

# Chapter 7: Practical Guidelines for CFD Simulation

Ibrahim Sezai

Department of Mechanical Engineering  
Eastern Mediterranean University

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## Guidelines on grid generation

### Boundary layers near solid walls:

Finer meshes are required near walls to resolve the sharp changes in the boundary layer.

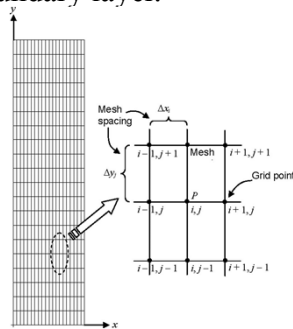


Fig. 1. A uniform rectangular mesh

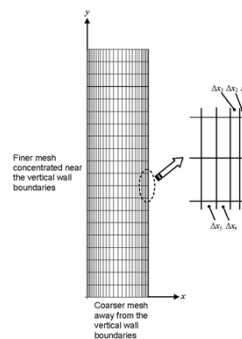


Fig. 2. A non-uniform rectangular mesh (stretched mesh)

Triangular (2D) or tetrahedral (3D) cells are ineffective for resolving wall boundary layers compared to quadrilateral (2D) or hexahedral (3D) cells.

Local refinement of meshes can be done using Cartesian meshes to capture high gradients at these localities.

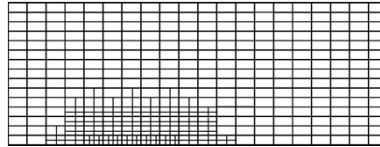


Fig.3. A structured Cartesian mesh without matching cell faces near the bottom boundary.

It should be noted that the locally refined region shown in the above figure can also be achieved through the use of other types of elements, such as triangular and quadrilateral elements.

Unstructured meshes are well suited for handling arbitrary shape geometries, specially for domains having high curvature boundaries.

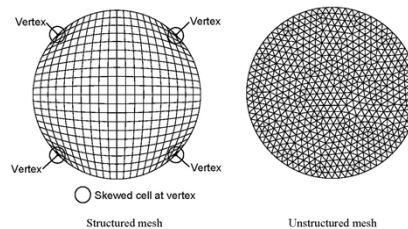


Fig. 4. A structured and an unstructured mesh for a circular cylinder.

Note the highly skewed cells at the four vertices (left). This type of mesh leads to numerical instabilities and inaccurate results.

It might have been preferable to re-mesh the geometry with an unstructured mesh (right).

## Block-structured or multiblock mesh

The mesh is assembled from a number of structured blocks attached to each other.

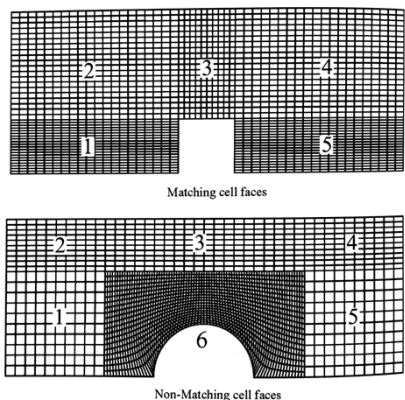


Fig. 5. Multi-block structured mesh with matching and non-matching cell faces.

## An example of an H-grid

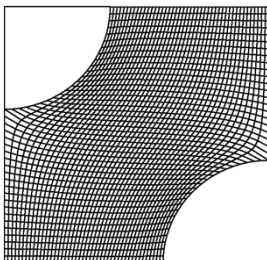


Fig. 6. Generation of a structured H-grid for the flow calculation in a symmetry segment of a staggered tube bank.

## An example of O-grids

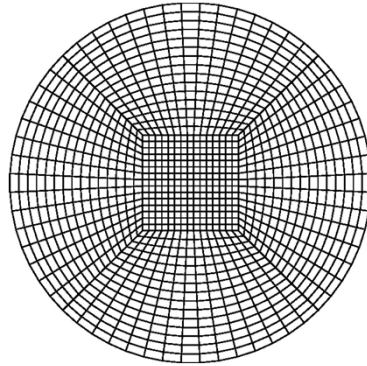


Fig. 7. The highly skewed cells of the circular cylinder in Fig. 4 can be removed through the use of O-grid, as shown in Fig. 7.

## An example of overlapping (chimera) grids

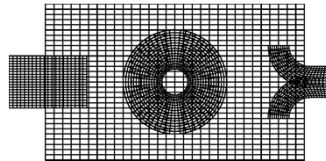


Fig. 8. A structured overlapping grid for a cylinder in a channel with inlet-outlet mappings.

