9. The CFD Process

- Pre-processing
- **Solving**:
  - **discretisation**
  - **solution of equations**
- Post-processing

- **Pre-processing**:
  - **governing equations**
  - **boundary conditions**
  - **grid-generation**
- Solving
- Post-processing

- Pre-processing
- Solving
- **Post-processing:**
  - **analysis**
  - **visualisation**

Commercial Codes

Vendor	Code
CD adapco	Star CD Star CCM+
Ansys	FLUENT CFX
Flow Science	FLOW3D
EXA	PowerFLOW

Web portal: **http://www.cfd-online.com/**

The Computational Mesh

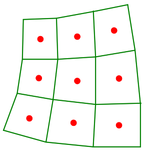
Mesh Generation

- **Function:**
  - to decompose the domain into control volumes
- **Constraints:**
  - flow geometry
  - capabilities of the solver
- **Output:**
  - cell vertices (x, y, z)
  - connectivity data

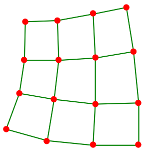
Mesh Arrangements

- Node locations (cell centres / vertices)
- Staggered / co-located
- Cell shapes (tetrahedra / hexahedra / arbitrary polyhedra)
- Structured (single- or multi-block) / unstructured
- Cartesian / curvilinear (orthogonal / non-orthogonal)
- …

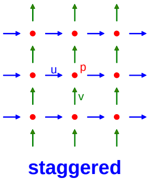
Storage Locations



cell-centred



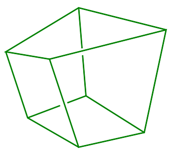
cell-vertex



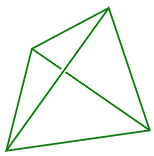
staggered

Cell Shapes

- **2-d:** triangles, quadrilaterals, …
- **3-d:** tetrahedra, hexahedra, …



hexahedron



tetrahedron

Areas and Volumes

- **Vector areas** are needed to compute **fluxes**:

  mass flux: $\rho \mathbf{u} \bullet \mathbf{A}$

  diffusive flux: $-\Gamma \nabla \phi \bullet \mathbf{A}$

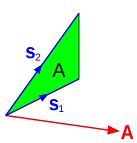
- **Volumes** are needed to compute **amounts in cells** and **cell averages**:

  amount in cell: $\rho V \phi$

Face Areas

Triangles

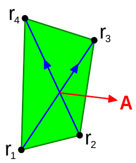
$\mathbf{A} = \frac{1}{2} \mathbf{s}_1 \wedge \mathbf{s}_2$



Quadrilaterals

- 4 points are not necessarily coplanar
- Vector area is independent of spanning surface

$\mathbf{A} = \frac{1}{2} \mathbf{d}_{13} \wedge \mathbf{d}_{24} = \frac{1}{2} (\mathbf{r}_3 - \mathbf{r}_1) \wedge (\mathbf{r}_4 - \mathbf{r}_2)$



Some Vector Calculus (*Not Examinable*)

$$\nabla \equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$$ is both a vector and a differential operator

Gradient: $$grad(\phi) \equiv \nabla\phi \quad \equiv \left(\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z}\right)$$

Divergence: $$div\,\mathbf{f} \equiv \nabla \bullet \mathbf{f} \quad \equiv \frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z}$$

Curl: $$curl\,\mathbf{f} \equiv \nabla \wedge \mathbf{f} \quad \equiv \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ f_x & f_y & f_z \end{vmatrix}$$

Integral Theorems

Gauss' Divergence Theorem: $$\int_V \nabla \bullet \mathbf{f} \;\; \mathrm{d}V = \oint_{\partial V} \mathbf{f} \bullet \mathrm{d}\mathbf{A}$$

Stokes' Theorem: $$\int_A \nabla \wedge \mathbf{f} \bullet \mathrm{d}\mathbf{A} = \oint_{\partial A} \mathbf{f} \bullet \mathrm{d}\mathbf{s}$$

Volumes

Position vector: $\mathbf{r} \equiv (x, y, z)$

Divergence: $$\nabla \bullet \mathbf{r} = \frac{\partial x}{\partial x} + \frac{\partial y}{\partial y} + \frac{\partial z}{\partial z} = 3$$

Integrate over an arbitrary closed volume, V:

$$\int_V \nabla \bullet \mathbf{r} \;\; \mathrm{d}V = \int_V 3 \;\; \mathrm{d}V$$

Use the divergence theorem:

$$\oint_{\partial V} \mathbf{r} \bullet \mathrm{d}\mathbf{A} = 3V$$

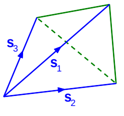
$$V = \frac{1}{3}\oint_{\partial V} \mathbf{r} \bullet \mathrm{d}\mathbf{A}$$

