

Introduction to Computational Fluid Dynamics (CFD) – Part I

CFD Fundamentals

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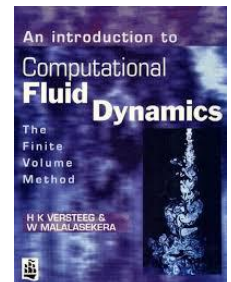
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Outline

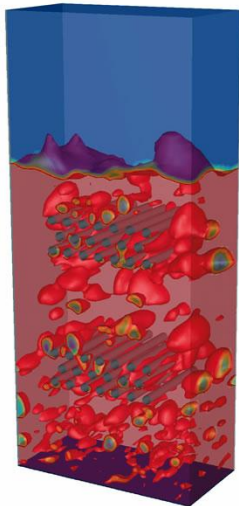
- Introduction
 - What is CFD?
 - Advantages of CFD over experiments
- How does it work?
 - Pre-processor, Solver, Post-processing
 - Solver - finite volume approach
 - 1D, steady-state diffusion problem
 - Using centre differencing scheme
 - Discretisation schemes
 - Importance of grid and its quality
 - Simulation stability and stability
 - Best practices

Ref: “An introduction to CFD – The finite volume method” by Versteeg and Malalasekera

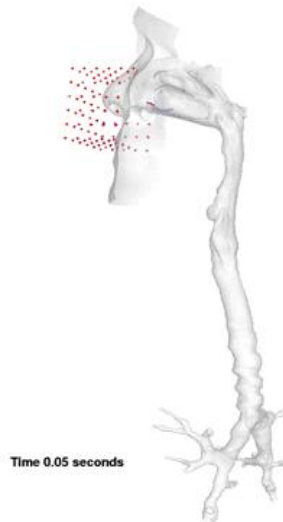


What is CFD?

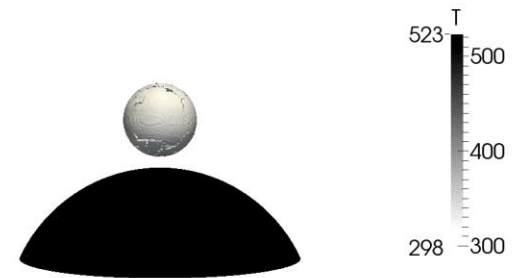
- *CFD is the analysis of systems involving fluid flow, heat transfer, mass transfer and associated phenomena such as chemical reactions by means of computer-based simulation.*
- *It is prediction tool based on the solution of governing equations of mass, momentum and energy conservation.*
- *Few examples:*



Bubbles in a
Fluidized beds



Particle migrations
through patients' airways
during breathing cycle



Interaction of liquid
droplets on spherical
hot surface

Advantages of CFD

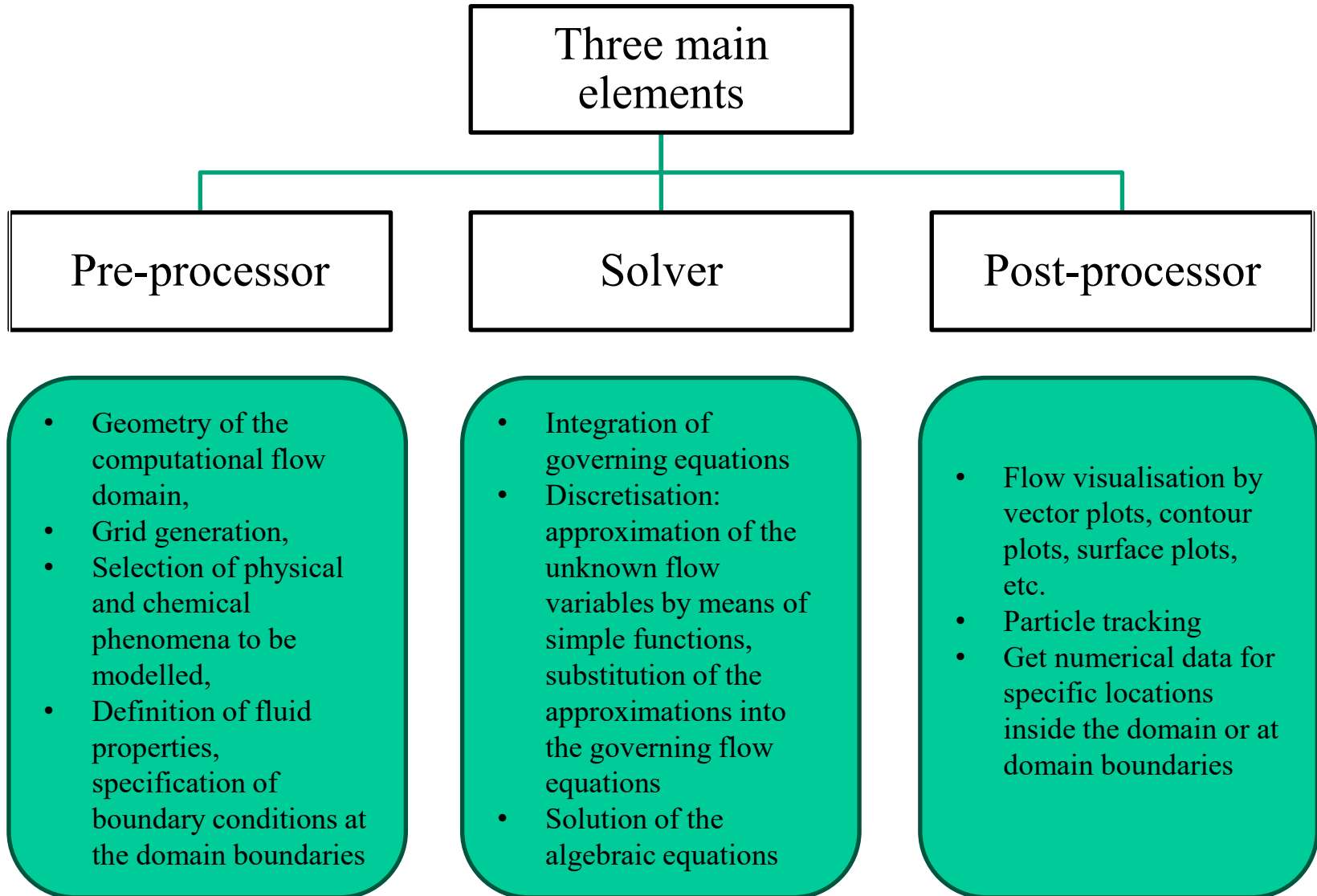
Provides several advantages over experiment-based approaches:

- Substantial reduction of lead times and costs of new designs
- Ability to study systems where controlled experiments are difficult or impossible to perform
- Ability to study systems under hazardous conditions at and beyond their normal performance limits (e.g. safety studies and accident scenarios)
- Practically unlimited level of detail of results

The variable cost of an experiment, in terms of facility and/or man-hour costs, is proportional to the number of data points and the number of configurations tested. In contrast, CFD codes can produce extremely large volumes of results at virtually no added expense.

Overall, less costly and less time consuming

How CFD works



How CFD works

Inlet fluid

- Material
- Velocity
- Temp.



Required solution:
What will be the velocity field,
pressure profiles, temperature
distributions in the flow domain?

Pre-processing:

- *Create geometry – CAD drawing (we use Ansys-DesignModeller in lab-1)*
- *Generate grid – Meshing the geometry → divide the flow domain in several sub domains*
- *Specify boundary conditions – boundary values*

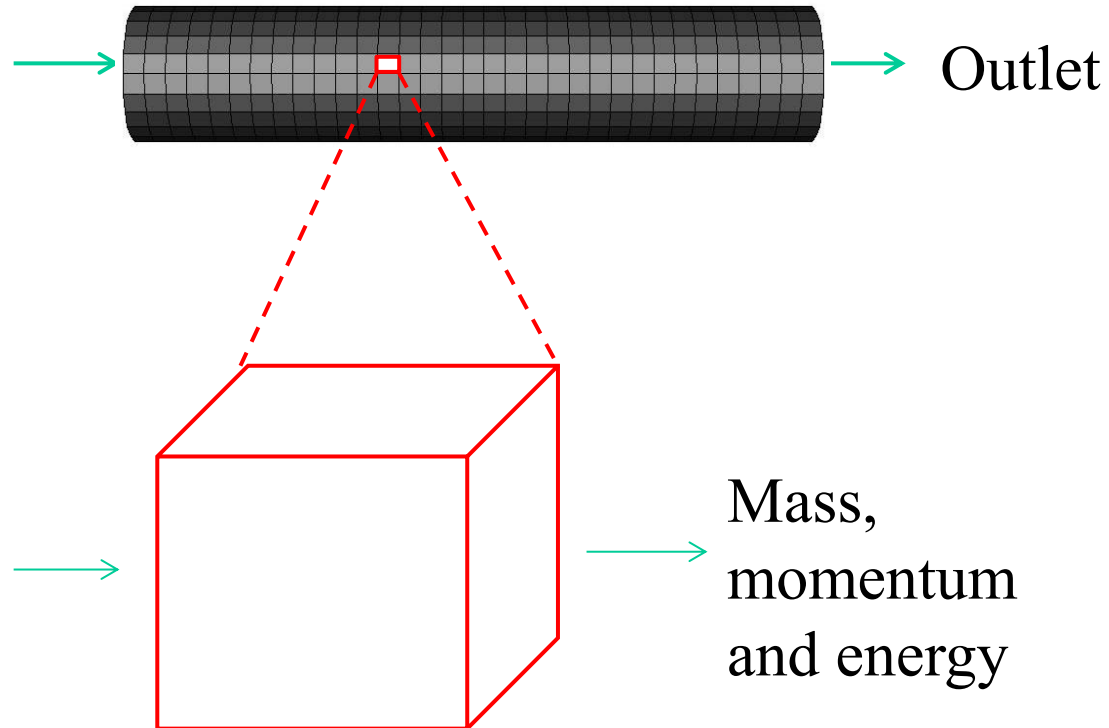
How CFD works

Inlet fluid

- Material
- Velocity
- Temp.

Solver:

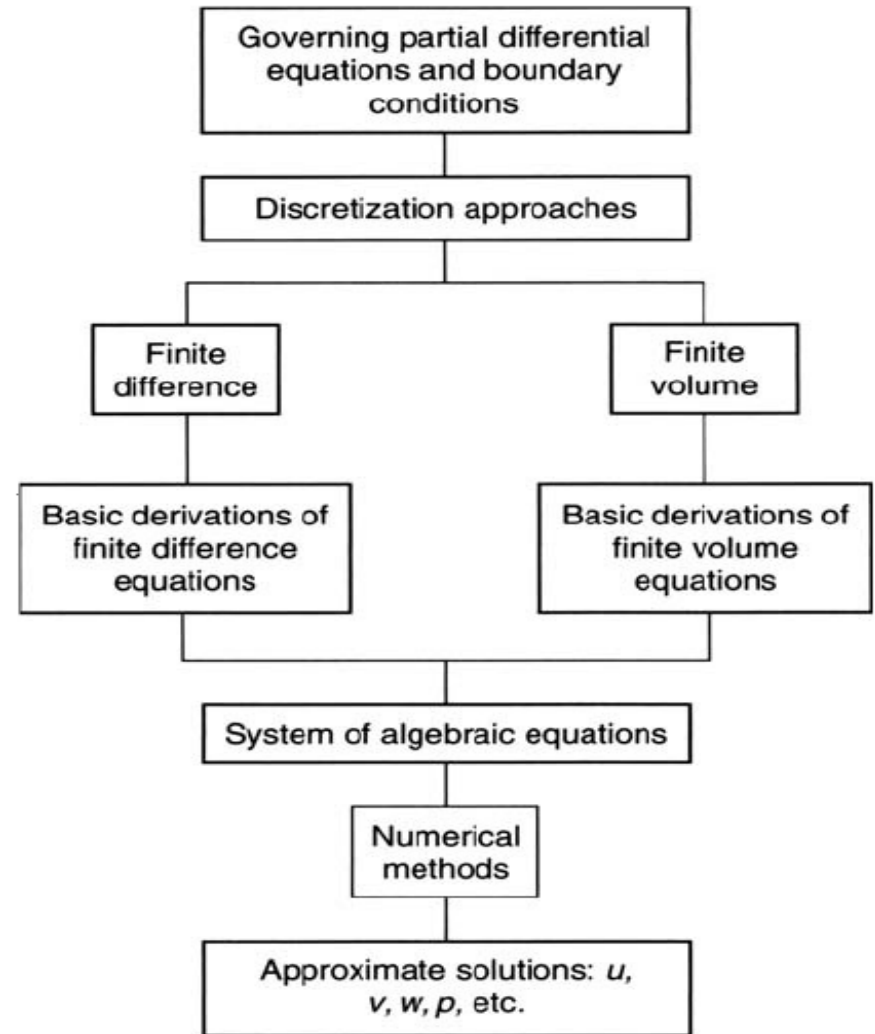
Mass,
momentum
and energy



- Apply governing equation on each control volume – **the equations of change**
 - Discretisation
 - Solution of algebraic equations
- } Numerical solution of governing equations

Solver: Computational Solution Procedure

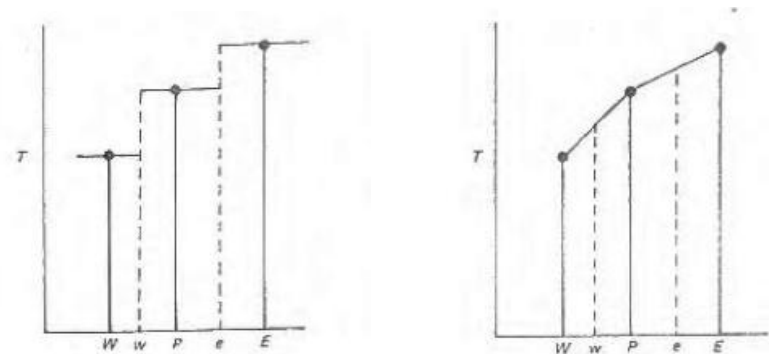
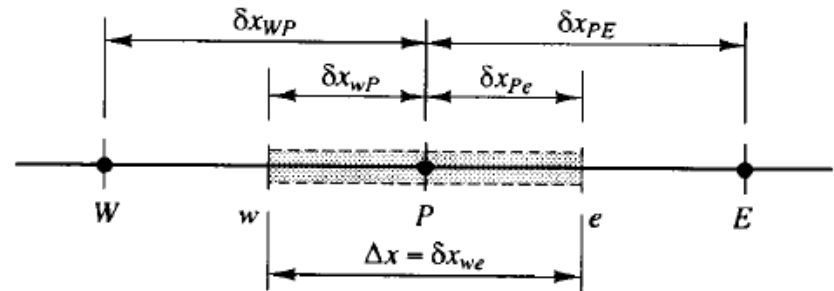
- Integration of the governing equations of fluid flow over all the control volume of the solution domain.
- Discretisation involves the substitution of a variety of finite-difference-type approximations for the terms in the integrated equation representing flow processes such as convection, diffusion, and sources. This converts the integral equations into a system of algebraic equations.
- Solution of the algebraic equations by an iterative method.



Finite Volume Method

- Introduced by Macdonald (1971) and MacCormack and Paullay (1972) for the solution of 2D unsteady Euler equation
- Rizzi and Inouye (1973) extended this to three dimensional flows
- Also known as control volume method as the domain is divided into a number of nonoverlapping volumes such that there is one control volume around each grid point

- The governing equation is integrated over each control volume
- Piecewise profiles expressing the variation of ϕ between the grid points are used to evaluate the integrals



Stepwise profile

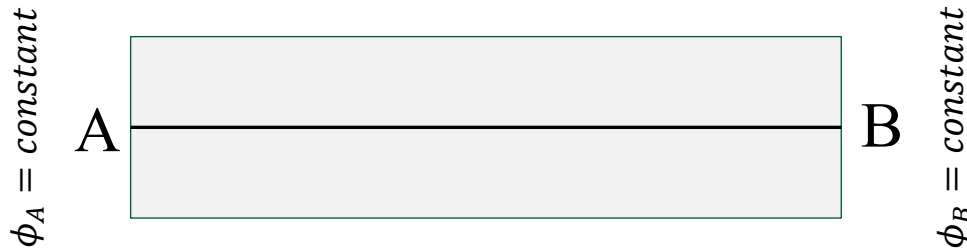
Piecewise linear profile 10

FVM: 1D, steady-state, diffusion

- Consider a steady state diffusion of property ϕ in a 1D domain. The process is governed by:

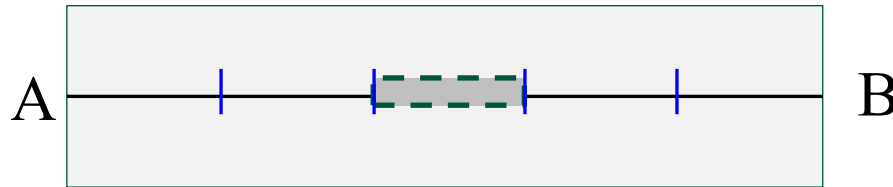
$$\frac{d}{dx} \left(\Gamma \frac{d\phi}{dx} \right) + S = 0$$

- Where Γ is the diffusion coefficient and S is the source term. Boundary value of ϕ (at points A and B in the diagram/geometry below) are defined.