This approach is attractive, because the structured mesh blocks can be placed freely in the domain to fit any geometrical boundary while satisfying the essential resolution requirements.

Information between the grids is achieved through the interpolation process.

## Hybrid grids

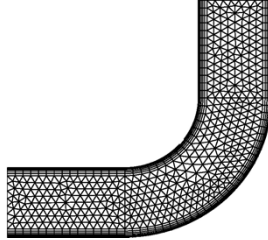
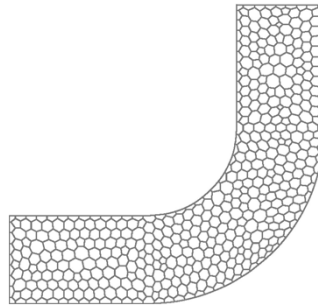


Fig. 9. A grid consisting of structured quadrilateral elements near the walls and unstructured triangular elements in the remaining part of the 90° bend.

As a common practice, grid quality is usually enhanced through the placement of quadrilateral or hexahedral elements in resolving boundary layers near solid walls, while triangular or tetrahedral elements are generated for the rest of the flow domain. This leads to both accurate solutions and better convergence.

## Polyhedral cells

Fig. 10. A grid consisting of polyhedral elements.



A polyhedral mesh can be created via cell agglomeration. As a result:

- Number of cells are reduced.
- Mesh quality is improved.
- Leads to better convergence.

Polyhedral meshes are relatively new, but gaining significant traction in CFD community.

## Test runs

- Initially, it is recommended to make test runs using a coarse mesh.
- This gives the opportunity to evaluate the computer's storage and running time.
- By this way it is also possible to assess the convergence or divergence behavior of the calculations.
- Test runs provide the means of rectifying possible sources of solution errors such as physical modeling or human errors.
- Making test runs on a fine grid may lead to divergence of the calculations, due to large gradients of the diffusion terms near walls, if the initial conditions are poorly chosen.

- For example, consider the diffusion term for flow in a duct.
- For the initial conditions  $\phi_{\text{fluid}} \approx 0$  and  $\phi_{\text{wall}} = 1$ , the term  $\partial^2 \phi / \partial y^2$  will be very large near the horizontal wall.
- This term will be larger for a finer mesh.
- As a result, for poor initial conditions, divergence problems may be encountered for a fine mesh.

- One practical way to overcome the poor initial guesses, or unresolved steep gradients in the flow field is through the use of under-relaxation factors.
- The other strategy is to initially solve the problem on a coarse mesh.
- The solution of this mesh is later interpolated onto a fine mesh.
- This strategy is available in many commercial codes.

## Grid quality: Aspect ratio of grid

- Grid aspect ratio of the cell:  $AR = \Delta y / \Delta x$

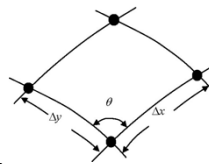
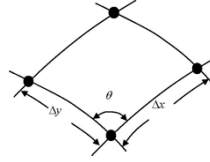


Fig. 11.

- Generally, cells with a very large aspect ratio can cause problems. In interior regions use  $0.2 < AR < 5$ .
- In near wall boundaries  $AR < 0.2$  or  $AR > 5$  can be used.
- As a result accuracy increases and convergence difficulties are alleviated.
- Also, abrupt changes in cell size can lead to convergence problems.

## Grid quality: grid distortion or skewness

- Grid distortion or skewness relates to angle  $\theta$  between the gridlines.



- It is desirable to have  $\theta = 90^\circ$  (orthogonal grids).
- If  $\theta < 45^\circ$  or  $\theta > 135^\circ$ , then accuracy decreases and leads to instabilities.
- The angle between the gridlines and the boundary of the computational domain (specially the wall, inlet or outlet boundaries) should be maintained as close as possible to  $90^\circ$ .

- For 2-D meshes, equiangle skewness is defined as

$$Q_{EAS} = \max \left( \frac{\theta_{\max} - \theta_{\text{equal}}}{180^\circ - \theta_{\text{equal}}}, \frac{\theta_{\text{equal}} - \theta_{\min}}{\theta_{\text{equal}}} \right)$$

- For triangular cells  $\theta_{\text{equal}} = 60^\circ$
- For quadrilateral cells  $\theta_{\text{equal}} = 90^\circ$
- It can be shown that  $0 < Q_{EAS} < 1$ .
- $Q_{EAS}$  should be as small as possible.

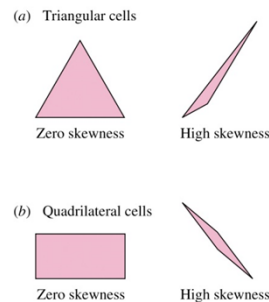


Fig. 12.