Volumes

Arbitrary volume: $$V = \frac{1}{3}\oint_{\partial V} \mathbf{r} \bullet \mathrm{d}\mathbf{A}$$

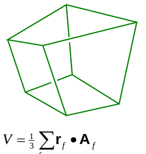
General polyhedron: $$V = \frac{1}{3}\sum_{faces} \mathbf{r}_f \bullet \mathbf{A}_f$$

Tetrahedron



$$V = \tfrac{1}{6}\mathbf{s}_1 \bullet \mathbf{s}_2 \wedge \mathbf{s}_3$$

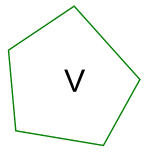
Hexahedron



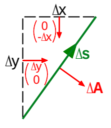
$$V = \tfrac{1}{3}\sum_{faces} \mathbf{r}_f \bullet \mathbf{A}_f \qquad \mathbf{r}_f = \tfrac{1}{4}(\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3 + \mathbf{r}_4)$$

2-D Case

- Treat as cells of unit depth
- The "volume" of the cell is then the planar area



- Outward "face area" vectors derived from **Cartesian projections**:



$$\Delta\mathbf{A} = \begin{pmatrix} \Delta y \\ -\Delta x \end{pmatrix}$$

(cell boundary traversed anticlockwise)

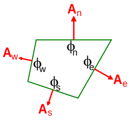
Cell-Averaged Derivatives

$$\left(\frac{\partial\phi}{\partial x}\right)_{av} \equiv \frac{1}{V}\int_V \frac{\partial\phi}{\partial x}\,\mathrm{d}V \quad = \frac{1}{V}\int_V \nabla\bullet(\phi\mathbf{e}_x)\,\mathrm{d}V \quad = \frac{1}{V}\oint_{\partial V} \phi \;\mathrm{d}A_x \qquad \boxed{\left(\frac{\partial\phi}{\partial x}\right)_{av} = \frac{1}{V}\sum_{faces}\phi_f A_{fx}}$$

$$(\nabla\phi)_{av} = \frac{1}{V}\oint_{\partial V} \phi \;\mathrm{d}\mathbf{A} \qquad \boxed{(\nabla\phi)_{av} = \frac{1}{V}\sum_{faces}\phi_f \mathbf{A}_f}$$

Hexahedra:

$$(\nabla\phi)_{av} = \frac{1}{V}(\phi_w\mathbf{A}_w + \phi_e\mathbf{A}_e + \phi_s\mathbf{A}_s + \phi_n\mathbf{A}_n + \phi_b\mathbf{A}_b + \phi_t\mathbf{A}_t)$$



Cartesian cell:

$$\frac{\partial\phi}{\partial x} = \frac{\phi_e - \phi_w}{\Delta x} \quad = \frac{\phi_e A - \phi_w A}{A\Delta x} \quad = \frac{1}{V}(\phi_e A_{ex} + \phi_w A_{wx})$$

Example

A tetrahedral cell has vertices at A$(2, -1, 0)$, B$(0, 1, 0)$, C$(2, 1, 1)$ and D$(0, -1, 1)$.

(a) Find the outward vector areas of all faces. Check that they sum to zero.
(b) Find the volume of the cell.
(c) If the values of ϕ at the centroids of the faces (indicated by their vertices) are

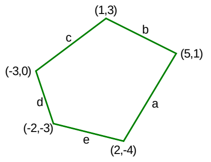
$\phi_{BCD} = 5, \quad \phi_{ACD} = 3, \quad \phi_{ABD} = 4, \quad \phi_{ABC} = 2,$

find the volume-averaged derivatives $\left(\frac{\partial\phi}{\partial x}\right)_{av}, \left(\frac{\partial\phi}{\partial y}\right)_{av}, \left(\frac{\partial\phi}{\partial z}\right)_{av}$

Example

In a 2-dimensional unstructured mesh, one cell has the form of a pentagon. The coordinates of the vertices are as shown in the figure, whilst the average values of a scalar ϕ on edges $a - e$ are:

$$\phi_a = -7, \quad \phi_b = 8, \quad \phi_c = -2, \quad \phi_d = 5, \quad \phi_e = 0$$



Find:

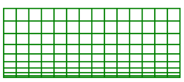
(a) the area of the pentagon;

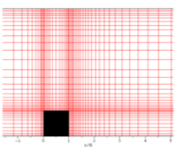
(b) the cell-averaged derivatives $\left(\frac{\partial\phi}{\partial x}\right)_{av}, \left(\frac{\partial\phi}{\partial y}\right)_{av}$