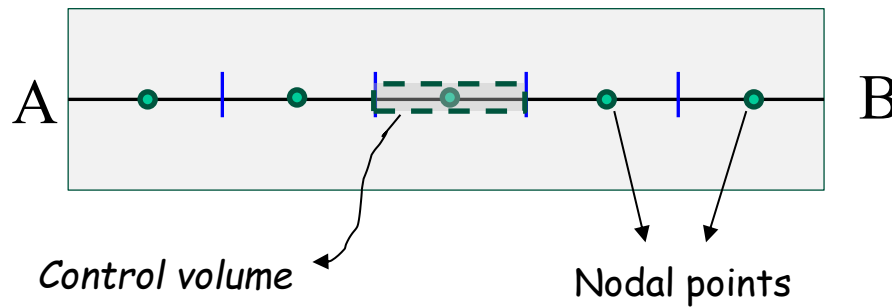


FVM: 1D, steady-state, diffusion

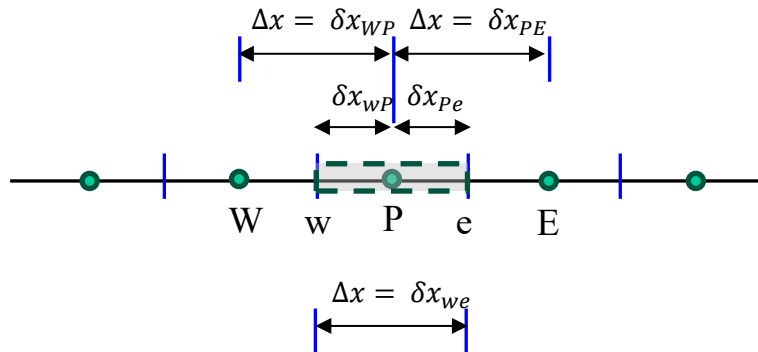
- Step 1: Grid generation



Divide the domain in 5 equal control volumes



Let us put a number of nodal points in the space between A and B



Nomenclature:

P = any node

E = node at east of P

W = node at west of P

e = boundary of CV at east of P

w = boundary of CV at west of P

FVM: 1D, steady-state, diffusion

- Step 2: Discretisation

Integration of the governing equation over a control volume to yield a discretised equation at its nodal point P.

$$\int \frac{d}{dx} \left(\Gamma \frac{d\phi}{dx} \right) + \int S = \left(\Gamma A \frac{d\phi}{dx} \right)_e - \left(\Gamma A \frac{d\phi}{dx} \right)_w + \bar{S} \Delta V = 0$$

A = cross sectional area of control volume face, ΔV = volume of the control volume, $\bar{S}$ = average value of source over the control volume

The equation states that the diffusive flux of ϕ leaving the east face minus the diffusive flux of ϕ entering the west face is equal to the generation of ϕ .

FVM: 1D, steady-state, diffusion

- Step 2: Discretisation

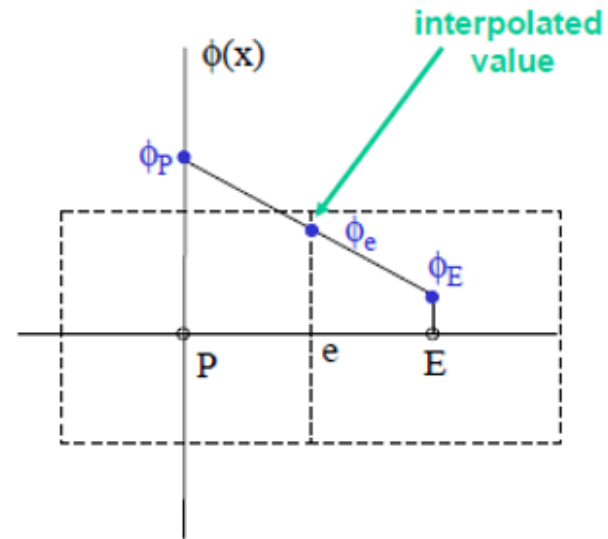
The diffusion coefficient Γ and the gradient $\frac{d\phi}{dx}$ at east “e” and west “w” are required.

Applying [central differencing](#) or linear approximation,

$$\Gamma_w = \frac{\Gamma_W + \Gamma_P}{2}, \quad \Gamma_e = \frac{\Gamma_P + \Gamma_E}{2}$$

$$\left(\Gamma A \frac{d\phi}{dx} \right)_e = \Gamma_e A_e \left(\frac{\phi_E - \phi_P}{\delta x_{PE}} \right)$$

$$\left(\Gamma A \frac{d\phi}{dx} \right)_w = \Gamma_w A_w \left(\frac{\phi_P - \phi_W}{\delta x_{WP}} \right)$$



$$\bar{S}\Delta V = S_u + S_p\phi_p \quad \text{Source term as a linear function of property } \phi. \text{ (assumption)}$$

FVM: 1D, steady-state, diffusion

- Step 2: Discretisation

Substitute the above equations in the discretised equation:

$$\Gamma_e A_e \left(\frac{\phi_E - \phi_P}{\delta x_{PE}} \right) - \Gamma_w A_w \left(\frac{\phi_P - \phi_W}{\delta x_{WP}} \right) + (S_u + S_p \phi_p) = 0$$

$$\left(\frac{\Gamma_e}{\delta x_{PE}} A_e + \frac{\Gamma_w}{\delta x_{WP}} A_w - S_p \right) \phi_p = \left(\frac{\Gamma_w}{\delta x_{WP}} A_w \right) \phi_W + \left(\frac{\Gamma_e}{\delta x_{PE}} A_e \right) \phi_E + S_u$$

In a simple form:

$$a_p \phi_p = a_W \phi_W + a_E \phi_E + S_u$$

a_W	a_E	a_p
$\left(\frac{\Gamma_w}{\delta x_{WP}} A_w \right)$	$\left(\frac{\Gamma_e}{\delta x_{PE}} A_e \right)$	$a_W + a_E - S_p$

FVM: 1D, steady-state, diffusion

- Step 2: Solution

Discretised equation for node P (on previous slide) is an algebraic equation. Similar equation can be set up for all nodes in the flow domain.

For control volumes that are adjacent to the domain boundaries the general discretised equation is modified to incorporate boundary conditions.