- $(Q_{EAS})_{\max} = 0.83$
- $(Q_{EAS})_{\max} = 0.76$
- $(Q_{EAS})_{\max}^{(c)} = 0.87$
- $(Q_{EAS})_{\max} = 0.76$

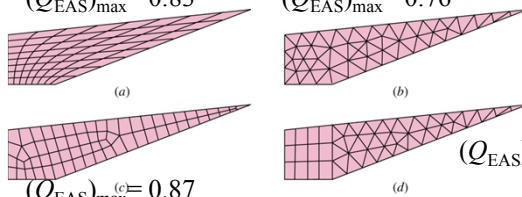
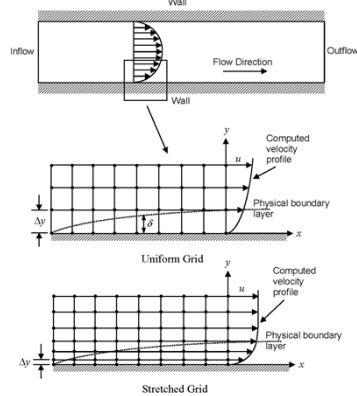


Fig. 13.



## Local refinement

One local refinement technique that is widely used in many CFD applications is the concept of a stretched grid.



Insufficient number of grids to resolve the boundary layer at all.

Boundary layer can be resolved to some extent.

Fig. 14. Two-schematic illustrations demonstrating the need for local refinement in the near vicinity of the bottom wall to resolve the physical boundary layer.

## Local refinement

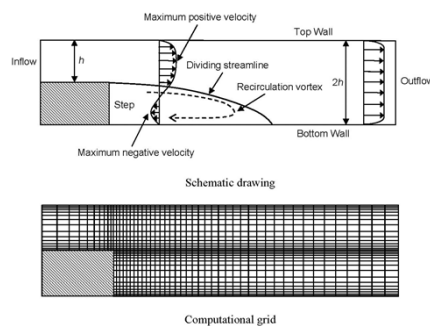
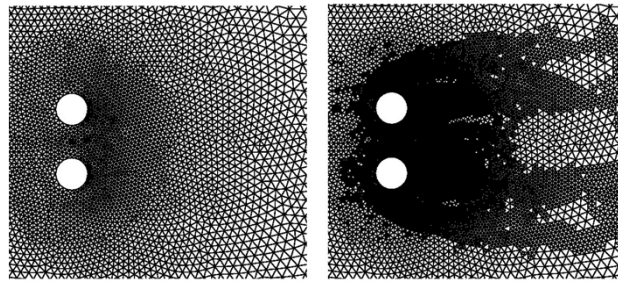


Fig. 15. A schematic drawing for the backward-facing step geometry and the computational grid to capture the essential feature of the recirculation vortex.

In applying the stretched grid, care must be exercised to avoid sudden changes in the grid size.

## Solution adaptation

- Solution adaptation, usually through the use of an adaptive grid, is a grid network that automatically or dynamically clusters the grid nodal points in regions where large gradients exist in the flow field.



Before

After

Fig. 16. A demonstration of solution adaptation through the use of triangular meshes for the fluid flowing over two cylinders. Grids are subdivided or recombined continuously according to solution during computer run.

- The advantages of an adaptive grid:
  1. Increased accuracy for a fixed number of grid points
  2. Fewer grid points required for a given accuracy.
- Most commercial codes offer some form of automated grid adaptation.
- However, the grid quality might not improve as a consequence of activating the feature in these codes.

## Boundary conditions

### Typical conditions

#### ■ Wall

- No-slip ( $u = v = w = 0$ )
- Slip (tangential stress = 0, normal velocity = 0)
- With specified suction or blowing
- With specified temperature or heat flux

#### ■ Inflow

#### ■ Outflow

#### ■ Interface Condition, e.g., Air-water free surface

#### ■ Symmetry and Periodicity

Usually set through the use of a graphical user interface (GUI) – click & set

## Guidelines for boundary conditions

- All boundary conditions used in CFD are based on two types: Dirichlet and Neumann.

$$\phi = f \quad (\text{Dirichlet bc})$$

$$\partial\phi/\partial n = f \quad (\text{Neumann bc})$$

where  $f$  is a specified function.

- In many real applications, there is great difficulty in prescribing some of the boundary conditions at the inlet and outlet of the computational domain.

