# GENERAL INTRODUCTION: HISTORICAL BACKGROUND AND SPECTRUM OF APPLICATIONS

## 1.1 INTRODUCTION

Analysis of physical problems in any area of engineering and science involves a multipronged approach:

- Idealized physical model: experiments on scale models of the problem
- Mathematical model: Theoretical analysis (analytical solution) / approximate numerical solution.

Physical Problem

Experimental Analysis

Mathematical Modeling
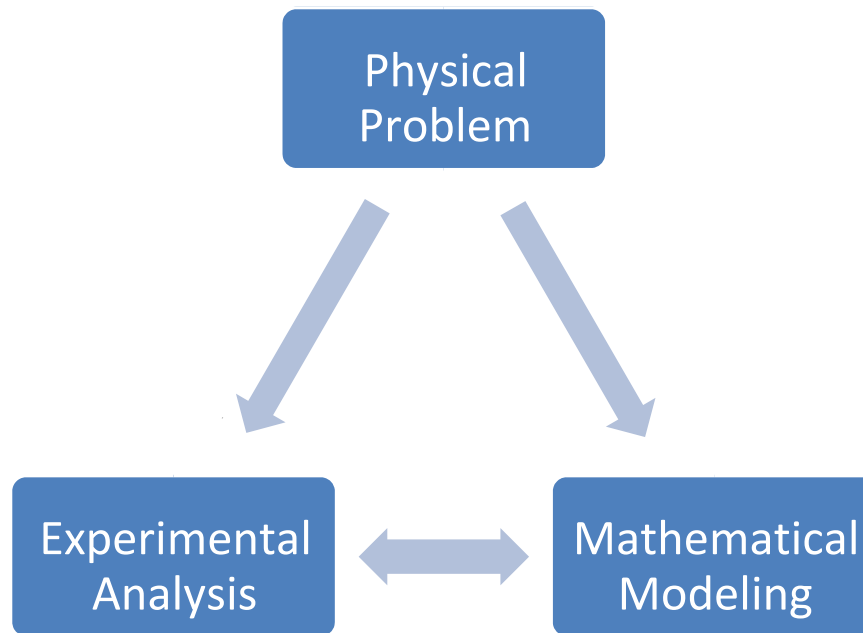
Both physical experiments and analytical/numerical simulations complement each other.
Both the approaches have their own limitations, advantages and disadvantages:

- **Physical experiments**  o These are usually very time consuming and expensive to set up o There are limitations on extrapolation of the results obtained on scaled model of a problem to the actual prototype.
    - o **BUT** the experimentally observed data provides the **closest possible approximation** of the physical reality within the limits of experimental errors.
- **Numerical Simulation** o Mathematical modelling is based on a set of assumptions with regard to the variation of the problem variables, constitutive relations and material properties.
    - o Numerical simulation process introduces **additional approximation errors** in the solution. Hence, results of any analytical or numerical study must be carefully validated against physical experiments to establish their practical usefulness.

o   However, once validated, a numerical simulation can be easily performed on the **full scale prototype**, and thereby eliminate the need of extrapolation.

## 1.2 WHAT IS CFD?

Mathematical modelling of a continuum problem leads to a set of differential, integral or integro-differential equations. Exact analytical solution of such equations is limited to problems in simple geometries. Hence, for most of the problems of practical interest, an approximate numerical solution is sought. In the context of mechanics, *the science and practice of obtaining approximate numerical solution using digital computers* is termed **Computational Mechanics**. For thermo-fluid problems, this approach is popularly known as **Computational Fluid Dynamics** (**CFD**). Thus,

> *CFD is essentially a branch of continuum mechanics which deals with numerical simulation of fluid flow and heat transfer problems.*

Note that although word *heat transfer* is missing from *CFD*, it is an intrinsic part of this discipline.

CFD deals with **approximate numerical** solution of governing equations based on the fundamental conservation laws of physics, namely mass, momentum and energy conservation. The CFD solution involves

• Conversion of the governing equations for a continuum medium into a set of discrete algebraic equations using a process called discretization.
• Solution of the discrete equations can using a high speed digital computer to obtain the numerical solution to desired level of accuracy.

## 1.3 HISTORICAL PERSPECTIVE

Although development of some of the techniques used in CFD dates back to pre-digital era, history of CFD is intrinsically linked to the advent of the digital computers in late 1950s. It is highly debatable as to who did the first CFD simulation of a flow problem. Hence, instead of looking at chronology of the history of CFD, we focus on the evolution of CFD for motivational and application perspective.