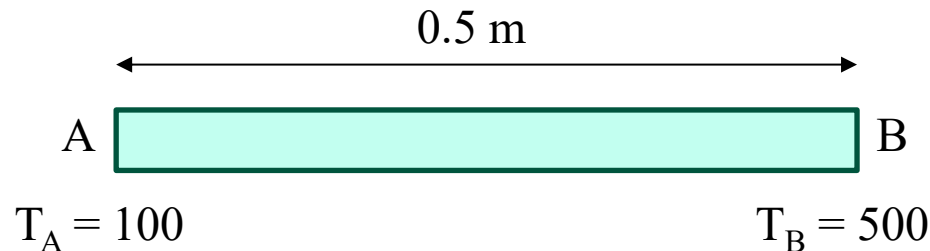
The resulting system of linear algebraic equations is then solved to obtain the distribution of property ϕ at nodal points.

FVM: 1D, steady-state, diffusion

Classroom example

Consider the problem of source-free conduction in an insulated rod whose ends are maintained at constant temperature of 100 C and 500 C respectively. The one-dimensional problem is governed by

$$\frac{d}{dx} \left(k \frac{dT}{dx} \right) = 0$$

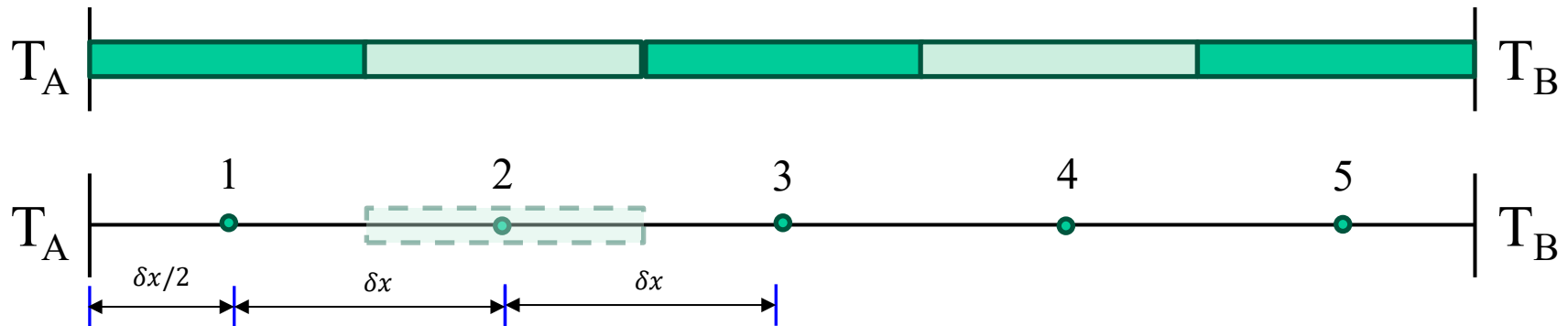


Calculate the steady state temperature distribution in the rod. Thermal conductivity k equals 1000 W/m/K, cross-section area A is $10 \times 10^{-3} \text{ m}^2$.

FVM: 1D, steady-state, diffusion

Classroom example

Let us divide the length of the rod into five equal control volumes.



The grid contains 5 control volume with each having node at the centre. Therefore, the geometry has 5 nodes.

FVM: 1D, steady-state, diffusion

Classroom example

For each of nodes 2, 3 and 4, temperature values to the east and west are available as nodal values. For these nodes, discretised equation for each node can be written as:

$$\left(\frac{k_e}{\delta x_{PE}} A_e + \frac{k_w}{\delta x_{WP}} A_w - \cancel{S_p} \right) T_p = \left(\frac{k_w}{\delta x_{WP}} A_w \right) T_W + \left(\frac{k_e}{\delta x_{PE}} A_e \right) T_E + \cancel{S_u} \quad \begin{matrix} = 0 \\ = 0 \end{matrix}$$

In a simple form:

$$a_p T_p = a_W T_W + a_E T_E$$

a_W	a_E	a_p
$\left(\frac{k_w}{\delta x_{WP}} A_w \right)$	$\left(\frac{k_e}{\delta x_{PE}} A_e \right)$	$a_W + a_E$

$$A_w = A_e = A, k_w = k_e = k$$

FVM: 1D, steady-state, diffusion

Classroom example

For nodes 1 and 5 (boundary nodes), special treatment is required.

For node 1, discretised equation for each node can be written as:

$$kA \left(\frac{T_E - T_P}{\delta x} \right) - kA \left(\frac{T_P - T_A}{\delta x/2} \right) = 0$$

$$\left(\frac{k}{\delta x} A + \frac{2k}{\delta x} A \right) T_P = 0 \times T_W + \left(\frac{k}{\delta x} A \right) T_E + \left(\frac{2k}{\delta x} A \right) T_A$$

In a simple form:

$$a_p T_p = a_W T_W + a_E T_E + S_u$$

a_W	a_E	a_p	S_p	S_u
0	$\left(\frac{k}{\delta x} A \right)$	$a_W + a_E - S_p$	$-\frac{2k}{\delta x} A$	$\left(\frac{2k}{\delta x} A \right) T_A$

FVM: 1D, steady-state, diffusion

Classroom example

For node 5, discretised equation for each node can be written as:

$$kA \left(\frac{T_B - T_P}{\delta x/2} \right) - kA \left(\frac{T_P - T_W}{\delta x} \right) = 0$$

$$\left(\frac{k}{\delta x} A + \frac{2k}{\delta x} A \right) T_P = \left(\frac{k}{\delta x} A \right) T_W + 0 \times T_E + \left(\frac{2k}{\delta x} A \right) T_B$$

In a simple form:

$$a_p T_p = a_W T_W + a_E T_E + S_u$$

a_W	a_E	a_p	S_p	S_u
$\left(\frac{k}{\delta x} A \right)$	0	$a_W + a_E - S_p$	$-\frac{2k}{\delta x} A$	$\left(\frac{2k}{\delta x} A \right) T_B$

