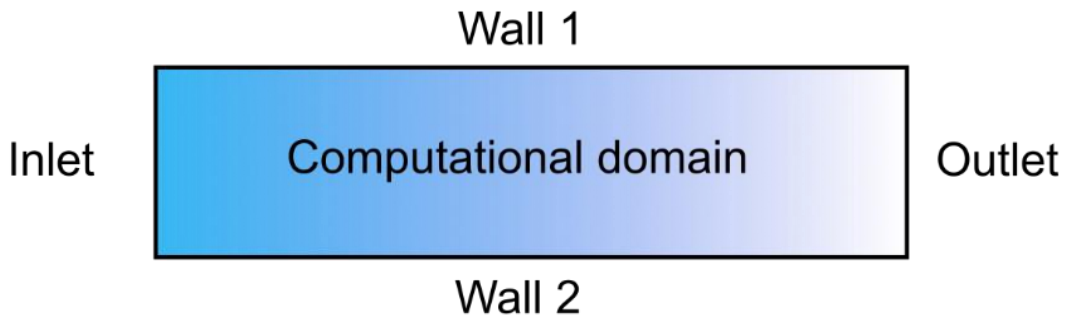
- Appropriate BCs are required to obtain accurate results!

General BCs:

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

Specific types of BCs:

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

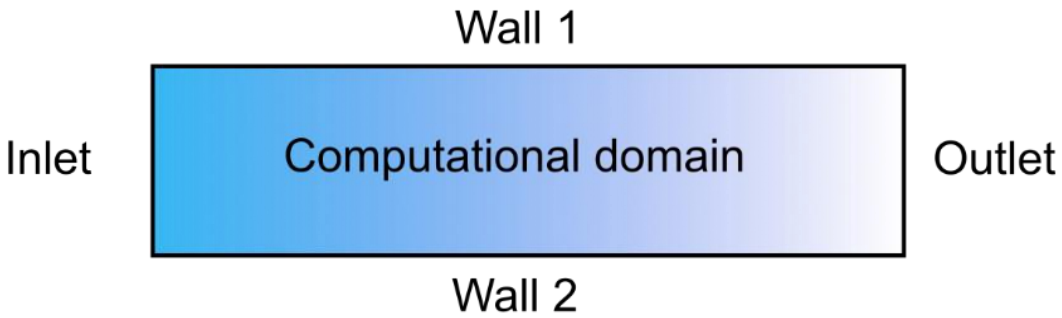


Wall boundary conditions

- One of the simplest BCs.
- Fluid cannot pass through a wall, so the normal velocity component (relative to the wall) is set to zero.
- 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 the wall temperature or the wall heat flux must be specified (but not both).
- BCs for other transport equations must also be specified (e.g., turbulence).

Wall boundary conditions (2)

- We can also specify zero shear stress along free surfaces to simulate an “inviscid” wall.
- This way, **we can simulate the free surface** of a swimming pool.
- However, this suppresses waves on the free surface and the associated pressure fluctuations.
- **For turbulent flows, wall roughness may be specified** through 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, …)
- ❑ Unspecified BCs (outflow, …)

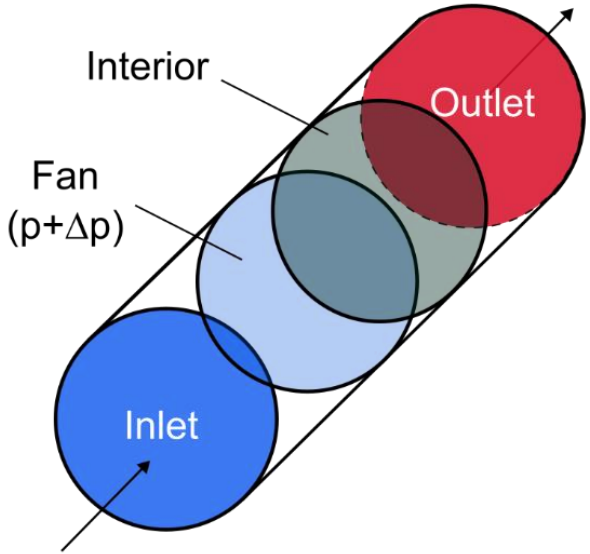
- If the energy equation or other scalar equations (e.g., turbulence) are solved, their boundary values must also be specified.

