

LECTURE NOTE 1

MCE 521: Computational Fluid Dynamics

ENGR. ALIYU, S. J.

MCE 521

Advanced Computational Dynamics

Modelling engineering systems using ordinary and partial differential equations; finite difference schemes; and weighted residual methods and spectral methods. All necessary theories in order for students to be able to use commercial computational fluid dynamics (CFD) software proficiently.

1 Introduction 1

- Importance of Fluids
- Fluids in the pure sciences
- Fluids in technology
- The Study of Fluids
- The theoretical approach
- Experimental fluid dynamics
- Computational fluid dynamics

Introduction

It takes little more than a brief look around for us to recognize that fluid dynamics is one of the most important of all areas of physics—life as we know it would not exist without fluids, and without the behavior that fluids exhibit. The air we breathe and the water we drink (and which makes up most of our body mass) are fluids. Motion of air keeps us comfortable in a warm room, and air provides the oxygen we need to sustain life. Similarly, most of our (liquid) body fluids are water based. And proper motion of these fluids within our bodies, even down to the cellular level, is essential to good health. It is clear that fluids are completely necessary for the support of carbon-based life forms.

But the study of biological systems is only one (and a very recent one) possible application of a knowledge of fluid dynamics. Fluids occur, and often dominate physical phenomena, on all macroscopic (non-quantum) length scales of the known universe—from the mega-par-secs of galactic structure down to the micro and even nano-scales of biological cell activity. In a more practical setting, we easily see that fluids greatly influence our comfort (or lack thereof); they are involved in our transportation systems in many ways; they have an effect on our recreation (e.g., basketballs and footballs are inflated with air) and entertainment (the sound from the speakers of a TV would not reach our ears in the absence of air), and even on our sleep (water beds!). From this it is fairly easy to see that engineers must have at least a working knowledge of fluid behavior to accurately analyze many, if not most, of the systems they will encounter. It is the goal of these lecture notes to help students in this process of gaining an understanding of, and an appreciation for, fluid motion—what can be done with it, what it might do to you, how to analyze and predict it. In this introductory chapter we will begin by further stressing the

importance of fluid dynamics by providing specific examples from both the pure sciences and from technology in which knowledge of this field is essential to an understanding of the physical phenomena (and, hence, the beginnings of a predictive capability—e.g., the weather) and/or the ability to design and control devices such as internal combustion engines. We then describe three main approaches to the study of fluid dynamics: i) theoretical, ii) experimental and iii) computational.

Importance of Fluids

We have already emphasized the overall importance of fluids in a general way, and here we will augment this with a number of specific examples. We somewhat arbitrarily classify these in two main categories:

- i) Physical and natural science, and
- ii) Technology. Clearly, the second of these is often of more interest to an engineering student, but in the modern era of emphasis on interdisciplinary studies, the more scientific and mathematical aspects of fluid phenomena are becoming increasingly important.

Fluids in the pure sciences

The following list, which is by no means all inclusive, provides some examples of fluid phenomena often studied by physicists, astronomers, biologists and others who do not necessarily deal in the design and analysis of devices. The accompanying figures highlight some of these areas.

1. Atmospheric sciences

- (a) Global circulation: long-range weather prediction; analysis of climate change (global warming)
- (b) Meso-scale weather patterns: short-range weather prediction; tornado and hurricane warnings; pollutant transport



2. Oceanography

- (a) Ocean circulation patterns: causes of El Niño, effects of ocean currents on weather and climate
- (b) Effects of pollution on living organisms



3. Geophysics

(a) Convection (thermally-driven fluid motion) in the Earth's mantle: understanding of plate tectonics, earthquakes, volcanoes

(b) Convection in Earth's molten core: production of the magnetic field



4. Astrophysics

(a) Galactic structure and clustering

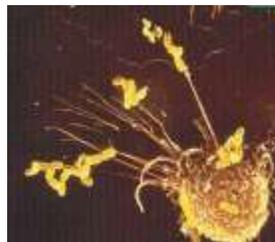
(b) Stellar evolution—from formation by gravitational collapse to death as a supernovae, from which the basic elements are distributed throughout the universe, all via fluid motion



5. Biological sciences

(a) Circulatory and respiratory systems in animals

(b) Cellular processes



1.1.2 Fluids in technology

As in the previous case, we do not intend this list of technologically important applications of fluid dynamics to be exhaustive, but mainly to be representative. It is easily recognized that a complete listing of fluid applications would be nearly impossible simply because the presence of fluids in technological devices is ubiquitous. The following provide some particularly interesting and important examples from an engineering standpoint.

1. Internal combustion engines—all types of transportation systems



2. Turbojet, scramjet, rocket engines—aerospace propulsion systems



3. Waste disposal

- (a) Chemical treatment
- (b) Incineration
- (c) Sewage transport



4. Pollution dispersal—in the atmosphere (smog); in rivers and oceans



5. Steam, gas and wind turbines, and hydroelectric facilities for electric power generation

6. Pipelines



- (a) Crude oil and natural gas transferral
- (b) Irrigation facilities
- (c) Office building and household plumbing
- 7. Fluid/structure interaction
 - (a) Design of tall buildings
 - (b) Continental shelf oil-drilling rigs
 - (c) Dams, bridges, etc.
 - (d) Aircraft and launch vehicle airframes and control systems
- 8. Heating, ventilating and air-conditioning (HVAC) systems
- 8. Heating, ventilating and air-conditioning (HVAC) systems
- 9. Cooling systems for high-density electronic devices—digital computers from PCs to supercomputers
- 10. Solar heat and geothermal heat utilization
- 11. Artificial hearts, kidney dialysis machines, insulin pumps
- 12. Manufacturing processes
 - (a) Spray painting automobiles, trucks, etc.
 - (b) Filling of containers, e.g., cans of soup, cartons of milk, plastic bottles of soda
 - (c) Operation of various hydraulic devices
 - (d) Chemical vapor deposition, drawing of synthetic fibers, wires, rods, etc.

We conclude from the various preceding examples that there is essentially no part of our daily lives that is not influenced by fluids. As a consequence, it is extremely important that engineers be capable of predicting fluid motion. In particular, the majority of engineers who are not fluid dynamicists still will need to interact, on a technical basis, with those who are quite frequently; and a basic competence in fluid dynamics will make such interactions more productive.