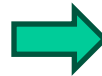
FVM: 1D, steady-state, diffusion

Classroom example

The discretisation process has yielded one equation for the nodal points 1 to 5. As per the values given in the problem statement, $k = 1000 \text{ W/m/K}$, $A = 10 \times 10^{-3} \text{ m}^2$, and $\delta x = 0.5/5 = 0.1 \text{ m}$

$$\frac{k}{\delta x} A = 100 \text{ W/K}$$

Node	a_W	a_E	S_u	S_P	a_p
1	0	$\left(\frac{kA}{\delta x}\right)$	$\left(\frac{2kA}{\delta x}\right)T_A$	$-\frac{2k}{\delta x}A$	$a_W + a_E - S_P$
2	$\left(\frac{kA}{\delta x}\right)$	$\left(\frac{kA}{\delta x}\right)$	0	0	$a_W + a_E$
3	$\left(\frac{kA}{\delta x}\right)$	$\left(\frac{kA}{\delta x}\right)$	0	0	$a_W + a_E$
4	$\left(\frac{kA}{\delta x}\right)$	$\left(\frac{kA}{\delta x}\right)$	0	0	$a_W + a_E$
5	$\left(\frac{kA}{\delta x}\right)$	0	$\left(\frac{2k}{\delta x}A\right)T_B$	$-\frac{2k}{\delta x}A$	$a_W + a_E - S_P$



Node	a_W	a_E	S_u	S_P	a_p
1	0	100	$200T_A$	-200	300
2	100	100	0	0	200
3	100	100	0	0	200
4	100	100	0	0	200
5	100	0	$200T_B$	-200	300

FVM: 1D, steady-state, diffusion

Classroom example

Applying the discretised equation,

$$a_p T_p = a_W T_W + a_E T_E + S_u$$

The resulting set of algebraic equations are:

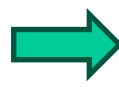
$$300T_1 = 100T_2 + 200T_A$$

$$200T_2 = 100T_1 + 100T_3$$

$$200T_3 = 100T_2 + 100T_4$$

$$200T_4 = 100T_3 + 100T_5$$

$$300T_5 = 100T_4 + 200T_B$$


$$\begin{bmatrix} 300 & -100 & 0 & 0 & 0 \\ -100 & 200 & -100 & 0 & 0 \\ 0 & -100 & 200 & -100 & 0 \\ 0 & 0 & -100 & 200 & -100 \\ 0 & 0 & 0 & -100 & 300 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \end{bmatrix} = \begin{bmatrix} 200T_A \\ 0 \\ 0 \\ 0 \\ 200T_B \end{bmatrix}$$

FVM: 1D, steady-state, diffusion

Classroom example

If $T_A = 100$ and $T_B = 500$, the solution of the matrix is:

$$\begin{bmatrix} 300 & -100 & 0 & 0 & 0 \\ -100 & 200 & -100 & 0 & 0 \\ 0 & -100 & 200 & -100 & 0 \\ 0 & 0 & -100 & 200 & -100 \\ 0 & 0 & 0 & -100 & 300 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \end{bmatrix} = \begin{bmatrix} 20000 \\ 0 \\ 0 \\ 0 \\ 100000 \end{bmatrix}$$

$$\begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \end{bmatrix} = \begin{bmatrix} 140 \\ 220 \\ 300 \\ 380 \\ 460 \end{bmatrix}$$

The exact solution is a linear distribution between the specified boundary temperature: $T = 800x + 100$.

FVM: Discretisation schemes

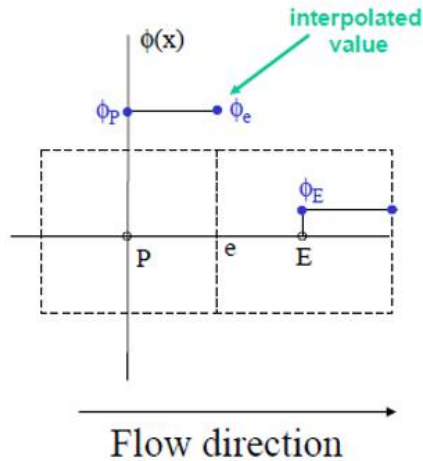
In the classroom example, we applied “central differentiation” scheme to approximate the value of gradient at cell boundary.

Other discretisation schemes:

- first order upwind,
- power law scheme,
- second order upwind,
- QUICK – quadratic upwind interpolation for convective kinetics

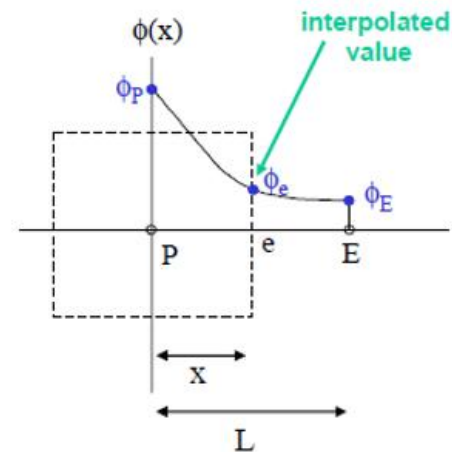
FVM: Discretisation schemes

First order upwind



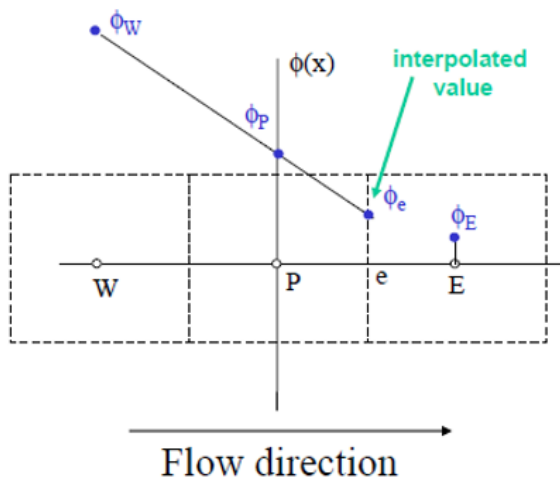
Value of ϕ at the face is the same as the cell centered value in the cell upstream of the face

Power law



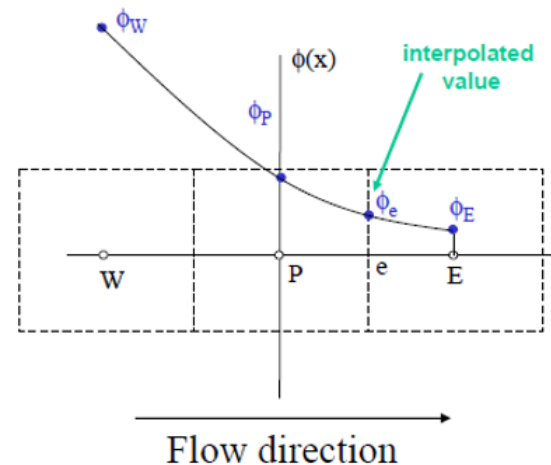
Face value is determined from an exponential profile through the cell values

Second order upwind



Value of ϕ at the face is determined from the values in the two cells upstream of the face

QUICK



A quadratic curve is fitted through two upstream nodes and one downstream node

FVM: Convergence, consistent, stability

Results generated by a CFD code are at best as good as the physics embedded in it and at worst as good as its operator.

