CHAPTER 3

COMPUTATIONAL FLUID DYNAMICS

3.1 INTRODUCTION

Computational fluid dynamics is the science to predict fluid flow, heat and mass transfer, chemical reactions and related phenomena by solving the mathematical governing equations. It complements the testing and experimentation by reducing the total effort required in the laboratory. It works with the mathematical model by satisfying conservation, momentum and energy equations for the fluid flowing. It requires simplifying assumptions and appropriate boundary conditions for solving the problem. CFD applies numerical methods called discretization to develop approximations of the geometry equations of the fluid flow. Computers have been employed to solve the fluid flow problems for many years. Numerous programs have been written to solve either specific problems or specific classes of problems. From the mid-1970s, the complex mathematics required to generalize the algorithms began to be understood, and general purpose CFD solvers were developed. These began to appear in the early 1980s with very powerful computers, as well as an in-depth knowledge of fluid dynamics, and large amounts of time to set up simulations. Consequently, CFD was a tool used almost exclusively in research.

Recent advances in computing power, together with powerful graphics and interactive 3D manipulation of models, have made the process of creating a CFD model and analyzing results much less labor intensive,
reducing time and, hence, cost. Advanced solvers contain algorithms that enable robust solutions of the flow field in a reasonable time. As a result of these factors, Computational Fluid Dynamics is now an established industrial design tool, helping to reduce design time scales and improve processes throughout the engineering world. CFD provides a cost-effective and accurate alternate to scale model testing, with variations on the simulation being performed quickly, with obvious advantages. CFD is made possible by the advent of digital computer to study and analyze the simulation of fluids using modeling and numerical methods. Fluid dynamics is made simple using computer integration and pushed away the Analytical Fluid Dynamics (AFD) and Experimental Fluid Dynamics (EFD). CFD plays a major role because (i). It is a Simulation-based design rather than building and testing, (ii). Simulation of fluid flow phenomena that is tedious or hazardous for analytical or experimental analysis. CFD is widely used in every field where there is any flow of energy.

3.2 HISTORY OF FLUID DYNAMICS

Archimedes (287 – 212 BC) Greece, initiated the fields of statics, hydrostatics and pycnometry. He invented water screw which can be used to lift and transport water and granular materials. Leonardo da Vinci, (1452 – 1519) Italy, recognized and described the form and structure of the natural phenomena. His contribution to fluid mechanics was presented in a nine chapter dissertation which covered the study on water surface, movement of water, water waves, eddies, falling water, free jets, interference of waves, and other newly observed phenomena.

Isaac Newton (1643 – 1727) England, contributed the well known three laws of motion. Newton’s II law of motion, Newton’s law of viscosity, reciprocity principle, relationship between the speed of waves at a liquid surface and wavelength are the key contributions to fluid mechanics by him.
During the eighteenth and nineteenth century, significant works were done to describe the fluid motion. Daniel Bernoulli (1700 – 1782) derived the Bernoulli’s equation; Leonhard Euler (1707 – 1783) derived the Euler’s equation and described the conservation of mass and conservation of momentum and also explained the velocity potential theory. Claude Louis Marie Henry Navier (1785 – 1836) and George Gabriel Stokes (1819 – 1903) introduced viscous flow in Euler’s equation and developed Navier-Stokes equation.

Oshorne Reynolds (1842 – 1912) introduced Reynold’s number to govern the transition of fluid from laminar to turbulent.

During the twentieth century, most works were done on defining boundary layer and turbulence theory. Ludwig Prandtl (1875 – 1953) introduced the boundary layer theory, mixing length concept, compressible flows and the Prandtl number.