The Study of Fluids

We begin by introducing the “intuitive notion” of what constitutes a fluid. As already indicated we are accustomed to being surrounded by fluids—both gases and liquids are fluids—and we deal with these in numerous forms on a daily basis. As a consequence, we have a fairly good intuition regarding what is, and is not, a fluid; in short we would probably simply say that a fluid is “anything that flows.” This is actually a good practical view to take, most of the time. But we will later see that it leaves out some things that are fluids, and includes things that are not. So if we are to accurately analyze the behavior of fluids it will be necessary to have a more precise definition. It is interesting to note that the formal study of fluids began at least 500 hundred years ago with the work of Leonardo da Vinci, but obviously a basic practical understanding of the behavior of fluids was available much earlier, at least by the time of the ancient Egyptians; in fact, the homes of well-to-do Romans had flushing toilets not very different from those in

modern 21st-Century houses, and the Roman aqueducts are still considered a tremendous engineering feat. Thus, already by the time of the Roman Empire enough practical information had been accumulated to permit quite sophisticated applications of fluid dynamics. The more modern understanding of fluid motion began several centuries ago with the work of L. Euler and the Bernoullis (father and son), and the equation we know as Bernoulli's equation (although this equation was probably deduced by someone other than a Bernoulli). The equations we will derive and study in these lectures were introduced by Navier in the 1820s, and the complete system of equations representing essentially all fluid motions were given by Stokes in the 1840s. These are now known as the Navier–Stokes equations, and they are of crucial importance in fluid dynamics. For most of the 19th and 20th Centuries there were two approaches to the study of fluid motion: theoretical and experimental. Many contributions to our understanding of fluid behavior were made through the years by both of these methods. But today, because of the power of modern digital computers, there is yet a third way to study fluid dynamics: computational fluid dynamics, or CFD for short. In modern industrial practice CFD is used more for fluid flow analyses than either theory or experiment. Most of what can be done theoretically has already been done, and experiments are generally difficult and expensive. As computing costs have continued to decrease, CFD has moved to the forefront in engineering analysis of fluid flow, and any student planning to work in the thermal-fluid sciences in an industrial setting must have an understanding of the basic practices of CFD if he/she is to be successful. But it is also important to understand that in order to do CFD one must have a fundamental understanding of fluid flow itself, from both the theoretical, mathematical side and from the practical, sometimes experimental, side. We will provide a brief introduction to each of these ways of studying fluid dynamics in the following subsections.

The theoretical approach

Theoretical/analytical studies of fluid dynamics generally require considerable simplifications of the equations of fluid motion mentioned above. We present these equations here as a prelude to topics we will consider in detail as the course proceeds. The version we give is somewhat simplified, but it is sufficient for our present purposes.

$$\nabla \cdot \mathbf{U} = 0 \text{ (conservation of mass)}$$

and

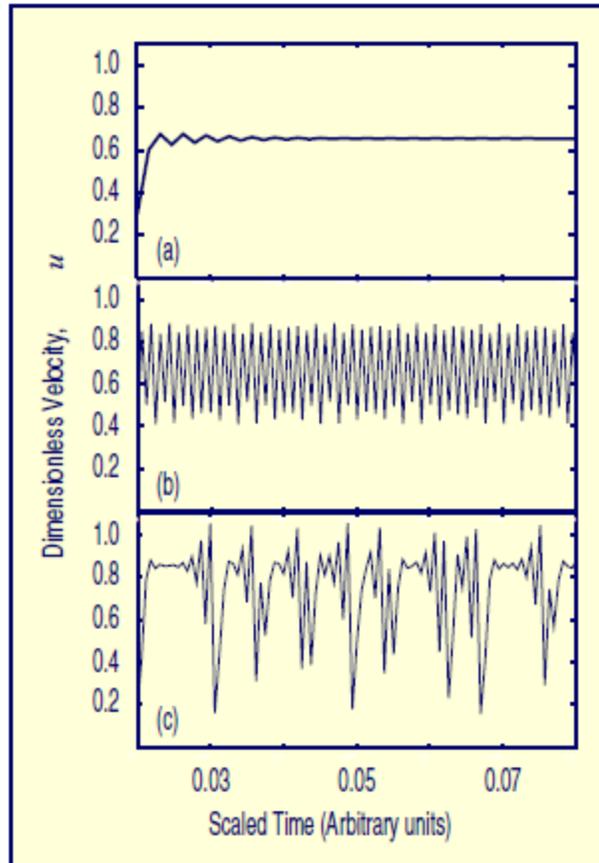
$$\frac{D\mathbf{U}}{Dt} = -\nabla P + \frac{1}{Re} \nabla^2 \mathbf{U} \text{ (balance of momentum) .}$$

These are the Navier–Stokes (N.–S.) equations of incompressible fluid flow. In these equations all quantities are dimensionless, as we will discuss in detail later: $\mathbf{U} \equiv (u, v, w)^T$ is the velocity vector; P is pressure divided by (assumed constant) density, and Re is a dimensionless parameter known as the Reynolds number. We will later see that this is one of the most important parameters in all of fluid dynamics; indeed, considerable qualitative information about a flow field can often be deduced simply by knowing its value.

In particular, one of the main efforts in theoretical analysis of fluid flow has always been to learn to predict changes in the qualitative nature of a flow as Re is increased. In general, this is a very difficult task far beyond the intended purpose of these lectures. But we mention it here to emphasize the importance of proficiency in applied mathematics in theoretical studies of fluid flow. From a physical point of view, with geometry of the flow situation fixed, a flow field

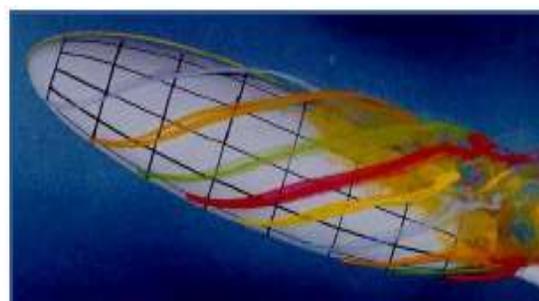
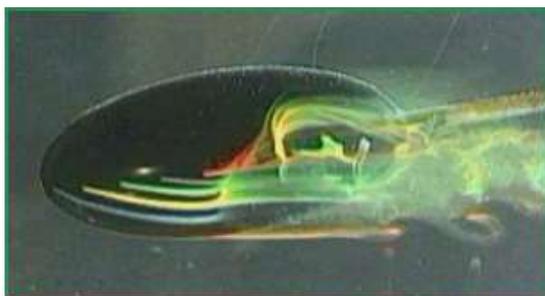
generally becomes “more complicated” as Re increases. This is indicated by the accompanying time series of a velocity component for three different values of Re . In part (a) of the figure Re is low, and the flow ultimately becomes time independent. As the Reynolds number is increased to an intermediate value, the corresponding time series shown in part (b) of the figure is considerably complicated, but still with evidence of somewhat regular behavior. Finally, in part (c) is displayed the high- Re case in which the behavior appears to be random. We comment in passing that it is now known that this behavior is not random, but more appropriately termed chaotic.