Internal boundary conditions

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

Classification of Internal BCs:

- ❑ Interior BCs (the flow passes through them)
- ❑ Fan BCs (induce a pressure rise/drop across the fan)



Symmetry and periodic boundary conditions

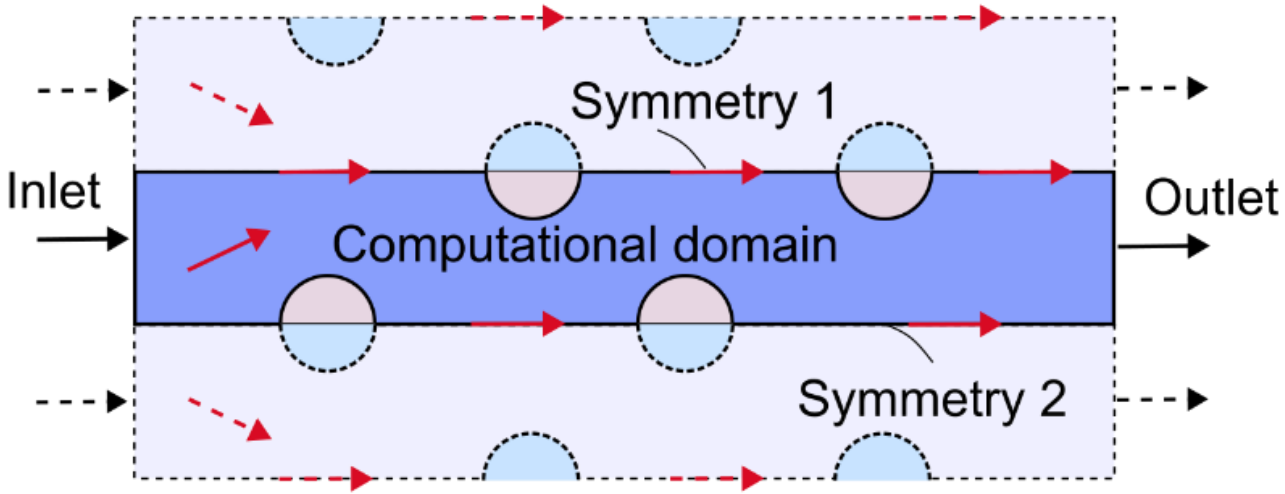
- They are not walls, inlets or outlets of the computational domain.
- They take advantage of periodicity or symmetry in the domain.

Classification of Symmetry/Periodic BCs:

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

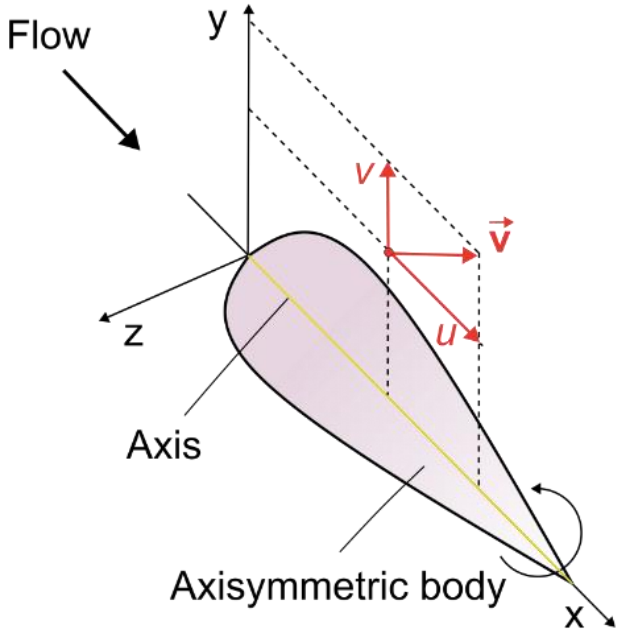
Symmetry boundary conditions

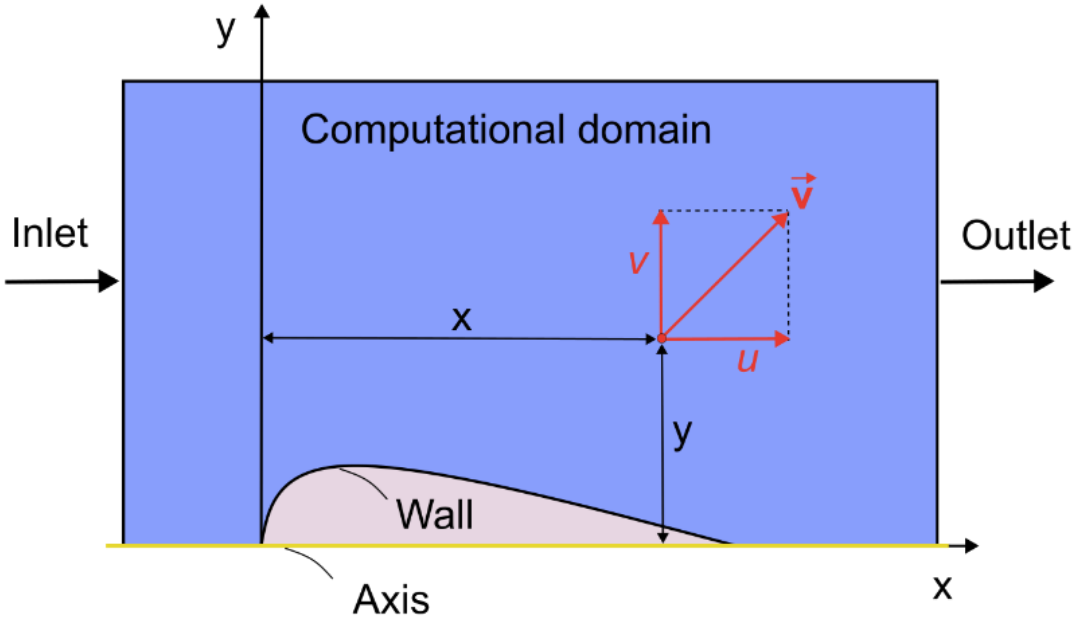
Symmetry *(plane symmetric)*



Symmetry boundary conditions (2)