Theodore von Karman (1881-1963) described the von Karman vortex street. Geoffrey Ingram Taylor (1886-1975) proposed the statistical theory of turbulence and the Taylor microscale. Andrey Nikolaevich Kolmogorov (1903-1987) described the Kolmogorov scales and the universal energy spectrum. George Keith Batchelor (1920-2000) contributed the theory of homogeneous turbulence. Lewis Fry Richardson (1881 – 1953) developed the weather prediction system in 1922. He attempted to calculate weather for a single eight-hour period which ended in failure. His model's enormous calculation requirements led Richardson to reach a solution and called it as forecast-factory. During 1960’s, Los Alamos contributed the following numerical methods: Particle-In-Cell, Marker-and-Cell, Vorticity-Stream function Methods, Arbitrary Lagrangian-Eulerian, $k$-$\varepsilon$ turbulence model. During 1970’s a group working under D. Brian Spalding, at Imperial College, London, developed Parabolic flow codes (GENMIX), Vorticity-Stream
function based codes, SIMPLE algorithm and the TEACH code. In 1980, Suhas V. Patankar published Numerical Heat Transfer and Fluid Flow, which is probably the most influential book on CFD.

3.3 CFD TECHNIQUES

Many CFD techniques are used in practical. Most common one is the finite volume method. Other techniques include finite element, finite difference, spectral methods, boundary element, vortex based methods, etc. Important methods are explained below.

3.3.1 Finite Volume Method

This method was first documented by Evans & Harlow in the year 1957 at Los Alamos and Gentry, Martin & Daley in the year 1966. It is most common because variables are continuously differentiable across shocks and mass, momentum and energy are always conserved. This method have advantages of memory and speed for very large problems, no limitations for cell shape, iterative solvers are well developed. The methodology includes

(i) Dividing the domain into control volumes,
(ii) Investigate the differential equation,
(iii) Apply the divergence theorem,
(iv) Evaluate the derivative terms,
(v) Solve iteratively.
### 3.3.2 Finite Difference Method

It is the oldest of the three finite element, finite difference and finite volume method. This technique was proposed by Richardson. The advantage is that it is easy to implement and disadvantages are it is restricted to simple grids and does not conserve mass, momentum and energy on grids. The basic methodology includes,

(i) Discretization of the domain by structured mesh,

(ii) The differential form of the equations are converted into algebraic form

(iii) Derivatives are evaluated using Taylor Series expansion

(iv) Solve iteratively.

### 3.3.3 Finite Element Method

This method was first used by courant in 1943 and later in 1960 Clough named this method as Finite Element Method. The advantages of this method are high accuracy on coarse grids, excellent for viscous flow and free surface problems. The limitations of this method include it is very slow for large problems and not suited for turbulent flow problems.
GEOMETRY

The first step in all problems as in figure 3.1 is geometry. It describes the shape of the problem to be analyzed. It consists of volumes, faces (surfaces), edges (curves) and vertices (points). Geometries can be created either by top-down or bottom-up. In top-down approach, the computational domain is created by performing logical operations on primitive shapes such as cylinders, bricks, and spheres. In bottom-up approach, the computational domain first creates vertices, create edges with these vertices, create faces with these edges, and create volumes with these faces. Geometries can be created using the same pre-processor also. This is the first preprocessing stage. It is the interactive process with its objective to create the geometry of the region of interest, a closed geometric solid and
mesh the same to provide an input to the physics preprocessor. Meshing can be performed with the help of other meshing tools also. The basic steps include

a) Define the geometry of the interested region
b) Create regions of fluid flow, solid body, and name the surfaces of the boundary
c) Set the mesh parameters

Mesh can be performed automatically and geometry can be imported from most of the CAD packages with its native format.

a) Select an appropriate coordinate
b) Specify the domain size and shape
c) Check for any simplifications
d) What kinds of shapes needed to be used to best resolve the geometry
e) Geometry is usually created using commercial software, either using ProE or Flow Lab

**PHYSICS**

Physics include flow conditions and fluid properties. Flow conditions include the types of flow and other parameters such as inviscid, viscous, laminar or turbulent, etc. Fluid properties include the properties of fluids such as density, viscosity, and thermal conductivity, etc. Flow conditions and properties are usually presented in dimensional form in industrial commercial CFD software, and as non-dimensional variables in research codes. Users should specify the required models and the boundary conditions. This is the second preprocessing stage which is used to create
input required by the solver. The mesh file is loaded in to the physics preprocessor. The physical model to be included in the simulation is defined with their properties and boundary conditions.