We also point out that the N.–S. equations are widely studied by mathematicians, and they are said to have been one of two main progenitors of 20th-Century mathematical analysis. (The other was the Schrödinger equation of quantum mechanics.) In the current era it is hoped that such mathematical analyses will shed some light on the problem of turbulent fluid flow, often termed “the last unsolved problem of classical mathematical physics.” We will from time to time discuss turbulence in these lectures because most fluid flows are turbulent, and some understanding of it is essential for engineering analyses. But we will not attempt a rigorous treatment of this topic. Furthermore, it would not be possible to employ the level of mathematics used by research mathematicians in their studies of the N.–S. equations. This is generally too difficult, even for graduate students.



Experimental fluid dynamics

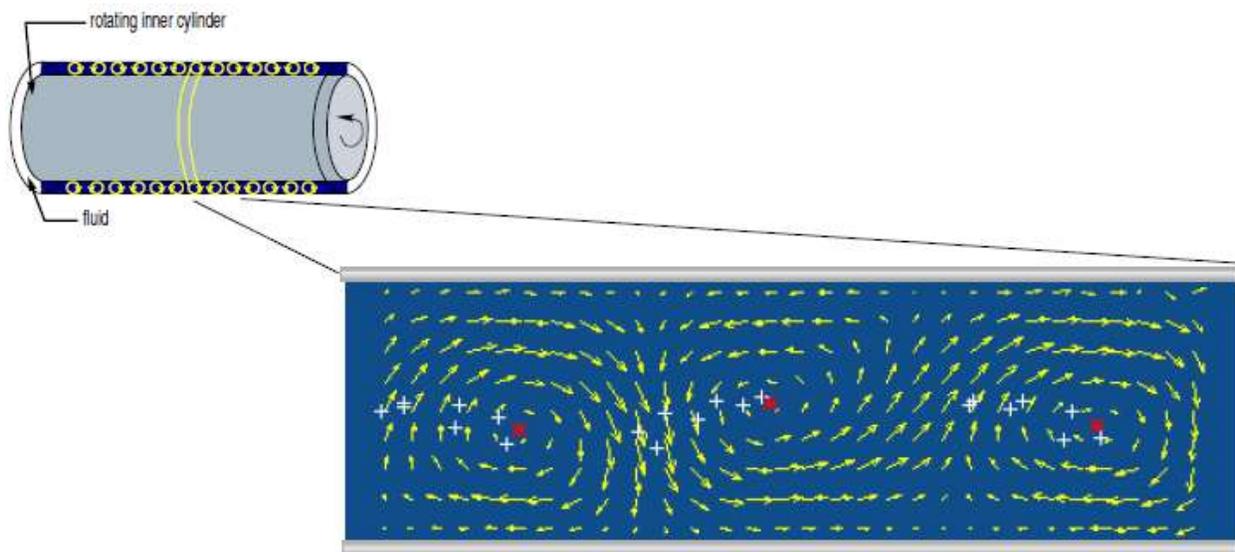
In a sense, experimental studies in fluid dynamics must be viewed as beginning when our earliest ancestors began learning to swim, to use logs for transportation on rivers and later to develop a myriad assortment of containers, vessels, pottery, etc., for storing liquids and later pouring and using them. Rather obviously, fluid experiments performed today in first class fluids laboratories are far more sophisticated. Nevertheless, until only very recently the outcome of most fluids experiments was mainly a qualitative (and not quantitative) understanding of fluid motion. An indication of this is provided by the adjacent pictures of wind tunnel experiments. In each of these we are able to discern quite detailed qualitative aspects of the flow over different prolate spheroids. Basic flow patterns are evident from colored streaks, even to the point of indications



of flow “separation” and transition to turbulence. However, such diagnostics provide no information on actual flow velocity or pressure—the main quantities appearing in the theoretical equations, and needed for engineering analyses. There have long been methods for measuring pressure in a flow field, and these could be used simultaneously with the flow visualization of the above figures to gain some quantitative data. On the other hand, it has been possible to accurately measure flow velocity simultaneously over large areas of a flow field only recently. If point measurements are sufficient, then hot-wire anemometry (HWA) or laser-doppler velocimetry (LDV) can be used; but for field measurements it is necessary to employ some form of particle image velocimetry (PIV). The following figure shows an example of such a measurement for fluid between two co-axial cylinders with the inner one rotating. This corresponds to a two-dimensional slice through a long row of toroidally-shaped (donutlike) flow structures going into and coming out of the plane of the page, i.e., wrapping around the circumference of the inner cylinder. The arrows indicate flow direction in the plane; the red asterisks show the center of the “vortex,” and the white pluses are locations at which detailed time series of flow velocity also have been recorded. It is clear that this quantitative detail is far superior to the simple visualizations shown in the previous figures, and as a consequence PIV is rapidly becoming the preferred diagnostic in many flow situations.