Structured Grids

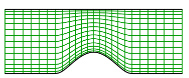
Control volumes indexed by (i, j, k)

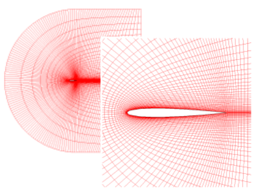
Cartesian



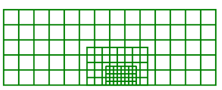


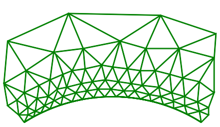
Curvilinear

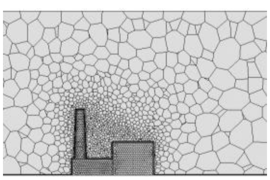




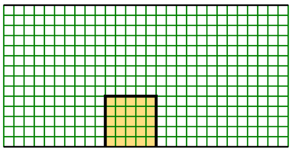
Unstructured Grids







Fitting Complex Boundaries
– Blocking Out Cells



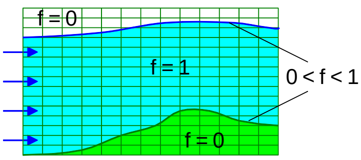
- Implemented by a source-term modification:

$$a_P\phi_P - \sum_F a_F\phi_F = b_P + s_P\phi_P \qquad b_P \to 0, \quad s_P \to -(large\ number)$$

$$\phi_P = \frac{\sum a_F\phi_F}{large\ number} \approx 0$$

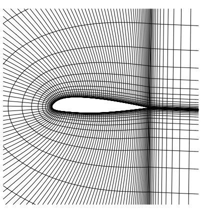
- A lot of redundant matrix operations for cells inside block

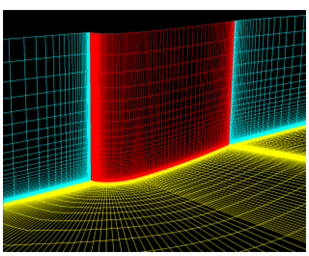
Fitting Complex Boundaries
– Volume-of-Fluid (VOF) Approach



- One way of handling **free-surface** calculations.
- For **moving** surfaces, solve a transport equation for **fluid fraction** *f*.

Fitting Complex Boundaries
– Curvilinear (Body-Fitted) Grids





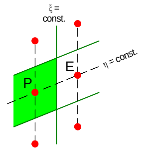
Curvilinear Grids

$$\frac{d}{dt}(amount) + \sum_{faces}(advection + diffusion) = source$$

Diffusion:

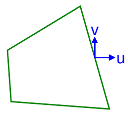
– also require derivatives **parallel** to cell faces

$$-\Gamma \frac{\partial \phi}{\partial n} A \neq -\Gamma \left(\frac{\phi_E - \phi_P}{\Delta_{PE}} \right) A$$



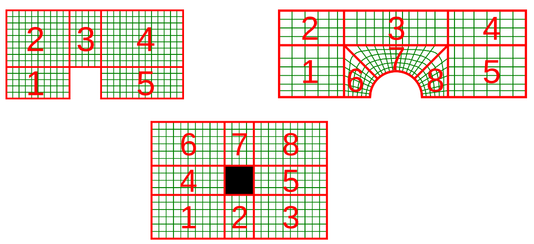
Advection:

– all velocity components contribute to mass flux



Fitting Complex Boundaries

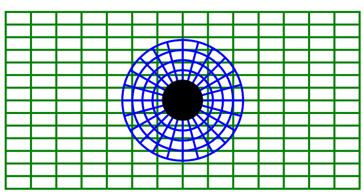
– Multi-Block Grids



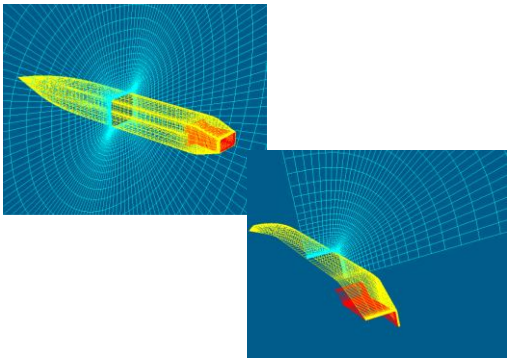
- Multiple structured blocks
- Grid lines may or may not match at block boundaries
- Arbitrary interfaces allow non-coincident grid vertices
- Sliding grids used for rotating machinery