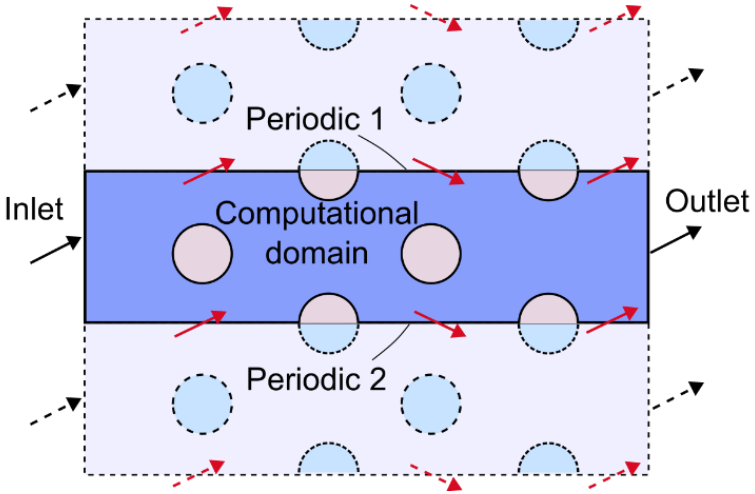
***Axis** (axisymmetric)*



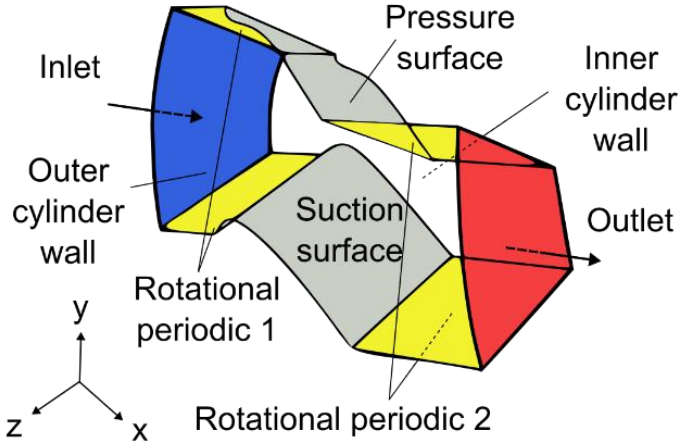


Periodic boundary conditions

Translational periodic

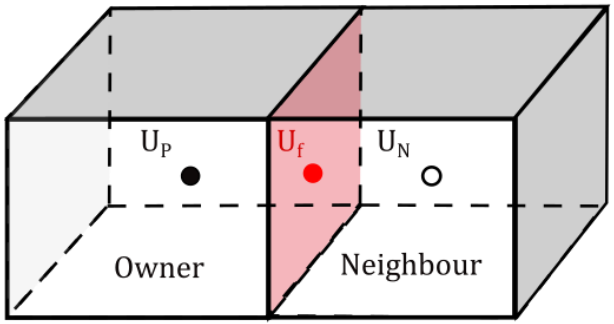


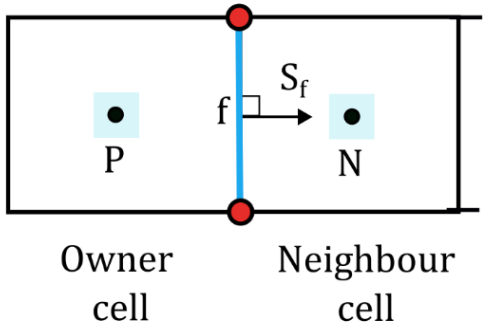
Rotational periodic



Discretization schemes for convective terms

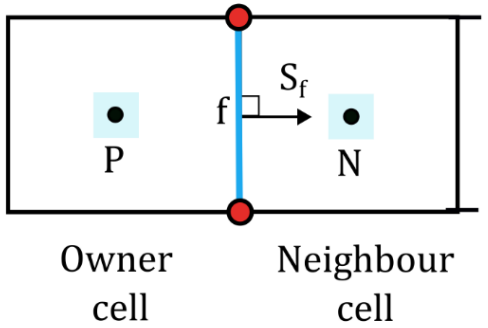
- Also known as **interpolation schemes**.
- **Values are usually stored at cell centroids**.
- For fluxes (gradients), **we need values at cell faces**.
- There are several ways to determine the cell face values.





Discretization schemes for convective terms (2)

- The face values of U (U_f) are found using an appropriate scheme.
- **Assumption about how U varies between two cell centers**.



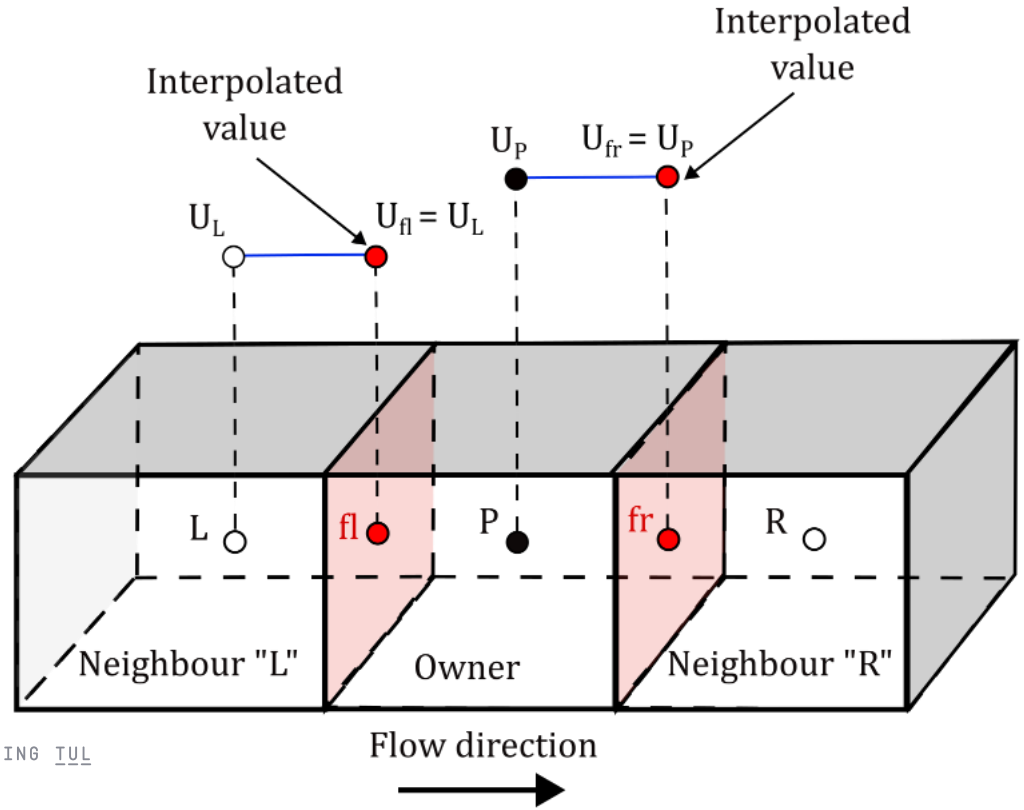
Most commonly used schemes for convective terms:

- ❑ 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**.
- The value of U at the face equals the value at the cell center UPSTREAM of 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 starting** a calculation.