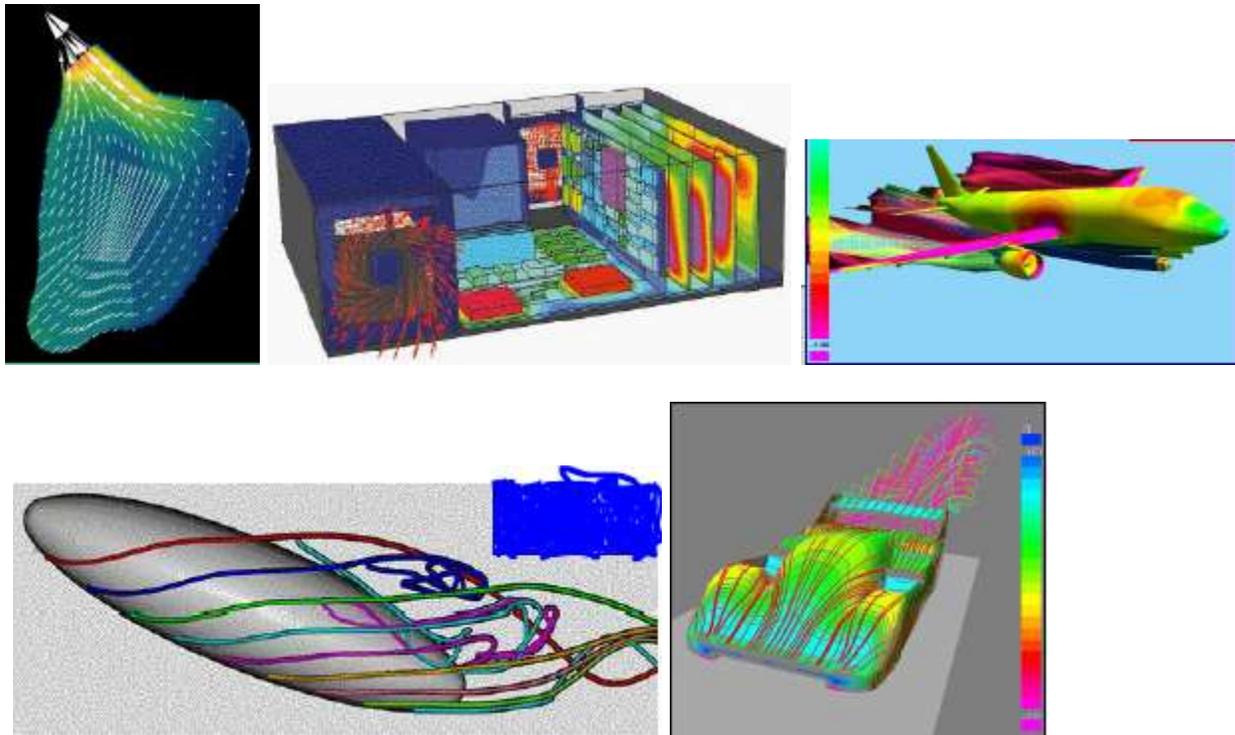
Computational fluid dynamics

We have already noted that CFD is rapidly becoming the dominant flow analysis technique, especially in industrial environments. CFD codes are available from many commercial vendors and as “freeware” from government laboratories, and many of these codes can be implemented on anything from a PC (often, even a laptop) to modern parallel supercomputers. In fact, it is not



difficult to find CFD codes that can be run over the internet from any typical browser. Here we display a few results produced by such codes to indicate the wide range of problems to which CFD has already been applied, and we will briefly describe some of the potential future areas for its use. The figure in the lower left-hand corner provides a direct comparison with experimental

results shown in an earlier figure. The computed flow patterns are very similar to those of the experiment, but in contrast to the experimental data the calculation provides not only visualization of qualitative flow features but also detailed quantitative output for all velocity component values and pressure, typically at on the order of 10^5 to 10^6 locations in the flow field. The upper left-hand figure displays predictions of the instantaneous flow field in the left ventricle of the human heart. Use of



CFD in biomedical and bioengineering areas is still in its infancy, but there is little doubt that it will ultimately dominate all other analysis techniques in these areas because of its generality and flexibility. The center figure depicts the pressure field over the entire surface of an airliner (probably a Boeing 757) as obtained using CFD. It was the need to make such predictions for aircraft design that led to the development of CFD, initially in the U. S. aerospace industry and NASA laboratories, and CFD was the driving force behind the development of supercomputers. Calculations of the type shown here are routine today, but as recently as a decade ago they would have required months of CPU time. The upper right-hand figure shows the temperature field and a portion (close to the fan) of the velocity field in a (not-so-modern) PC. This is a very important application of CFD simply because of the large number of PCs produced and sold every year worldwide. The basic design tradeoff is the following. For a given PC model it is necessary to employ a fan that can produce sufficient air flow to cool the computer by forced convection, maintaining temperatures within the operating limits of the various electronic devices throughout the PC. But effectiveness of forced convection cooling is strongly influenced by details of shape and arrangement of circuit boards, disk drives, etc. Moreover, power input to the fan(s), number of fans and their locations all are important design parameters that influence, among other things,

the unwanted noise produced by the PC. Finally, the lower right-hand figure shows pressure distribution and qualitative nature of the velocity field for flow over a race car, as computed using CFD. In recent years CFD has played an ever-increasing role in many areas of sports and athletics—from study and design of Olympic swimwear to the design of a new type of golf ball providing significantly longer flight times, and thus driving distance (and currently banned by the PGA). The example of a race car also reflects current heavy use of CFD in numerous areas of automobile production ranging from the design of modern internal combustion engines exhibiting improved efficiency and reduced emissions to various aspects of the manufacturing process, per se, including, for example, spray painting of the completed vehicles. It is essential to recognize that a CFD computer code solves the Navier–Stokes equations, given earlier, and this is not a trivial undertaking—often even for seemingly easy physical problems. The user of such codes must understand the mathematics of these equations sufficiently well to be able to supply all required auxiliary data for any given problem, and he/she must have sufficient grasp of the basic physics of fluid flow to be able to assess the outcome of a calculation and determine, among other things, whether it is “physically reasonable”—and if not, decide what to do next.

1.1 What is CFD?

Computational Fluid Dynamics or CFD is the analysis of systems involving fluid flow, heat transfer and associated phenomena such as chemical reactions by means of computer-based simulation. The technique is very powerful and spans a wide range of industrial and non-industrial application areas. Some examples are:

- aerodynamics of aircraft and vehicles: lift and drag
- hydrodynamics of ships
- power plant: combustion in IC engines and gas turbines
- turbomachinery: flows inside rotating passages, diffusers etc.
- electrical and electronic engineering: cooling of equipment including microcircuits
- chemical process engineering: mixing and separation, polymer moulding
- external and internal environment of buildings: wind loading and heating/ ventilation
- marine engineering: loads on off-shore structures
- environmental engineering: distribution of pollutants and effluents
- hydrology and oceanography: flows in rivers, estuaries, oceans
- meteorology: weather prediction
- biomedical engineering: blood flows through arteries and veins

From the 1960s onwards the aerospace industry has integrated CFD techniques into the design, R&D and manufacture of aircraft and jet engines. More recently the methods have been applied to the design of internal combustion engines, combustion chambers of gas turbines and furnaces. Furthermore, motor vehicle manufacturers now routinely predict drag forces, under-bonnet air flows and the in- car environment with CFD. Increasingly CFD is becoming a vital component in the design of industrial products and processes.