**Early Applications**
• The early beginning of the CFD can be traced to numerical simulations for aerospace applications at Douglas, Boeing, NASA, and Lockheed in 1960s based on panel methods.
  o The codes based on panel methods still play an important role in the computer aided design of modern day aircraft.
• Meteorologists were the next early users of CFD for weather forecasting applications. Large eddy simulation models for atmospheric turbulent flows appeared in early 1970s.

**Algorithmic Front**

- 1960s: Development of Particle-In-Cell (PIC), Marker-and-Cell (MAC) and VorticityStream function methods at NASA.
- 1970s: Development of parabolic flow codes (GENMIX), Vorticity-Stream function based codes, and the SIMPLE algorithm by the research group of Professor D. Brian Spalding, at Imperial College, London.
- 1980 onwards vigorous research activity in various parts of the globe addressing different aspects of CFD: new discretization methods, turbulence modelling, numerical algorithms, grid generation methods, post-processing and visualization, parallel implementation etc.

**Impact of Developments in CAD on Industrial Applications of CFD**
- Industrial applications of CFD boosted by the availability of commercial CFD codes in 1980s.
- Developments in CAD and FEA have inspired development of commercial CFD codes with user-friendly graphical user interface, in-built geometry and solid modelling, and visual post-processing capabilities.
- Availability of commercial and open-source GUI based codes which offer CAD interoperability has led to the integration of CFD analysis in the design cycle.

## 1.4 APPLICATIONS OF CFD

CFD is being used for fundamental research as well as industrial R&D. CFD analysis forms an integral part of design cycle in most of the industries: from aerospace, chemical and transportation to bio-medical engineering. The length scales range from planetary boundary layers to micro-channels in electronic equipments. Following is a short-list of some of more prominent applications of CFD:
- Meteorology: weather forecasting
- Aerospace: design of wings to complete aircraft aerodynamic design
- Turbomachines: design of hydraulic, steam, gas, and wind turbines; design of pumps, compressors, blower, fans, diffusers, nozzles.
- Engines: combustion modelling in internal combustion engines
- Electronics: cooling of micro-circuits
- Chemical process engineering
- Energy systems: analysis of thermal and nuclear power plants, modelling of accident situations for nuclear reactors.
- Hydraulics and hydrology: flow in rivers, channels, ground aquifers, sediment transport.
- HVAC: Design of ducts, placement of heating/cooling ducts for optimum comfort in a building
- Surface transport: aerodynamic design of vehicles
- Marine: hydrodynamic design of ships, loads on off-shore structures
- Biomedical: simulation of blood flow through arteries and veins, fluid flow in renal and ocular systems.
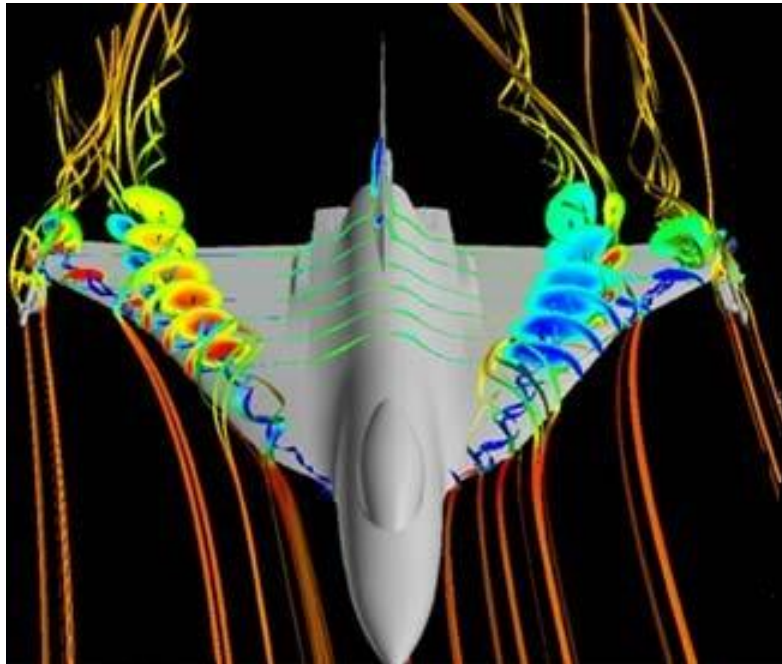- Fundamental flow physics: dynamics of laminar, transitional and turbulent flows.
- ………