## Guidelines for inlet boundary conditions

- Inlet and outlet boundaries are categorized as
  - 1) velocity-specified conditions and
  - 2) pressure-specified conditions
- At a **velocity inlet**, we specify the velocity of the incoming flow.  $T$ ,  $k$ ,  $\varepsilon$  should also be specified if energy and turbulence equations are to be solved.
- At a **pressure inlet**, we specify the total (stagnation) pressure (static+dynamic) at the inlet face.
- For example, if the flow is coming from a pressurized tank then  $p_{\text{inlet}} = p_{\text{tank}}$ .
- If the flow is coming from the far field, then  $p_{\text{inlet}} = p_{\text{surroundings}}$ .

- Pressure is not specified at a **velocity inlet**, as this would lead to mathematical over-specification, since pressure and velocity are coupled in the momentum equations. Rather, pressure at a velocity inlet adjusts itself to match the rest of the flow field.
- In a similar fashion, velocity is not specified at a **pressure inlet** or **outlet**

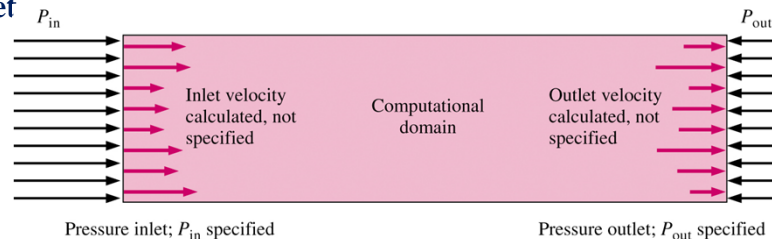


Fig. 16b At a **pressure inlet** or **pressure outlet**, we specify the pressure on the face, but we cannot specify the velocity through the face. As the CFD solution converges, the velocity adjusts itself such that the prescribed pressure boundary conditions are satisfied.

## Configurations for a simple duct flow

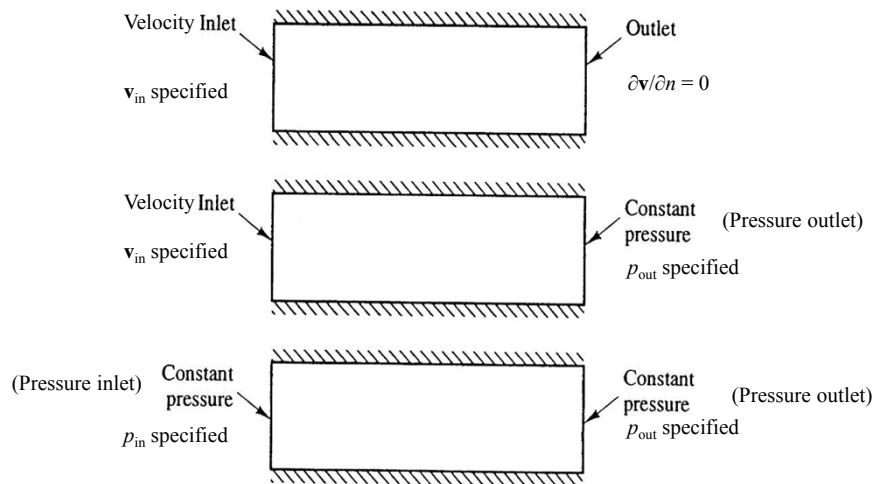


Fig. 17 Configurations for a simple duct flow.

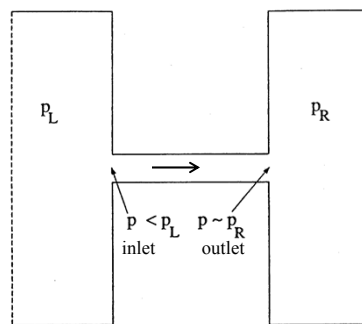


Fig. 18 Flow in a pipe joining two plenums at different pressures.

Consider the pipe connecting the two reservoirs. If  $p_L > p_R$ , the flow is from left (L) to right (R).

Let the **static pressures** at the inlet and outlet, be  $p_{in}$  and  $p_{out}$ .

$$\text{At inlet: } p_{in} = p_L - 0.5\rho_{in}|\mathbf{v}_{in}|^2$$

$$\text{At outlet: } p_{out} = p_R$$

## Boundary conditions for a heated cylinder

Consider a two-dimensional, buoyant flow of air around an isothermal, heated horizontal cylinder. Only one-half of the cylinder need be modeled due to symmetry.