The ultimate aim of developments in the CFD field is to provide a capability comparable to other CAE (Computer-Aided Engineering) tools such as stress analysis codes. The main reason why CFD has lagged behind is the tremendous complexity of the underlying behaviour, which precludes a description of fluid flows that is at the same time economical and sufficiently complete. The availability of affordable high performance computing hardware and the introduction of user- friendly interfaces have led to a recent upsurge of

interest and CFD is poised to make an entry into the wider industrial community in the 1990s.

As explained above, flows and related phenomena can be described by partial differential (or integro-differential) equations, which cannot be solved analytically except in special cases. To obtain an approximate solution numerically, we have to use a *discretization method* which approximates the differential equations by a system of algebraic equations, which can then be solved on a computer. The approximations are applied to small domains in space and/or time so the numerical solution provides results at *discrete locations* in space and time. Much as the accuracy of experimental data depends on the quality of the tools used, the accuracy of numerical solutions is dependent on the quality of discretizations used. Contained within the broad field of computational fluid dynamics are activities that cover the range from the automation of well-established engineering design methods to the use of detailed solutions of the Navier-Stokes equations as substitutes for experimental research into the nature of complex flows. *CFD is the numerical solving of partial differential equations on a discretized system that given the available computer resources best approximates the real geometry and fluid flow phenomena of interest.*

In other words CFD is a tool, similar to experimental tools, used to gain greater physical insight into problems of interest. Thus, based on

- geometry
- fluid flow physics
- computer

we then select the appropriate:

- governing equations
- numerical method
- grid system

and then examine the results in order to gain physical insight and understanding.

At one end, one can purchase design packages for pipe systems that solve problems in a few seconds or minutes on personal computers or workstations. On the other, there are codes that may require hundreds of hours on the largest super-computers. The range is as large as the field of fluid mechanics itself, making it impossible to cover all of CFD in a single work. Also, the field is evolving so rapidly that we run the risk of becoming out of date in a short time. CFD is finding its way into process, chemical, civil, and environmental engineering. Optimization in these areas can produce large savings in equipment and energy costs and in reduction of environmental pollution.

Clearly the investment costs of a CFD capability are not small, but the total expense is not normally as great as that of a high quality experimental facility. Moreover, there are several unique advantages of CFD over experiment-based approaches to fluid systems design:

- substantial reduction of lead times and costs of new designs
- ability to study systems where controlled experiments are difficult or impossible to perform (e.g. very large systems)
- 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 hire 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 and it is very cheap to perform parametric studies, for instance to optimise equipment performance.

We also note that, in addition to a substantial investment outlay, an organisation needs qualified people to run the codes and communicate their results and briefly consider the modelling skills required by CFD users.

How does a CFD code work?

CFD codes are structured around the numerical algorithms that can tackle fluid flow problems. In order to provide easy access to their solving power all commercial CFD packages include sophisticated user interfaces to input problem parameters and to examine the results. Hence all codes contain three main elements: (i) a pre-processor, (ii) a solver and (iii) a post-processor. We briefly examine the function of each of these elements within the context of a CFD code.

Pre-processor

Pre-processing consists of the input of a flow problem to a CFD program by means of an operator-friendly interface and the subsequent transformation of this input into a form suitable for use by the solver. The user activities at the pre-processing stage involve:

- Definition of the geometry of the region of interest: the computational domain.
- Grid generation-the sub-division of the domain into a number of smaller, non-overlapping sub-domains: a grid (or mesh) of cells (or control volumes or elements).
- Selection of the physical and chemical phenomena that need to be modelled.
- Definition of fluid properties.
- Specification of appropriate boundary conditions at cells which coincide with or touch the domain boundary.

The solution to a flow problem (velocity, pressure, temperature etc.) is defined at nodes inside each cell. The accuracy of a CFD solution is governed by the number of cells in the grid. In general, the larger the number of cells the better the solution accuracy. Both the accuracy of a solution and its cost in terms of necessary computer hardware and calculation time are dependent on the fineness of the grid. Over 50% of the time spent in industry on a CFD project is devoted to the definition of the domain geometry and grid generation. In order to maximise productivity of CFD personnel all the major codes now include their own CAD-style interface and/or facilities to import data from proprietary surface modellers and mesh generators such as PATRAN and I-DEAS. Up-to-date pre-processors also give the user access to libraries of material properties for common fluids and a facility to invoke special physical and chemical process models (e.g. turbulence models, radiative heat transfer, combustion models) alongside the main fluid flow equations.

Solver

There are three distinct streams of numerical solution techniques: finite difference, finite element and spectral methods. In outline the numerical methods that form the basis of the solver perform the following steps:

- Approximation of the unknown flow variables by means of simple functions.
- Discretisation by substitution of the approximations into the governing flow equations and subsequent mathematical manipulations.
- Solution of the algebraic equations.

The main differences between the three separate streams are associated with the way in which the flow variables are approximated and with the discretisation processes. Finite difference methods. Finite difference methods describe the unknowns of the flow problem by means of point samples at the node points of a grid of co-ordinate lines. Truncated Taylor series expansions are often used to generate finite difference approximations of derivatives of ϕ in

terms of point samples of ϕ_j at each grid point and its immediate neighbours. Those derivatives appearing in the governing equations are replaced by finite differences yielding an algebraic equation for the values of ϕ_j at each grid point. Smith (1985) gives a comprehensive account of all aspects of the finite difference method.

Finite Element Method. Finite element methods use simple piecewise functions (e.g. linear or quadratic) valid on elements to describe the local variations of unknown flow variables ϕ_j . The governing equation is precisely satisfied by the exact solution ϕ . If the piecewise approximating functions for ϕ_j are substituted into the equation it will not hold exactly and a residual is defined to measure the errors. Next the residuals (and hence the errors) are minimised in some sense by multiplying them by a set of weighting functions and integrating. As a result we obtain a set of algebraic equations for the unknown coefficients of the approximating functions. The theory of finite elements has been developed initially for structural stress analysis.

Spectral Methods.

Spectral methods approximate the unknowns by means of truncated Fourier series or series of Chebyshev polynomials. Unlike the finite difference or finite element approach the approximations are not local but valid throughout the entire computational domain. Again we replace the unknowns in the governing equation by the truncated series. The constraint that leads to the algebraic equations for the coefficients of the Fourier or Chebyshev series is provided by a weighted residuals concept similar to the finite element method or by making the approximate function coincide with the exact solution at a number of grid points.

The finite volume method.

The finite volume method was originally developed as a special finite difference formulation.

It is central to four of the five main commercially available CFD codes: PHOENICS, FLUENT, FLOW3D and STAR-CD. The numerical algorithm consists of the following steps:

- Formal integration of the governing equations of fluid flow over all the (finite) control volumes 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.