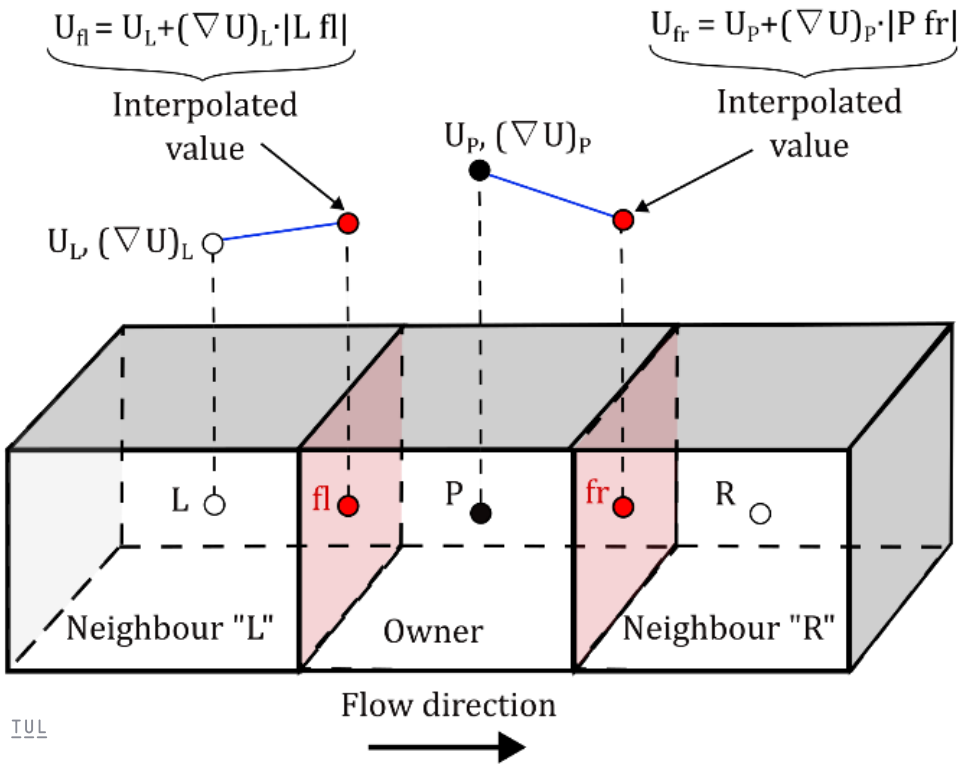
First-Order Upwind Scheme (2)



Second-Order Upwind Scheme

- The value of U at the face is computed from the cell centroid value and its gradient upstream of the face.
- **More accurate than First-Order Upwind** (also **DIRECTION-DEPENDENT!**).
- In regions with strong gradients, it can produce face values outside the range of the cell values (limiters may be applied).
- A popular scheme due to its good **trade-off between accuracy and stability**.

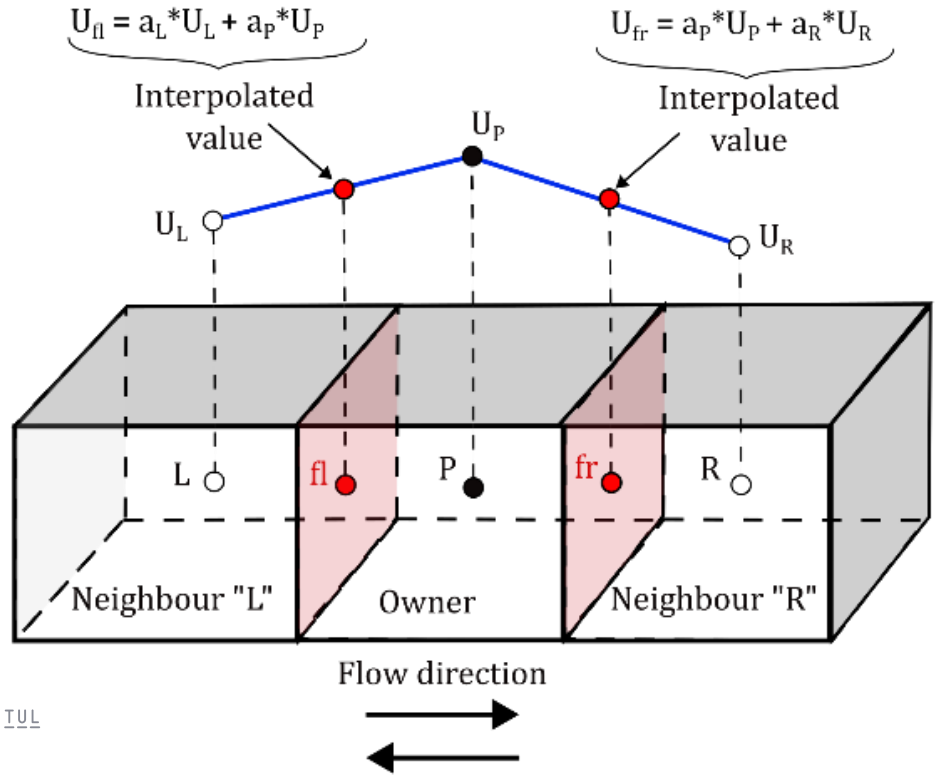
Second-Order Upwind Scheme (2)