**MESH**

Meshes should be well designed inorder to resolve the important flow parameters that are dependent upon flow condition parameters. Mesh can be generated either by the commercial codes or research code. Then the mesh together with the boundary conditions should be exported from commercial software which can be recognized by the research CFD code or other commercial CFD software. There are many different cells or elements and grids available according to the problem and the solver capabilities. There are different types of cells or elements in 2D and 3D as quadrilateral, tetrahedron, hexahedron or wedge. There are different types of grids as structured grid and unstructured grid. In the structured grid, the cells are arranged in i,j,k indexing. But it is not used for complicated geometries. The unstructured grid can be used for more complicated geometries that the cells are arranged in an arbitrary fashion. In structured grid, the face meshing is performed as multi-block geometry. Different types of hexahedral grids are used. The quality of the elements can be increased using edge meshing. In unstructured grid, the face meshing is performed using unstructured hexahedral grids. The different types of face meshing are map, sub-map, tri-primitive, pave and tri-pave.

The quality of mesh determines the accuracy of the solution. Hexahedral meshes will give more accurate solutions, especially if the grid lines are aligned with the flow. The mesh density should be very high so that all the relevant features can be determined. The boundary layers should be meshed finely inorder to resolve the boundary layer flow. Quadrilateral,
hexahedral and wedge cells are preferred over triangular or tetrahedral cells to achieve higher quality of mesh.

There are three measures of mesh quality, namely skewness, smoothness and aspect ratio. Skewness is based on the equilateral volume and it applies for quadrilateral, triangles and tetrahedron mesh. For triangles and tetrahedral, skewness can be determined by

$$ \text{skewness} = \frac{\text{optimal cell size} - \text{cell size}}{\text{optimal cell size}} $$

For quadrilateral mesh, skewness can be determined by

$$ \text{skewness} = \left[ \frac{\theta_{\text{max}} - 90}{90}, \frac{90 - \theta_{\text{max}}}{90} \right] $$

Aspect ratio is defined as the ratio between its sides in different dimensions. In a rectangle, the aspect ratio is the ratio of longer side to its shorter side or it is also equal to the ratio of width to the height of the rectangle.

**SOLVE**

The component that solves the CFD problem is termed the solver. The solver produces the required results in a non-iterative process. A CFD problem is solved as follows. The partial differential equations are integrated over all the control volumes in the interested region which is equivalent to applying a basic conservation law to each control volume. These integral equations are converted to a system of algebraic equations by generating a set of approximations for the terms in the integral equations. Then these algebraic equations are solved iteratively. An iterative approach is required because of the nonlinear nature of the equations, and as the solution approaches the exact
solution, it is about to converge. For each iteration an error, or residual, is reported as a measure of the overall conservation of the flow properties. How close the final solution is to the exact solution depends on a number of factors, including the size and shape of the control volumes and the size of the final residuals. Complex physical processes, such as combustion and turbulence, are often modeled using empirical relationships. The approximations inherent in these models also contribute to differences between the CFD solution and the real flow. The solution process requires no user interaction and is, therefore, usually carried out as a batch process. The solver produces a results file that is then passed to the post-processor.

a) Setup the appropriate numerical parameters  
b) Choose appropriate solvers  
c) Select the appropriate solution procedure (e.g. incompressible flows)  
d) Solve the momentum, pressure equations and get flow field parameters, such as velocity, turbulence, pressure and integral quantities.

REPORT  

a) Reports show the time history of the residuals of the velocity, pressure and temperature, etc.  
b) Report shows the integral quantities, such as total pressure drop, friction factor in case of pipe flow, lift and drag coefficients in case of aerofoil, etc.  
c) XY plots show the centerline velocity/pressure distribution, friction factor distribution in case of pipe flow, pressure coefficient distribution in case of airfoil flow.
d) Analytical and experimental data can be included on the top of the XY plots for validation.