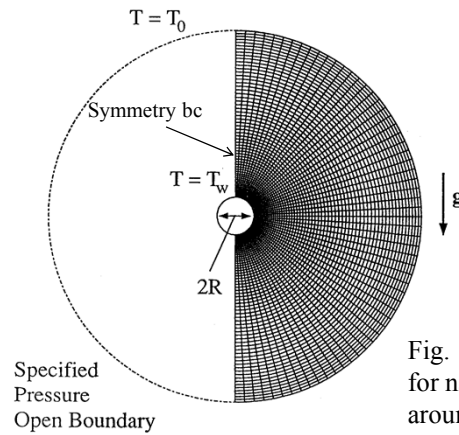


Fig. 19 Geometry and grid for natural convection around a heated cylinder.

## Inlet location for the backward-facing step flow

- Consider the backward-facing step flow problem.
- It is necessary to demonstrate that the interior solution is unaffected by the choice of location of the inlet, by using different upstream distances from the expansion region.
- If the inlet is too close, the velocity profile will be changing (developing flow) in the flow direction before the flow expansion region which significantly affects the recirculation region.

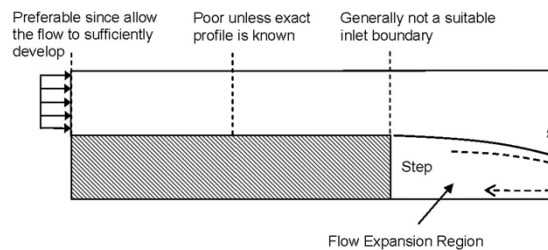


Fig. 20 Inlet locations for the backward-facing step problem.

## Guidelines for outlet boundary conditions

- At a **pressure outlet**, fluid flows out of the computational domain.
- We specify the static pressure along the outlet face. In many cases this is atmospheric pressure (zero gage pressure)
- For example, the pressure is atmospheric at the outlet of a subsonic exhaust pipe open to ambient air.

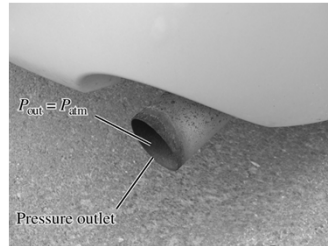


Fig. 21 When modeling an incompressible flow field, with the outlet of a pipe exposed to ambient air, the proper bc is a **pressure outlet** with  $P_{\text{out}} = P_{\text{atm}}$ . Shown here is the exhaust pipe of an automobile.

- Another option at an outlet is the **outflow** boundary condition.
- At an outflow boundary no flow properties are specified.
- Instead, flow properties such as  $\mathbf{v}$ ,  $T$ ,  $k$  and  $\varepsilon$  are forced to have zero gradients normal to the outflow direction.
- For example, if a duct is sufficiently long so that the flow is **fully developed** at the outlet, the **outflow** bc would be appropriate, since velocity does not change in the direction normal to the outlet face.
- Note that the flow direction is not constrained to be perpendicular to the outflow boundary as shown in Fig. 22.

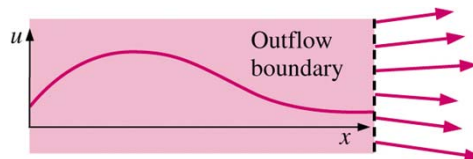


Fig. 22 At an outflow boundary  $\partial \mathbf{v} / \partial n = 0$ . Note that neither  $p$  or  $\mathbf{v}$  are specified.

## Pressure far field boundary condition

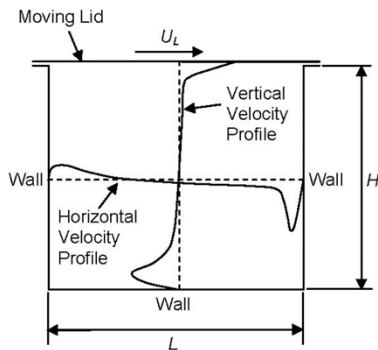
- Is used for **compressible flows** to account for the incoming or outgoing waves.
- Is used to specify mach number,  $p$  and  $T$  at an inlet.
- Same bc's can be applied at an outlet.
- When flow exits the domain, flow variables at outlet are extrapolated from interior of domain.

## Guidelines for wall boundary conditions

- Because of the **no-slip condition**, we usually set the **tangential component** of velocity at a stationary wall to zero
- In addition, since fluid cannot pass through a wall, the **normal component** of velocity is also set to zero.
- If the energy equation is being solved, either **wall temperature** or **wall heat flux** must be specified.
- If turbulence transport equations are being solved, wall roughness may need to be specified.
- In addition, users must choose among various kinds of turbulence wall treatments (**wall functions** or **low Reynolds number model wall treatments**).