Three mathematical concepts are useful in determining the success or otherwise of CFD algorithm.

- **Convergence:** property of a numerical method to produce a solution which approaches the exact solution as the grid spacing, control volume size is reduced to zero.
- **Consistent:** numerical schemes produce systems of algebraic equations which can be demonstrated to be equivalent to the original governing equation as the grid spacing tends to zero.
- **Stability:** is associated with damping of errors as the numerical method proceeds. If a technique is not stable, even roundoff errors in the initial data can cause wild oscillation or divergence.

FVM: Pressure-velocity coupling

- Pressure appears in all three momentum equations. The velocity field also has to satisfy the continuity equation. So even though there is no explicit equation for pressure, we do have four equations for four variables, and all set of equations is closed.
- So-called pressure-velocity coupling algorithms are used to derive equations for pressure from the momentum equations and the continuity equation.
- The most common algorithm is SIMPLE (semi-implicit Method for Pressure-Linked Equations).

FVM: Importance of mesh design and quality

- Pre-processing: Geometry creation and [meshing](#)
 - [Meshing](#): dividing flow domain into the number of subdomains
- Grid design or mesh design
 - Type of mesh to be used
 - Resolving the gradients
 - Controlling the growth of cells

FVM: Importance of mesh design and quality

- Type of mesh

If the geometry is simple

Always use **quad/ hex** cells

More cell count needed if tri/tets are used

If the geometry is complex

Try to decompose to fit quad/hex cells

At least use quad/hex cells along the wall - hybrid mesh

If not, grow prism layers on the boundary

Make use of additional tools to **reduce the cell count**

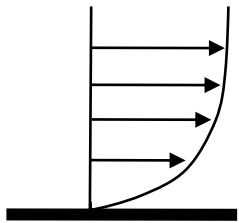
Size Function

Hex Core

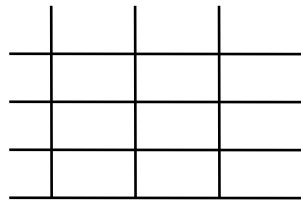
FVM: Importance of mesh design and quality

- Resolving gradient

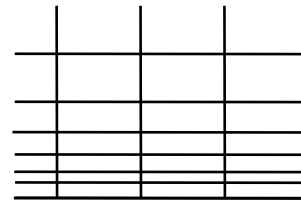
Use finer mesh in the areas of higher gradients



flow



inadequate



better

Capture all the pertinent flow features

Separation

Boundary layers

Shear layers

Shocks

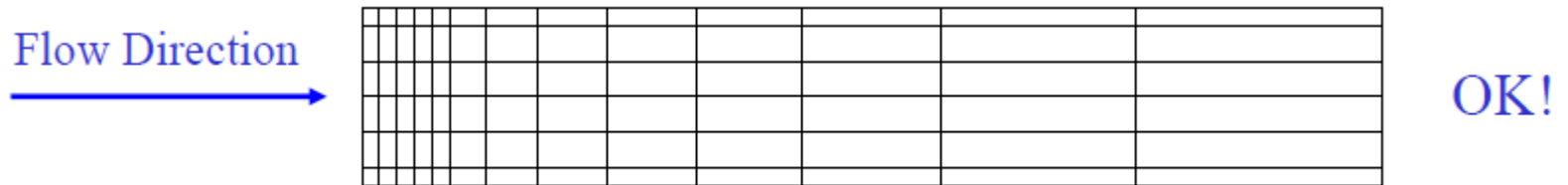
FVM: Importance of mesh design and quality

- Resolving gradient

Use cell aspect ratio (width/height) of unity, at places where flow is multi dimensional

- Quads do not offer any special advantage for such conditions

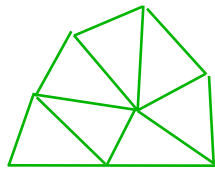
Stretch Quad/hex cells, where flow is fully developed and essentially one-dimensional



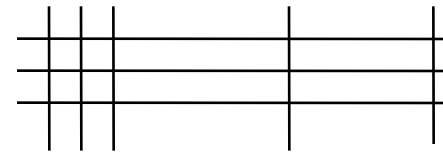
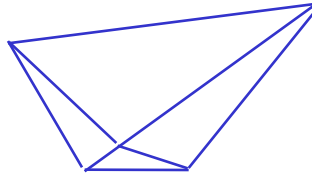
FVM: Importance of mesh design and quality

- Controlling the growth of cells

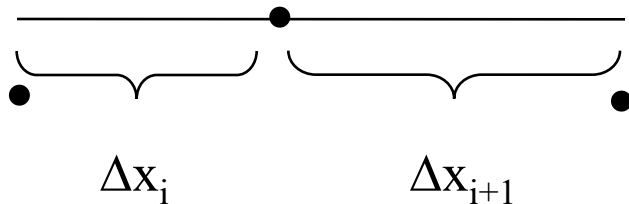
Change in cell/element size should be gradual (smooth)