**POST PROCESSING**

The post-processor is the component which is used to analyze, visualize and present the results interactively. Post-processing includes obtaining point values to complex animated sequences. Some important features of post-processors include

i. Visualization of the geometry and control volumes

ii. Vector plots showing the direction and magnitude of the flow

iii. Visualization of the variation of scalar variables through the domain

iv. Quantitative numerical calculations

v. Animation

vi. Charts showing graphical plots of variables

vii. Hardcopy and online output.

Post processing helps in analysis and visualization of the defined problem. In analysis, the derived variables and the integral parameters can be calculated. In visualization, the simple 2D and 3D contour plots, vector plots and streamlines can be visualized. Also animations can be obtained in post processing.

**MAIN SOURCES OF ERRORS**

a) Mesh too coarse.

b) High skewness.
c) Large jumps in volume between adjacent cells.

d) Large aspect ratios.

e) Interpolation errors at non-conformal interfaces.

f) Inappropriate boundary layer mesh.

3.5 MATHEMATICS OF CFD

The set of equations that describe the processes of momentum, heat and mass transfer are known as the Navier-Stokes equations. These partial differential equations were derived in the early nineteenth century and have no known general analytical solution but can be discretized and solved numerically. Equations describing other processes, such as combustion, can also be solved in conjunction with the Navier-Stokes equations. Often, an approximating model is used to derive these additional equations, turbulence models being a particularly important example. There are a number of different solution methods that are used in CFD codes. The most common one on which CFX is based is known as the finite volume technique. In this technique, the region of interest is divided into small sub-regions, called control volumes. The equations are discretized and solved iteratively for each control volume. As a result, an approximation of the value of each variable at specific points throughout the domain can be obtained. In this way, one derives a full picture of the behavior of the flow.

Additional information on the Navier-Stokes equations and other mathematical aspects of the CFX software suite is available in Basic Solver Capability Theory in the CFX-Solver Theory Guide. Andre Bakker (2002-2006) explained that this mathematical equation is used to model fluid flow, heat, and mass transfer in ANSYS CFX for single-phase, single and multi-component flow without combustion or radiation. It is designed to be a reference for those users who desire a more detailed understanding of the
mathematics underpinning the CFX-Solver, and is therefore not essential reading. CFD is used by engineers and scientists in a wide range of fields. Typical applications include Mixing vessels and chemical reactors in process industry, ventilation of buildings, such as atriums in building services, investigating the effects of fire and smoke in health and safety industry, combustion modeling and car aerodynamics in automobile industry, heat transfer within and around circuit boards in electronics field, dispersion of pollutants in air or water in environmental studies, optimization of combustion processes in power and energy studies, blood flow through grafted blood vessels in medical sciences.

CFD is used to determine the performance of a component at the design stage, and to analyze the difficulties in an existing component which helps to improve the design. The first step is to identify the region of interest. The geometry can be imported if CAD model exists. The geometry or the domain is then meshed and imported to the preprocessor. The boundary conditions and fluid properties are defined. The flow solver is run to iterate the result that shows the variation of pressure, velocity and other defined variables throughout the interested region. The results can be visualized and the clear understanding of the behavior of fluid in the interested region can be analyzed. The results can be validated with the analytical one which can lead to design modifications by changing the geometry of either the CAD model or the domain and see the effect of the modifications. On the whole, the process of performing a single CFD simulation can be divided into four components.

3.6 GOVERNING EQUATIONS

The following conservation laws of physics are the governing equations of CFD.

(i) Lagrangian Description and Eulerian Description
(ii) Conservation of mass

(iii) Newton’s second law

(iv) First law of thermodynamics

3.6.1 Lagrangian Description and Eulerian Description

A fluid flow field comprises of a large number of finite sized fluid particles which have mass, momentum, internal energy, and other properties. For each fluid particle, mathematical laws should be written. This is the Lagrangian description of fluid motion. The other view of fluid motion is the Eulerian description. In this, the properties change at a fluid element is studied in a fixed space and time (x,y,z,t), rather than following individual fluid particles as in lagrangian Description.

Figure 3.2 Lagrangian Description

Figure 3.3 Eulerian Description
### 3.6.2 Continuity Equation

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0
\]

### 3.6.3 Momentum Equation

According to Newton’s II law of motion, the rate of change of momentum is equal to the sum of all the forces.