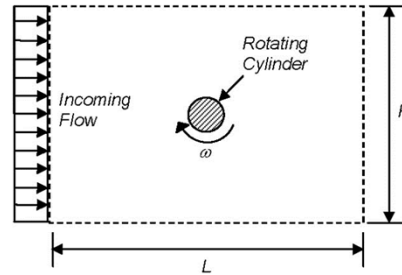


## Moving or rotating walls



Lid-driven cavity

A tangential velocity is imposed on the top boundary



Rotating cylinder in a fluid environment

A rotational speed is imposed on the circumferential surface of the rotating cylinder.

Fig. 23

Other more complex CFD problems may require the use of sliding or moving meshes to better emulate the motion of a rotating impeller stirring the fluid in a tank.

## An example of boundary conditions

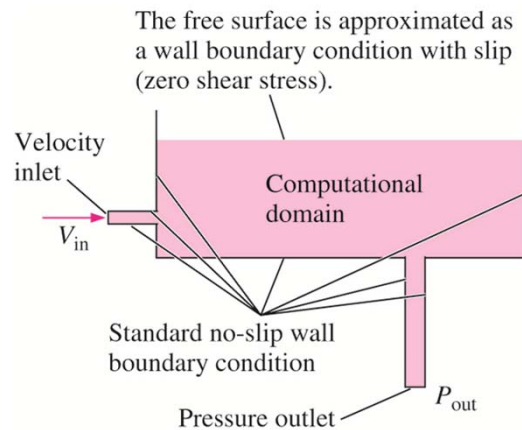


Fig.24 Boundary conditions for the simulation of a swimming pool.

## Symmetry boundary conditions

- Symmetry bc's are applied when the physical geometry and the flow field have mirror symmetry.
- At the symmetry plane:
  - The normal velocity is zero
  - The normal gradients of all variables are zero.
- The application of symmetry planes to the flow in the square duct problem below, can reduce the computational effort significantly, since only one fourth of the domain need to be simulated.

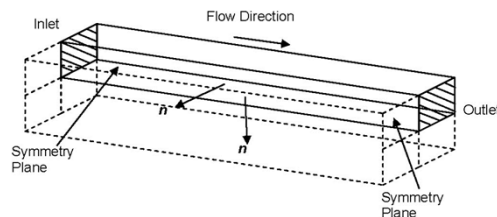
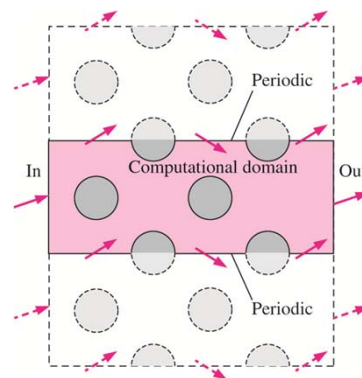


Fig. 25 Application of symmetry bc's for air flow through a square duct.

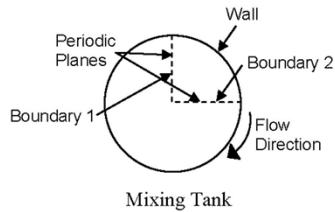
## Periodic boundary conditions

- The **periodic** boundary condition is useful when the geometry involves repetition.
- A pair of periodic planes must be used.
- The periodic planes should be identical.
- Mesh distribution in the two planes should be identical.
- The flow leaving one of the periodic planes is equal to the flow entering the other ( $\mathbf{v}$ ,  $T$ ,  $p$ , etc).
- The periodic boundary condition enables us to work with a computational domain that is much smaller than the full flow field, thereby conserving computer resources.

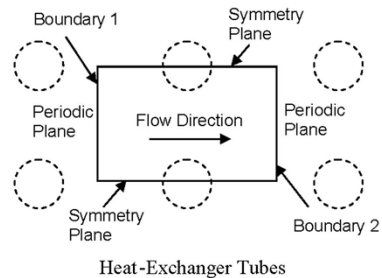


- Fig. 26 Domain chosen for simulating flow in a heat exchanger.
- Note that the velocity vectors crossing the two planes are identical.

## Examples of periodic boundary conditions



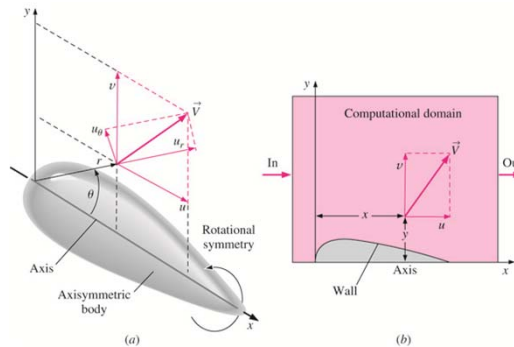
**Rotationally periodic case:**  
Flow field leaving “boundary 2” is enforced as an inlet flow condition at “boundary 1”.