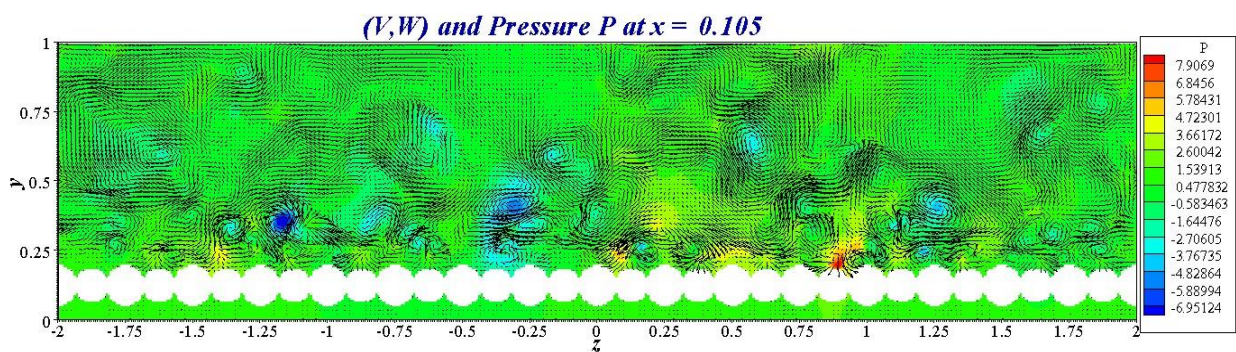Figure 1.1 CFD Simulation of complete fighter aircraft



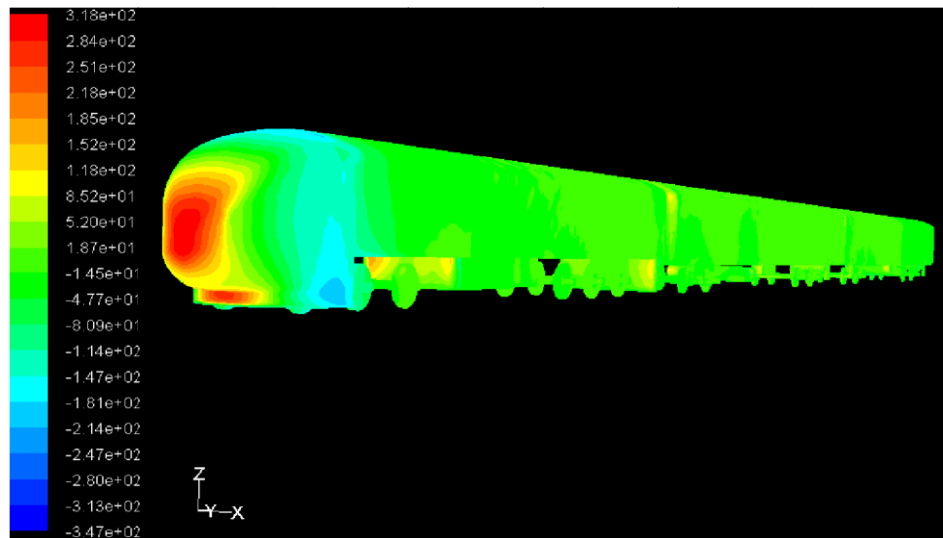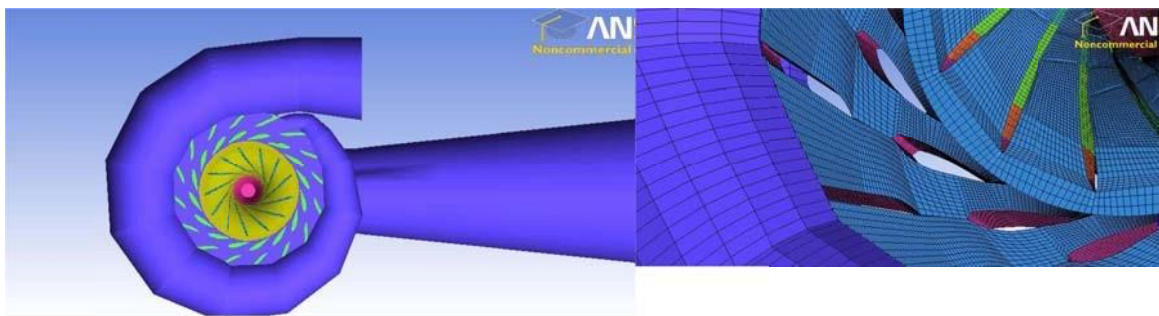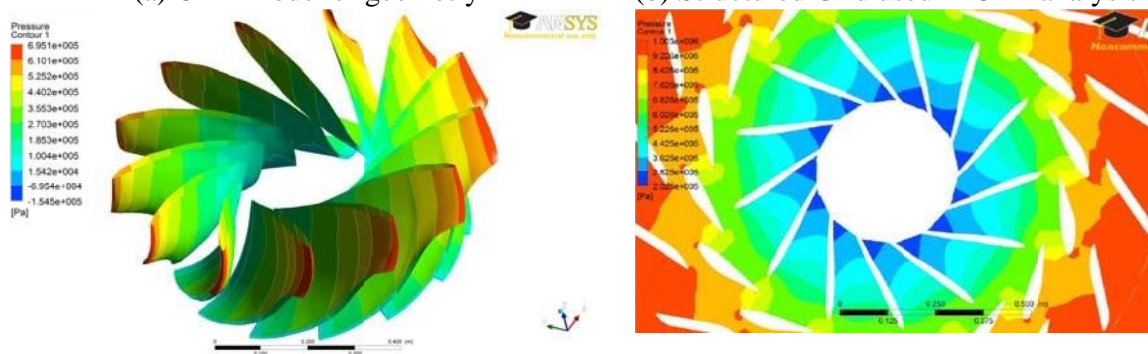Figure 1.2 Direct numerical simulation of flow over a rough-bed channel