Fitting Complex Boundaries

– Overlapping (Chimera) Grids



Use of Symmetry



Disposition of Grid Cells

- **Local refinement** where gradients are large:
  - solid boundaries
  - separation, reattachment and impingement points
  - discontinuities (shocks, hydraulic jumps)
- **Grid-dependence** tests necessary
- **Turbulent** calculations impose constraints:
  - low-Re calculations: $y^+ < 1$ (ideally)
  - wall-function calculations: $30 < y^+ < 150$ (ideally)

Multiple Levels of Grid

- Used to confirm **grid independence**
- Exploited by **multi-grid** methods
- Permit **estimation of error** (and solution improvement) by **Richardson extrapolation**

Richardson Extrapolation

Order n $\Leftrightarrow$ $\text{error} \propto \Delta^n$

$$\phi_\Delta - \phi^* = C\Delta^n$$
$$\phi_{2\Delta} - \phi^* = C(2\Delta)^n$$

$$\phi^* = \frac{2^n \phi_\Delta - \phi_{2\Delta}}{2^n - 1}$$

Improved solution by weighted average from two meshes

$$C\Delta^n = \frac{\phi_{2\Delta} - \phi_\Delta}{2^n - 1}$$

Estimate of error from difference between solutions on two meshes

Example

A numerical scheme known to be second-order accurate is used to calculate a steady-state solution on two regular Cartesian meshes A and B, where the finer mesh A has half the grid spacing of mesh B. The values of the solution ϕ at a particular point are found to be 0.74 using mesh A and 0.78 using mesh B. Use Richardson extrapolation to:

(a) estimate an improved value of the solution at this point;

(b) estimate the error at this point using the mesh-A solution.

Summary of Grids

- Dictated by:
  - flow geometry
  - solver capabilities
- Grid generator provides vertex and connectivity data
- Vector geometry to find areas, volumes and cell-averages
- Structured/unstructured meshes
- Complex geometries via:
  - blocked-out cells
  - volume-of-fluid methods
  - curvilinear (body-fitted) meshes
  - multiblock grids
  - chimera meshes
- Cell density higher in rapidly-varying regions

Boundary Conditions

Boundary Conditions

- **Inlet:**
  - velocity inlet
  - stagnation / reservoir inlet
- **Outlet:**
  - standard outlet
  - pressure boundary
  - radiation boundary
- **Wall:**
  - non-slip (rough/smooth; moving/stationary; adiabatic/heat-transfer)
  - slip
- **Symmetry plane**
- **Periodic boundary**
- **Free surface**

Flow Visualisation

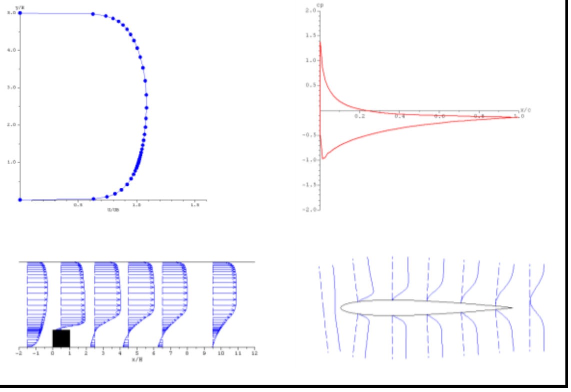
Uses of Flow Visualisation

- Understanding flow behaviour
- Locating important regions
- Summarising data
- Optimising design
- Finding reasons for non-convergence
- Publicity

Types of Plot

- x-y line graphs
- Contour plots
- Vector plots
- Streamline plots
- Mesh plots
- Composite plots

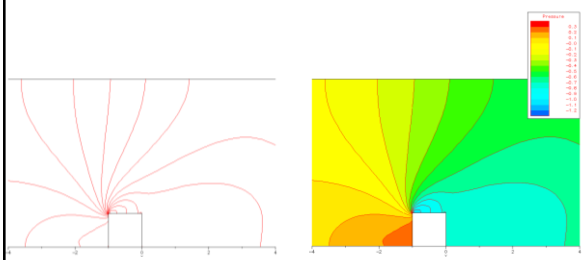
x-y Graphs



x-y Graphs
– Assessment

- Simple
- Widely-available software
- Precise and quantitative
- Direct comparison with experimental data
- Linear or logarithmic scales
- Limited view of flow field