**Cyclically periodic case:**  
Flow field leaving “boundary 2” is enforced as an inlet flow condition at “boundary 1”.  
Note that no flow crosses the symmetry plane.

## Axis boundary condition

The axis bc is applied to the axis of symmetry (here the  $x$ -axis) in an axisymmetric flow, since there is rotational symmetry about that axis.

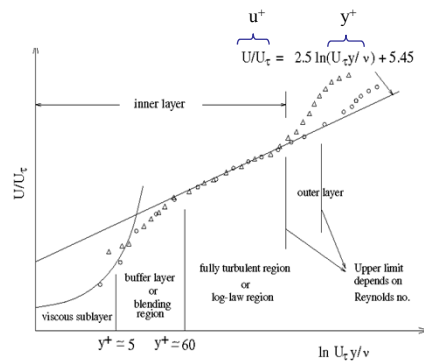


(a) A slice defining the  $xy$ - or  $r\theta$ - plane is shown, and the velocity components can be either  $(u, v)$  or  $(u_r, u_\theta)$ .

(b) The computational domain (light blue shaded region) for this problem is reduced to a plane in two dimensions ( $x$  and  $y$ ). In many CFD codes,  $x$  and  $y$  are used as axisymmetric coordinates, with  $y$  being understood as the distance from the  $x$ -axis.

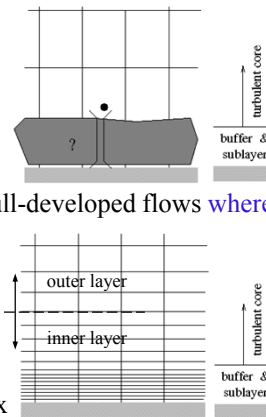
# Wall Boundary Conditions for Turbulent Flow

- Accurate near-wall modeling is important:
  - Successful prediction of frictional drag, pressure drop, separation, etc., depends on the fidelity of local wall shear predictions.
  - Near-wall modeling is used to supply boundary conditions for turbulent flows.
- Most k-ε and RSM turbulence models are not valid in the near-wall region:
  - Special near-wall treatment is required to provide proper BC's:
    - Standard wall functions
    - Non-Equilibrium wall functions
    - Enhanced wall treatment
- S-A, k-ω and SST models are capable of resolving the steep near-wall profiles, provided the mesh is sufficiently fine.



# Near-Wall Modeling Options

- In general, wall functions are a *collection or set of laws* that serve as boundary conditions for momentum, energy, and species as well as for turbulence quantities.
- **Wall Function Options**
  - 1) **The Standard and Non-equilibrium Wall Functions** (SWF and NWF) use the law of the wall to supply boundary conditions for turbulent flows.
    - The near-wall mesh can be relatively coarse.
    - It is used for equilibrium boundary layers and full-developed flows where log-law is valid.
  - 2) **Enhanced Wall Treatment Option**  
 Uses a single equation for the law of the wall by blending the linear and logarithmic laws as.
 
$$U^+ = e^{\Gamma} U_{lam}^+ + e^{1/\Gamma} U_{turb}^+$$
    - Suitable for low-Re flows or flows with complex near-wall phenomena.
    - Generally requires a fine near-wall mesh capable of resolving the viscous sub-layer (more than 10 cells within the inner layer)



## Placement of the first grid point for wall functions

- For standard or non-equilibrium wall functions, each wall-adjacent cell's centroid should be located within the log-law layer:  $y_p^+ \approx 30 - 300$
- For the enhanced wall treatment (EWT), each wall-adjacent cell's centroid should be located within the viscous sublayer:  $y_p^+ \approx 1$ 
  - EWT can automatically accommodate cells placed in the log-law layer.
- How to estimate the size of wall-adjacent cells before creating the grid:
  - $y_p^+ \equiv y_p u_\tau / \nu \Rightarrow y_p \equiv y_p^+ \nu / u_\tau \quad u_\tau \equiv \sqrt{\tau_w / \rho} = U_e \sqrt{c_f / 2}$
  - The skin friction coefficient can be estimated from empirical correlations:  
Flat Plate:  $\frac{\overline{C_f}}{2} \approx 0.037 \text{Re}_L^{-1/5}$     Duct:  $\frac{\overline{C_f}}{2} \approx 0.039 \text{Re}_D^{-1/4}$
- Use post-processing (e.g., xy-plot or contour plot) to double check the near-wall grid placement after the flow pattern has been established.