smooth change
in cell size



sudden change
in cell size — **AVOID!**



$$\frac{\Delta x_{i+1}}{\Delta x_i} \leq 1.2$$

Ideally, the maximum change in grid spacing should be 20%

FVM: Importance of mesh design and quality

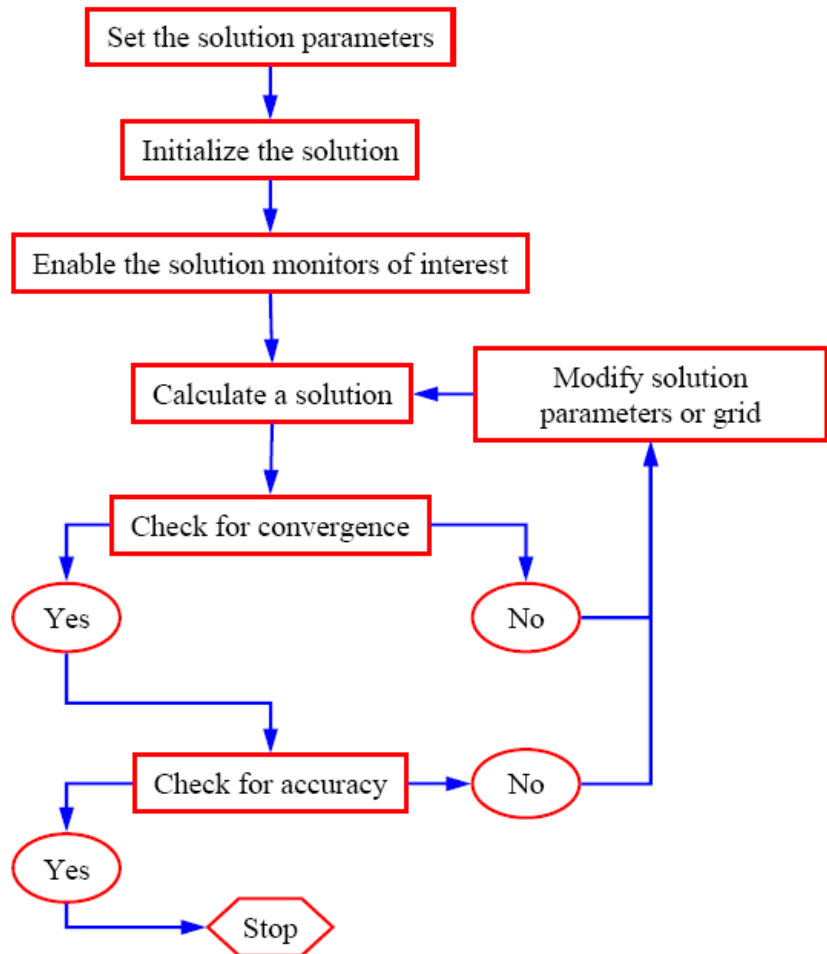
- Mesh quality
 - Skewness
 - Area/ Volume
 - Aspect ratio
 - Adjacent cell ratio

Summary

- CFD → can be used to predict flow and associated transport phenomena occurring at different time and space scales.
- Three important aspects: pre-processor, solver and post-processor.
- Finite volume approach:
 - We learned the application of FVM to 1D, steady state diffusion problem
 - Discretisation scheme: method to approximate a value of a variable at the boundaries of control volume.
 - Shape, size and number of control volumes: very critical to FVM simulations

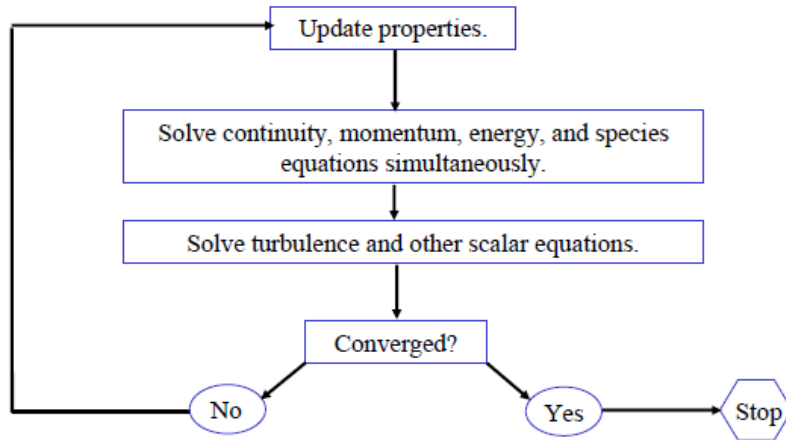
Fluent Solver Basics

- Solution parameters
 - Choosing the solver
 - Discretization schemes
- Initialization
- Convergence
 - Monitoring convergence
 - Stability
 - Setting Under-relaxation
 - Setting Courant number
 - Accelerating convergence
- Accuracy
 - Grid Independence
 - Adaption



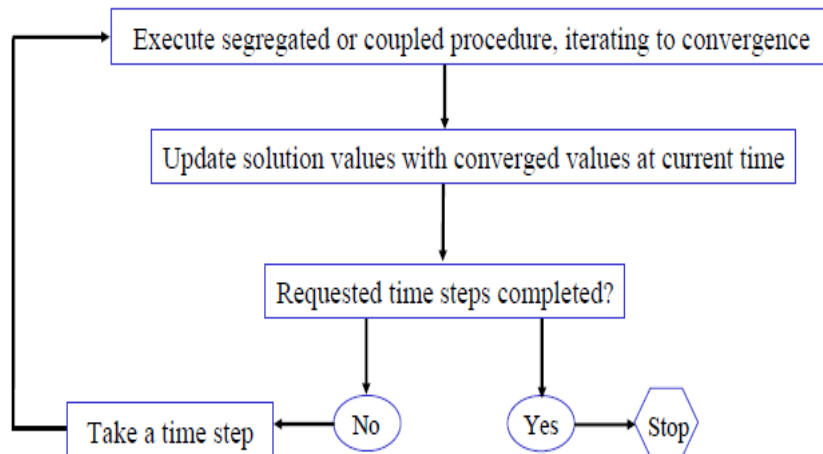
Fluent Solver Basics

Coupled solution procedure



For a given cell, equations for all variables are solved, and that process is then repeated for all cells.

Unsteady formulation



The user has to specify a time step that matches the time variation in the flow

If a time accurate solution is required, the solution should be converged at every time step. Otherwise, convergence at every time step may not be necessary.