The first step, the control volume integration, distinguishes the finite volume method from all other CFD techniques. The resulting statements express the (exact) conservation of relevant properties for each finite size cell. This clear relationship between the numerical algorithm and the underlying physical conservation principle forms one of the main attractions of the finite volume method and makes its concepts much more simple to understand by engineers than finite element and spectral methods. The conservation of a general flow variable ϕ_j , for example a velocity component or enthalpy, within a finite control volume can be expressed as a balance

Basics of Computational Fluid Dynamics

Concept of Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) is the simulation of fluids engineering systems using modeling (mathematical physical problem formulation) and numerical methods (discretization methods, solvers, numerical parameters, and grid generations, etc.). The process is as figure 1.

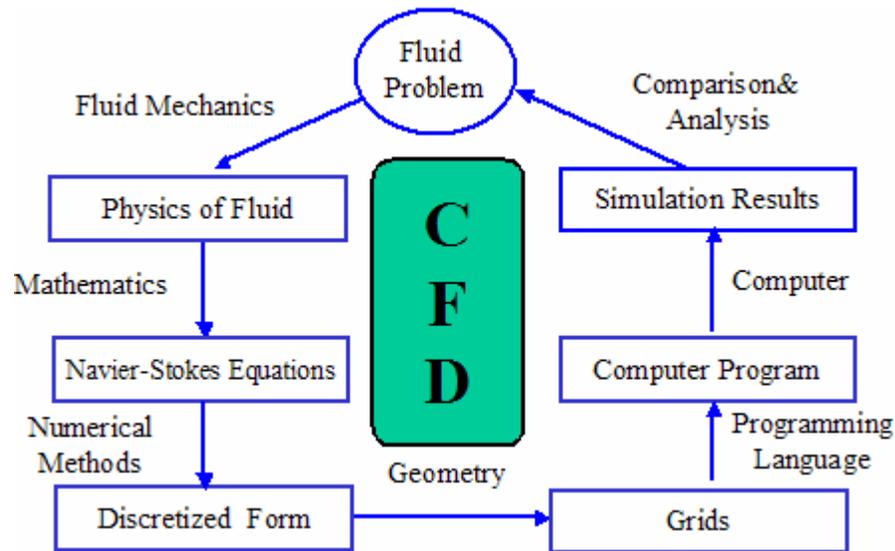


Figure 1 Process of Computational Fluid Dynamics

Firstly, we have a fluid problem. To solve this problem, we should know the physical properties of fluid by using Fluid Mechanics. Then we can use mathematical equations to describe these physical properties. This is Navier-Stokes Equation and it is the governing equation of CFD. As the Navier-Stokes Equation is analytical, human can understand it and solve them on a piece of paper. But if we want to solve this equation by computer, we have to translate it to the discretized form. The translators are numerical discretization methods, such as Finite Difference, Finite Element, Finite Volume methods. Consequently, we also need to divide our whole problem domain into many small parts because our discretization is based on them. Then, we can write programs to solve them. The typical languages are Fortran and C. Normally the programs are run on workstations or supercomputers. At the end, we can get our simulation results. We can compare and analyze the simulation results with experiments and the real problem. If the results are not sufficient to solve the problem, we have to repeat the process until find satisfied solution. This is the process of CFD.

Importance of Computational Fluid Dynamics

There are three methods in study of Fluid: theory analysis, experiment and simulation (CFD). As a new method, CFD has many advantages compared to experiments.

| | Simulation (CFD) | Experiment |
|-------------|------------------|----------------|
| Cost | Cheap | Expensive |
| Time | Short | Long |
| Scale | Any | Small/Middle |
| Information | All | Measured Point |
| Repeatable | Yes | Some |
| Safety | Yes | Some Dangerous |

Table 1 Comparison of Simulation and Experiment

Physics of Fluid

Fluid is liquid and gas. For example, water and air. Fluid has many important properties, such as velocity, pressure, temperature, density and viscosity. The density (ρ) of a fluid is its mass per unit volume. If the density of fluid is constant (or the change is very small), we call the fluid is incompressible fluid. If the density of fluid is not constant, we call the fluid is compressible fluid. Normally, we can treat water and air as incompressible fluid. If the fluid is incompressible, we can simplify the equations for this type of fluid.

$$\rho = \frac{M}{V} \left[\frac{kg}{m^3} \right] \text{ -----1}$$

The viscosity (μ) is an internal property of a fluid that offers resistance to flow. For example, to stir water is much easier than to stir honey because the viscosity of water is much smaller than honey.

$$\mu = \left[\frac{Ns}{m^2} \right] = [poise] \text{ -----2}$$

Table 2 shows the densities and viscosities of air, water and honey.

| Substance | Air (18°C) | Water (20°C) | Honey (20°C) |
|------------------------------|------------|--------------|--------------|
| Density (kg/m ³) | 1.275 | 1000 | 1446 |
| Viscosity (P) | 1.82e-4 | 1.002e-2 | 190 |

Navier-Stokes Equations

Conservation Law

Navier-Stokes equations are the governing equations of Computational Fluid Dynamics. It is based on the conservation law of physical properties of fluid. The principle of conservational law

is the change of properties, for example mass, energy, and momentum, in an object is decided by the input and output.

For example, the change of mass in the object is as follows

$$\frac{dM}{dt} = \dot{m}_{in} - \dot{m}_{out} \quad \text{-----3}$$

If $\dot{m}_{in} - \dot{m}_{out} = 0$, we have

$$\frac{dM}{dt} = 0 \quad \text{-----4}$$

Which means

$$M = \text{const} \quad \text{,,,,,,5}$$

Navier-Stokes Equation

Applying the mass, momentum and energy conservation, we can derive the continuity equation, momentum equation and energy equation as follows.