Figure 1.3 Pressure distribution around a high-speed train obtained from RANS simulation



(a) CAD model of geometry       (b) Structured Grid used in CFD analysis



(c) Pressure distribution over runner blades    (d) Pressure contours in stator and runner Figure
1.4 RANS simulation of turbulent flow in a Francis turbine

# NUMERICAL SIMULATION PROCESS

## 2.1 NUMERICAL SIMULATION PROCESS

Numerical simulation of a physical problem involves approximation of the problem geometry, choice of appropriate mathematical model and numerical solution techniques, computer implementation of the numerical algorithm and analysis of the data generated by the simulation. Thus, this process involves the following steps:

- Model the geometry of the problem domain.
- Choose appropriate mathematical model of the physical problem.
- Choose a suitable discretization method.
- Generate a grid based on the problem geometry and the discretization method.
- Use a suitable solution technique to solve the system of discrete equations.
- Set suitable convergence criteria for iterative solution methods. ◻ Prepare the numerical solution for further analysis

Let us have a bit more detailed look at the preceding steps. Each of these steps clearly reminds us of the approximations involved at each step of numerical simulation: from approximations/idealizations used in geometry modelling to solution process and postprocessing.

## 2.2 GEOMETRY MODELLING

The numerical simulation requires a computer representation of the problem domain. For most of the engineering problems, it may not be possible or even desirable to include all the geometric details of the system in its geometric model. The analyst has to make a careful choice regarding the level of intricate details to be chosen. For example, in the numerical simulation of flow field around an automobile, finer details of the front air-intake grills would be avoided. Incorporation of these finer features would make the grid generation process very difficult, but would hardly contribute to the accuracy of the velocity and pressure fields.

## 2.3 MATHEMATICAL MODELLING

An appropriate mathematical model for the problem has to be selected keeping in view the objective of the simulation, and physics of the flow problem. For example, one can opt for incompressible Navier-Stokes equations for low speed aerodynamics (Mach number < 0.3, e.g. flow over a car or train). Similarly, for high speed compressible flow over a whole aircraft, one may choose inviscid model (Euler's equation). The choice of the model also depends on the available computing resources and level of accuracy desired.

## 2.4 DISCRETIZATION METHOD

For computer simulation, the continuum mathematical model must be converted into a discrete system of algebraic equation using a suitable discretization procedure. There are many discretization approaches. The most popular are the finite difference method (FDM), the finite element method (FEM) and the finite volume method (FVM). Choice of the discretization method depends on the problem geometry, preference of the analyst and predominant trend in a particular application area. For instance, FEM is very popular for stress

analysis applications, whereas FDM has traditionally been more popular for simulation of turbulent flows. Similarly, commercial CFD codes have shown a distinct preference for the finite volume method.

## 2.5 GRID GENERATION

The problem domain is discretized into a mesh/grid appropriate to the chosen discretization method. The type of the grid also depends on the geometry of the problem domain. Structured grid is required for the finite difference method, whereas FEM and FVM can work with either structured or unstructured grids. In case of unstructured grids, care must be taken to ensure proper grading and quality of the mesh.

## 2.6 NUMERICAL SOLUTION

The discretization method applied to the mathematical model of the problem leads to a system of discrete equations: (a) a system of ordinary differential equations in time for unsteady problems, and (b) a system of algebraic equations for steady state model. For unsteady problems, time integration methods for initial value problems are employed, some of which transform the differential system to a system of algebraic equations at each time step. Iterative methods are usually employed to solve the system of algebraic equations, choice of methods being dependent on the type of the grid and size of the system.