## Near-Wall Modeling: Recommended Strategy

- Use SWF or NWF for most high  $Re$  applications ( $Re > 10^6$ ) for which you cannot afford to resolve the viscous sub-layer.
  - There is little gain from resolving the viscous sub-layer. The choice of core turbulence model is more important.
  - Use NWF for mildly separating, reattaching, or impinging flows.
- You may consider using EWT if:
  - The characteristic  $Re$  is low or if near wall characteristics need to be resolved.
  - The same or similar cases which ran successfully previously with the two-layer zonal model (in Fluent v5).
  - The physics and near-wall mesh of the case is such that  $y^+$  is likely to vary significantly over a wide portion of the wall region.
- *Try to make the mesh either coarse or fine enough to avoid placing the wall-adjacent cells in the buffer layer ( $y^+ = 5 \sim 30$ ).*

## Boundary Conditions at Inlet and Outlet

- When turbulent flow enters a domain at inlets or outlets (backflow), boundary conditions for  $k$ ,  $\varepsilon$ ,  $\omega$  and/or  $\overline{u'_i u'_j}$  must be specified, depending on which turbulence model has been selected.
- Preferably experimentally obtained values for these quantities should be used. If they are not available use the following approximations:

$$k_{inlet} = 3 / 2 (U_{inlet} I)^2$$

where  $I = u'/U$  is the turbulence intensity.

$$I = \begin{cases} 0.3\% & \text{for external aerodynamic flows over airfoils.} \\ 30\% & \text{for atmospheric boundary layer flows.} \\ 5\%-10\% & \text{for internal flows.} \end{cases}$$

- Similarly,  $\varepsilon_{inlet}$  can be approximated as

$$\varepsilon_{inlet} = C_\mu^{3/4} \frac{k^{3/2}}{L}$$

where  $L$  is the characteristic length scale.

- If the  $k$ - $\omega$  model is employed,  $\omega$  can be approximated by

$$\omega_{inlet} = \frac{k^{1/2}}{C_\mu^{1/4} L}$$

- For external flows remote from boundary layers take:  $1 < \mu_t / \mu < 10$
- For internal flows take  $(\mu_t)_{inlet} = \rho C_\mu (k^2 / \varepsilon)_{inlet}$

- If RSM model is used take the inlet values as

$$\overline{u_1'^2} = \overline{u_2'^2} = \overline{u_3'^2} = 2 / 3 k$$

$$\overline{u'_1 u'_2} = \overline{u'_1 u'_3} = \overline{u'_2 u'_3} = 0$$

## BC's for solid walls for $k$ , $\varepsilon$ and $\omega$

- Depends on whether low Reynolds number (LRN) turbulence models or wall function method is employed.

- **For LRN turbulence models** use the following at the walls:

$$k = 0 \quad \frac{\partial \varepsilon}{\partial n} = 0 \quad \varepsilon = \left( \frac{\partial v_i}{\partial n} \right)^2 \quad v_i = \text{velocity component tangential to the wall}$$

- For the LRN Wilcox  $k$ - $\omega$  model use  $\omega_{wall} = 10 \frac{6\mu}{0.075\rho(n_p)^2}$  where  $n_p$  is the distance of the first grid point to the wall.

- **For wall function method** use the following at the wall:

$$\frac{\partial k}{\partial n} = 0$$

- $\varepsilon$  is not applied at the wall but is calculated at the first computational grid point (CV center point P) as

$$\varepsilon_P = \frac{C_\mu^{3/4} k_P^{3/2}}{\kappa n_p}$$

- In cases where the non-equilibrium wall function is used,  $\varepsilon_P$  is calculated as

$$\varepsilon_P = \frac{1}{2n_p} \left[ \frac{2\mu}{\rho y_v} + \frac{C_\mu^{3/4} k_P}{\kappa} \ln \left( \frac{2n_p}{y_v} \right) \right] k_P$$

where  $y_v$  is the physical viscous sub-layer thickness computed from

$$y_v = \frac{y^* \mu}{\rho C_\mu^{1/4} k_P^{1/2}} \quad \text{and} \quad y^* = 11.225$$

## BC's at outlet or symmetry boundaries

- At outlet or symmetry boundaries, the Neumann boundary conditions are applicable:

$$\frac{\partial k}{\partial n} = 0; \quad \frac{\partial \varepsilon}{\partial n} = 0; \quad \frac{\partial \overline{u'_i u'_j}}{\partial n} = 0;$$

- In the free stream flow where the computational boundaries (symmetry boundaries) are far away from the region of interest, the following bc's can be used:

$$k \approx 0; \quad \varepsilon \approx 0; \quad \overline{u'_i u'_j} = 0$$

which results in the turbulent viscosity  $\mu_t \approx 0$ .