Continuity Equation

$$\frac{D\rho}{Dt} + \rho \frac{dU_i}{dx_i} = 0 \quad \text{-----} \quad 6$$

Momentum Equation

$$\rho \frac{dU_j}{dt} + \rho U_i \frac{dU_j}{dx_i} = \frac{dP}{dx_j} - \frac{d\tau_{ij}}{dx_i} + \rho g_j \quad \text{-----7}$$

Where

$$\tau_{ij} = \mu \left(\frac{dU_j}{dx_i} + \frac{dU_i}{dx_j} \right) + \frac{2}{3} \delta_{ij} \mu \frac{dU_k}{dx_k} \quad \text{-----} \quad 8$$

I: Local change with time

II: Momentum convection

III: Surface force

IV: Molecular-dependent momentum exchange (diffusion)

V: Mass force

Energy Equation

$$\rho C_\mu \frac{dT}{dt} + \rho C_\mu U_i \frac{dT}{dx_i} = -P \frac{dU_i}{dx_i} + \lambda \frac{d^2 T}{dx_i^2} - \tau_{ij} \frac{dU_j}{dx_i} \quad \text{-----} \quad 9$$

I : Local energy change with time

II: Convective term

III: Pressure work

IV: Heat flux (diffusion)

V: Irreversible transfer of mechanical energy into heat

If the fluid is compressible, we can simplify the continuity equation and momentum equation as follows.

Continuity Equation

$$\frac{dU_i}{dx_i} = 0 \quad \text{-----} \quad 10$$

Momentum Equation

$$\rho \frac{dU_j}{dt} + \rho U_i \frac{dU_j}{dx_i} = -\frac{dp}{dx_j} - \mu \frac{d^2 U_j}{dx_i^2} + \rho g_j \quad \text{-----} \quad 11$$

We now explain the notation used in the Navier-Stoke's equations; $\rho = \rho(x, y, z, t)$ is the density of the fluid at a point (x, y, z) at time t , $p = p(x, y, z, t)$ is the pressure on the fluid at a point (x, y, z) at time t . The symbol ∇ represents the gradient (column) vector $(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3})$ or $(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$. By ∇p we mean the (column) vector (p_x, p_y, p_z) , where the subscript indicates partial differentiation with respect to that variable. The symbol Δ represents the Laplacian and is given by $\nabla \cdot \nabla$ or $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ and is applied to each component of $U = (u, v, w)$. The parameters δ, η and μ are functions of (x, y, z) that describe the viscosity of the fluid. The function G is the (column) vector $(g_1(x, y, z, t), g_2(x, y, z, t), g_3(x, y, z, t))$ and models external forces acting on the fluid. In the modules we set $G = 0$. You can easily modify the codes to see

Introduction

Fluid dynamics is a classic discipline. The physical principles governing the flow of simple fluids and gases, such as water and air, have been understood since the times of Newton. Since about 1950 classic fluid dynamics finds itself in the company of computational fluid dynamics. This newer discipline still lacks the elegance and unification of its classic counterpart, and is in a state of rapid development. The purpose of this lecture note is:

- To introduce some notation that will be useful later;
- To recall some basic facts of vector analysis;
- To introduce the governing equations of laminar incompressible fluid dynamics;
- To explain that the Reynolds number is usually very large. In later notes this will be seen to have a large impact on numerical methods.

What is Computational Fluid Dynamics?

What is CFD?

Computational Fluid Dynamics can be defined as the field that uses computer resources to simulate flow related problems. To simulate a flow problem you have to use mathematical physical and programming tools to solve the problem then data is generated and analysed. This field has been developing for the past 30 years. During the last 10 years this field has just made a big jump especially due to the introduction of new computer hardware and software. University academics write their own mini sized codes to solve the problems they are usually assigned. These codes are usually not that user friendly and not very well documented. Before computational fluid dynamics was used on a wide scale. Engineers had to make small scale

models to validate how slender is their design. A design that is not aerodynamically efficient will have a negative impact on where the design will be used. So a bad car design will result in more fuel consumption. While a bad design for a plane might cause it to crash.



Figure 2 : A researcher puts a lorry model inside a wind tunnel for tests.

These experiments were done by immersing the model in a transparent fluid/gas and then applying flow conditions similar to the conditions the model would encounter. Next came was applying a colour dye to the flow which resulted in showing the flow pattern resulting from the flow. The set back of using such methods is that after you have got your blue print drawings from the design team you have to model your design in a work shop. Once the model has been made you will need to have the experimental set up apparatus in an allocated space in the engineering lab. Just to note that Wind tunnels are huge in size some of them can contain real scale model as illustrated in figure 2 below. While now you just need the flow modelling software, a good research team and lots of computer resources.



Figure 2: A panoramic view of the wind tunnel in the workshops, just to illustrate its tremendous size in comparison with a desktop computer. The researcher can be seen on the bottom right hand side of the picture.

The researchers advantage of CFD is that you can have a wind tunnel on your desktop without having to worry about choosing big fans or that your model will fit into the wind tunnel or not Figure 3 shows the size extent of a wind tunnel blowing fan. These problems can be solved in the

software by changing the scaling of the studied model or by modifying the value of the inflow velocity into the studied domain mesh.



Figure 3 : The Inlet duct of the blowing fan for the wind tunnel its reasonably large.

Computational Fluid Dynamics Theoretical Foundation:

1. Linear Algebra, example TDMA, Gauss ,.....etc

For a researcher working in CFD linear algebra is a must and has to be covered or refreshed, because with progress with time you will find that all your work revolves around matrix operations, plotting vector fields, vector operations, etc.

2. Numerical Analysis, example to know how to discretize first order, second order derivatives encountered in PDEs (Partial Differential Equations) and ODEs (Ordinary Differential Equations)

3. Tensor Calculus, example for applying the summation convention when tensor notation is used.

4. Fluid Mechanics, example to know how to use the Continuity Equation, Bernoulli Equation, Reynolds Number, Mach Number, etc

5. Programming:

Throughout your research you come across all sorts of codes, during this process you will need to quickly know how to approach the codes and to what details to look for and best ways to summarize the processes that take place in it.

6. Programming in General:

To know how to write a code through a step by step guide, The lecture note expresses it in Pascal but you can use its outline depending on what language your using, it's a 1995 edition but it's very useful for self study.

7. Fortran90.

You might be assigned during your PhD to generate data with a provided code, during the process of running the code you will sometimes have to go through the various parts of the code.

8. MATLAB.

MATLAB is a very user friendly software with lots of helpful online material and books not forgetting its excellent help. As a researcher you will have to learn this software due to its powerful tools in the data analysis part of your PhD.

9. Statistics and Probability.

If you're going to be working in the field of turbulence you will need statistical tools, while if you're going to work on reactive flows you will need initially statistical tools and later probability functions for later stages of your project once you get to the detailed side of chemistry.

10. Differential Equations and Computational PDEs.

11. Algorithm Theory.

12. Data Structures.

During the research process dealing with all sorts of matrices of different types is an issue that has to be accepted, depending on the studied problem.