### 3.6.4 Navier-Stokes Equation

Navier-Stokes equations (3D in Cartesian coordinates)

\[
\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} + \rho w \frac{\partial u}{\partial z} = -\frac{\partial p}{\partial x} + \mu \left[ \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right]
\]

\[
\rho \frac{\partial v}{\partial t} + \rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} + \rho w \frac{\partial v}{\partial z} = -\frac{\partial p}{\partial y} + \mu \left[ \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right]
\]

\[
\rho \frac{\partial w}{\partial t} + \rho u \frac{\partial w}{\partial x} + \rho v \frac{\partial w}{\partial y} + \rho w \frac{\partial w}{\partial z} = -\frac{\partial p}{\partial z} + \mu \left[ \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right]
\]

### 3.7 Numerical Schemes

There are number of schemes to find the face values. Most common are explained below.

(i) **First order upwind scheme**

It is the simplest numerical scheme which is used earlier. It is often the best scheme to start the calculation. The advantages of this scheme are that it is easy to implement and it results in very stable calculations. In this scheme, it is assumed that the interpolated value at the face is same as that in
the cell upstream of the face. This scheme only uses constants and ignores the first derivative and consecutive terms; hence it is considered as first order accurate.

(ii) **Power law scheme**

This is based on the analytical solution of the one dimensional convection-diffusion equation. The face value is determined from an exponential profile through the cell values.

(iii) **Second order upwind scheme**

This scheme is more accurate than the first order upwind scheme. It is necessary to apply limiters to the predicted face values. This scheme is more popular because of its accuracy and stability. The second order upwind scheme includes the first order derivative and ignores the second order derivative and consecutive terms; hence it is considered as second order accurate.

(iv) **QUICK scheme**

QUICK stands for Quadratic Upwind Interpolation for Convective Kinetics. It works with a quadratic curve fitted through two upstream nodes and downstream node. This scheme is very accurate and stable. This scheme includes the second order derivative but ignores the third order derivative; hence it is considered as third order accurate.

High order schemes will be more accurate but will be less stable and requires higher computational time. To increase the solution accuracy and stability, it is recommended to start calculations with first order upwind and after 100 iterations, switch over to the second order upwind.
3.8 CONVERGENCE

The general approach in the iterative process is that the change in the variable between iterations should be very small. At this convergence level, all the conservation equations in all cells will be in a specified tolerance. Also there will be no changes in the additional iterations at this level. Residuals measure the imbalance of error in conservation equations between the cells. It is common to plot the scaled residuals in the order of \(1E^{-3}\) to \(1E^{-4}\) or even less for convergence. The results will be accurate if the problem is properly converged. Before retrieving the results it is most important to plot and monitor the convergence of residuals. There are certain conditions in monitoring the residuals, which are as follows.

(i) If the residuals never meet the convergence level and it is no longer decreasing in the solution monitors, then it can be considered as the solution is converged.

(ii) If the residuals meet the convergence criterion and still decreasing, then the solution is not yet converged.

(iii) Low residuals do not mean a correct solution and high residuals never mean it yields a wrong solution.

(iv) Residuals are often higher for higher order discretization schemes compared with first order discretization.

(v) For models to calculate the forces on an object, the predicted force itself is to be monitored for convergence.

3.9 TYPES OF FLOW

There are different types of fluid flow, as
(i) **Laminar and turbulent flow**

Laminar flow is that type of flow in which the fluid particles moves in a regular, smooth, layered fashion. Turbulent flow is that type of flow in which the fluid particles move in a zig-zag manner. It can be predicted by the dimensionless Reynold’s number. The flow is laminar if the value of the Reynold’s number is less than 2000, and if it is greater than 4000, then the flow is turbulent. And if the value is between 2000 and 4000 the flow is unpredictable.

(ii) **Steady and unsteady flow**

Steady flow is that type of flow in which the flow properties at any point in space do not vary with respect to time, whereas in unsteady flow, the fluid flow properties vary with respect to time.