The convergence criterion for the iterative solvers depends on the accuracy as well as efficacy requirements. The tightness of the specified error tolerance would also depend on the precision chosen for numerical computations.

## 2.7 POST-PROCESSING

Numerical simulation provides values of field variables at discrete set of computational nodes. For analysis of the problem, the analyst would like to know the variation of different variables in space-time. Further, for design analysis, secondary variables such a stresses and fluxes must be computed. Most of the commercial CFD codes provide their own postprocessor which compute the secondary variables and provide variety of plots (contour as well as line diagrams) based on the nodal data obtained from simulation. These computations involve use of further approximations for interpolation of nodal data required in integration and differentiation to obtain secondary variables or spatial distributions.

## 2.8 VALIDATION

Numerical solution of a physical problem must be validated with available experimental data to ensure that it gives a reasonably accurate description of the physical reality. In general, numerical solution is sought for a problem for which no experimental results are available. For example, it is not feasible to perform experiments on a full scale prototype of an airplane or high-speed train. In such situations, validation of the simulation process is carried out with the scale model for which experimental data are available. Thereafter, the simulation process can be extended for numerical solution of the full-scale problem.

# APPROXIMATE SOLUTION TECHNIQUES

## 3.1 INTRODUCTION

Numerous approximate solution techniques have been developed for different types of problems in CFD. These methods can be classified into two categories:

- Mesh-based methods which require discretization of the problem domain into a mesh (or grid), e.g. finite difference, finite element, and finite volume methods.
- Mesh-free methods which primarily use a collection of nodes with no apparent connectivity, e.g. smooth particle hydrodynamics (SPH), mesh-less PetrovGalerkin (MLPG), lattice Boltzmann methods.

Of the preceding two types, mesh-based methods are more popular in CFD. Of these, finite volume method has been the most popular due to its simplicity and ease of application for problems in complex geometries. In fact, majority of commercial CFD packages (e.g. Fluent, StarCD, etc.) are based on finite volume method. In this lecture, we will have a brief overview of finite difference, finite element and finite volume methods.

## 3.2 FINITE DIFFERENCE METHOD (FDM)

The FDM is the oldest method for numerical solution of partial differential equations. This method is also the easiest method to formulate and program for problems on simple geometries. In FDM, the solution domain is discretized using a structured (usually Cartesian) grid. The conservation equations in differential form are approximated at each grid point by replacing the partial derivatives by finite difference approximations in terms of nodal values of the unknown variables. This process results in an algebraic equation for each node. These algebraic equations are collected for all the grid points and resulting system of discrete equations are solved to yield the approximate solution of the problem at the grid nodes.

The main disadvantage of the finite difference method is its restriction to simple geometries (although immersed boundary techniques do remove this restriction). We provide a detailed description of this method in the following section.

## 3.3 FINITE ELEMENT METHOD (FEM)

The finite element method is based on the division of the problem domain into a set of finite elements which are generally unstructured. The elements are usually triangles or quadrilaterals in two dimensions, and tetrahedra or hexahedra in three dimensions. Starting point of the method is conservation equation in differential form. The unknown variable is approximated using an interpolation procedure in terms of nodal values and a set of known functions (called shape functions). This approximation is substituted into the differential equation. The resulting residual (error) is minimized in an average sense using a weighted residual procedure. The weighted integral statement leads to a system of discrete equations in terms of unknown nodal values, which is solved to obtain the solution of the problem.

FEM is ideally suited to problems on complex geometries, and hence, this method has been very popular in computational solid mechanics. There is an extensive literature available on all aspects of this method: type of elements, shape functions, mesh generation, applications to different type of problems, etc. For detailed study of FEM, interested reader can refer to books by Zienkiewicz et al. (2005a, 2005b), Reddy (2005), Reddy and Gartling (2010) amongst others.

## 3.4 FINITE VOLUME METHOD (FVM)

The finite volume method is based on the integral form of conservation equations. The problem domain is divided into a set of non-overlapping control volumes (called finite volumes). The conservation equations are applied to each finite volume. The integrals occurring in the conservation equations are evaluated using function values at computational nodes (which are usually taken as centroids of finite volumes). This process involves use of approximate integral formulae and interpolation methods (to obtain the values of variables at surfaces of the CVs).

The FVM can accommodate any type of grid, and hence, it is naturally suitable for complex geometries. This explains its popularity for commercial CFD packages, which must cater to problems in arbitrarily complex geometries. This method has immensely benefited from the unstructured grid generation methods developed for the finite element method.