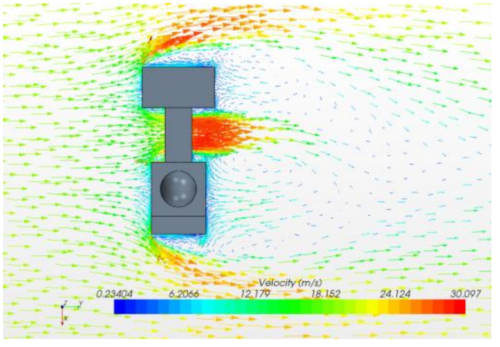
Contour Plots



Contour Plots
– Assessment

- Isoline (2-d) or isosurface (3-d)
- Optional smooth or discrete colour shading
- Global view of the flow
- Geometric spacing of lines indicates gradient
- Not as quantitative as line graphs
- Miss detail in small, but important, flow regions

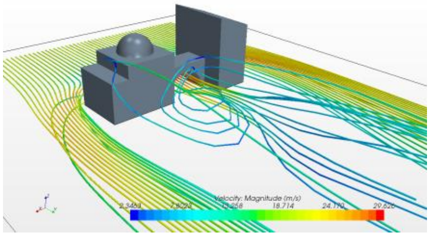
Vector Plots

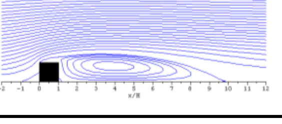


Vector Plots
– Assessment

- Direction and magnitude
- Used to plot vector quantities (velocity and stress)
- May be coloured to indicate magnitude
- Excellent first indication of flow behaviour
- Interpolation often necessary for non-uniform grids
- Not good in flows with wide range of magnitudes
- Miss important detail in small regions
- Orientation effects deceptive in 3d

Streamline Plots

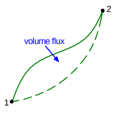


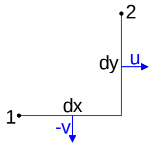


Calculating Streamlines

3-d: integrate **particle path** $\frac{d\mathbf{x}}{dt} = \mathbf{u}$

2-d: contour the **stream function**



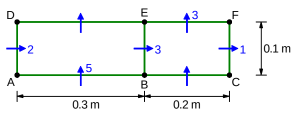


$$d\psi = u\,dy - v\,dx \quad = \textit{volume flux}$$

$$u = \frac{\partial \psi}{\partial y}, \qquad v = -\frac{\partial \psi}{\partial x}$$

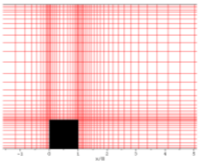
Example

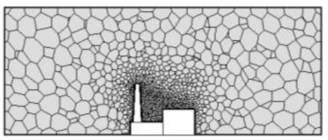
(a) Two adjacent cells in a 2-dimensional Cartesian mesh are shown below, along with the cell dimensions and some of the velocity components (in m s^{-1}) normal to cell faces. The value of the stream function ψ at the bottom left corner is $\psi_A = 0$. Find the value of the stream function at the other vertices B to F. (You may use either sign convention for the stream function.)

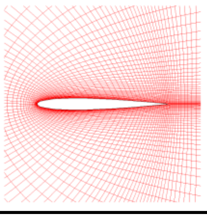


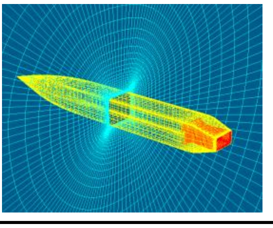
(b) Sketch the pattern of streamlines across the two cells in part (a).

Mesh Plots

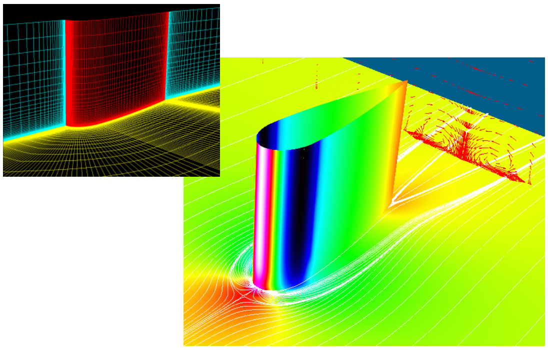




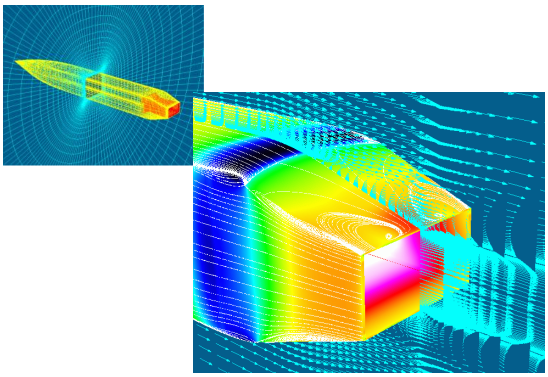




Composite Plots



Composite Plots



Composite Plots