Central-Differencing Scheme

- The value of U at the face is obtained by **linear interpolation between the upstream and downstream cells**.
- **More accurate than First-Order Upwind**.
- **May lead to oscillations** in the solution (divergence) if the local Peclet number is greater than 2.
- It is possible to switch to First-Order Upwind in cells where the Peclet number is greater than 2 (hybrid scheme).

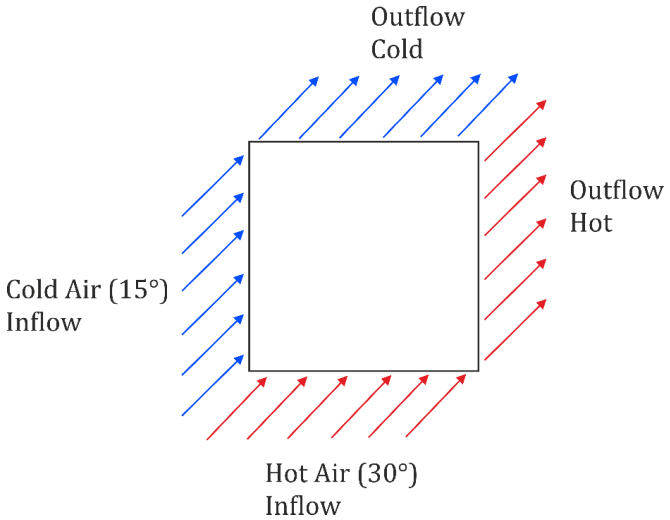
Central-Differencing Scheme (2)



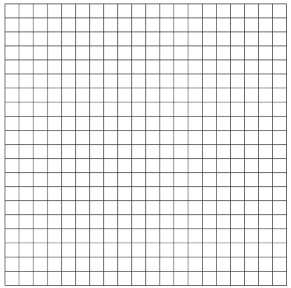
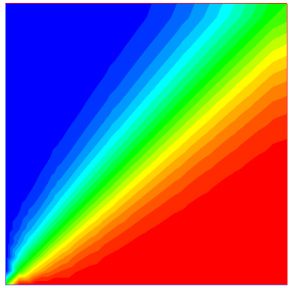
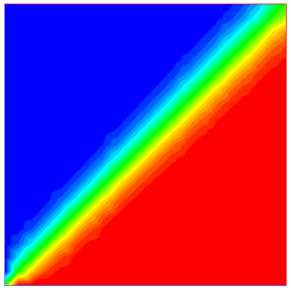
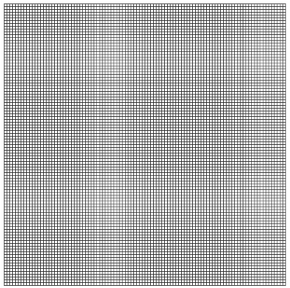
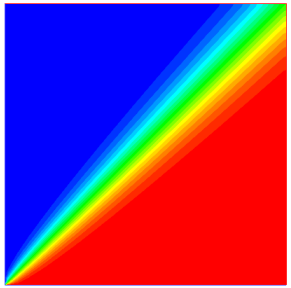
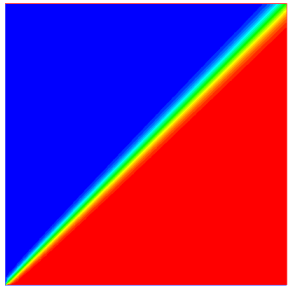
Accuracy and False Diffusion

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

Two parallel streams moving at the same velocity but at a different temperatures.



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 for convective terms**

Thank you.