13. Discrete Mathematics.

Steps to Set Up a Simulation

During the description of the following, the points might overlap every now and then. Planning for a simulation is advantageous, it helps you to focus for longer hours, keeps you focused on your target and confident that you will get to finish on target.

1. Choosing the problem like as case study or in most cases you are assigned a problem which might represent a air flow in a lecture room or air flow around a car, air flow around a building ...etc.

2. What parameters are of interest. That's if some hints had already been provided by the manufacturer or by the customer. If the researcher has been assigned the problem and has to start from scratch this leads him to run simulations for very simple cases , then to verify that the results if they are correct by comparing the data with experimental or available literature data. Once this objective is achieved the researcher would select the required parameters for study, makes a list of them and then starts running more detailed simulations. What is meant if we are interested in combustion case turbulence intensity is an attractive parameter to study which means it can illustrate the magnitude of mixing strength in the process. Another parameter to study and can give a good indication of the rate of mixing is through plotting the eddy viscosity frequency. Shear strain rate can give a good indication on flow break up leading to dissipation such an example is a jet blowing into a stagnant air in a room.

3. The user has to specify if it's an Internal flow case (looking at figure 4 which represents a throttle valve) or an external flow case (looking at figure 5 which refers to a wind turbine).

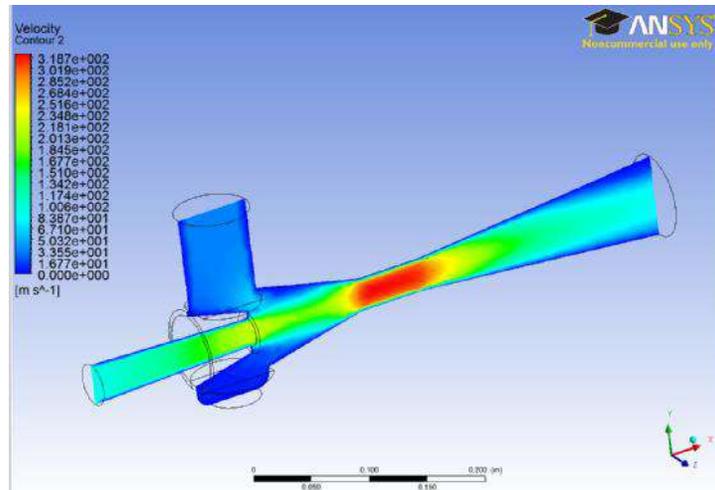


Figure 4: A throttle valve describes and internal flow example, where maximum velocity is achieved at the minimum area cross section (throat).

In some cases the researcher might have to break down the studied mesh into smaller domains due to that the available hardware resources are not sufficient for such a simulation unfortunately this is something that the user has to get used to as an obstacle that would occur every now and then. Options are provided with CFD software's in domain decomposition as an option which can be very helpful especially in study cases that have large meshes.

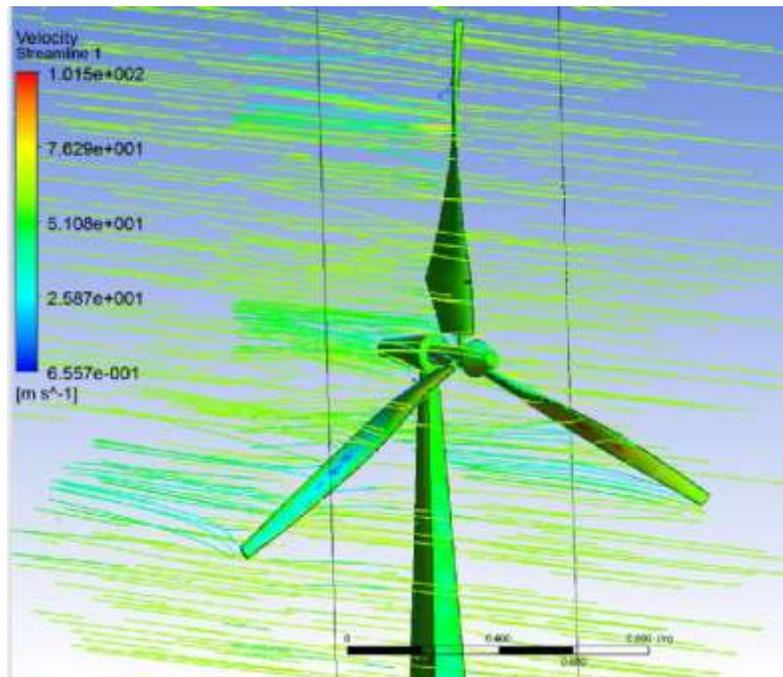


Figure 5: A wind turbine describes an external flow case.

4. Choosing a simulation model. These models all depend on what is wanted out of the simulation and what is being looked for. These models start from Direct Numerical Simulations to Reynolds Averaged Methods toetc.

5. Assessing the required hardware and software resources and what is available. Due to these challenges the user has to take into account these issues as an example simulation run time, calculation time on the desktop, data storage and simulation grid resolution, how many cores are requiredetc.
6. Specifying the boundary conditions in the simulation. These can refer to solid walls or inflow and outflow boundaries. At some cases moving boundaries are taken into account as cases in simulating flows in pumps, compressors, wind turbinesetc. At certain cases the smoothness of the boundaries have to be specified as smooth or rough boundaries.
7. Selecting the physical continuum which might be Air, Argon, Nitrogen,etc.
8. Selecting a Mesh type for the simulation. Will it be hexahedral or tri-diagonal ...etc. Usually CFD software has several meshing options to choose from.

Mathematical Flow Modelling

On the assumption that the problem is a flow problem:

1. Choosing the coordinates system, which specifies what space the student, will work on. Metric, Sobolev or Hilbert space..etc. At later stages this will lead the researcher to adopt specified mathematical methods that can only be used in these spaces.
2. Choosing the reference coordinate system, this is automatically taken at point (0,0,0) . The equations that you are going to solve are related to the coordinate system for the space relation. Once motion is going to be studied that means we will have a generated mesh velocity and acceleration to be taken in account. The use of velocity acceleration leads to the conclusion that derivatives are going to be used. Once derivatives come into account that means at later stages we will need to use some kind of discretization method.
3. The studied domain geometry and dimensions. Is it a box, rectangular, sphere or cylinder or a complex domain?. This relates to the required scales to be captured by the simulation. Another factor is the studied object. As an example the Navier-Stokes equations are applicable at certain length ranges at small scales Lattice-Boltzmann might be better at a smaller scale schrodinger equation that all depends on using the Knudsen number to verify the scale of the studied case.
4. Then comes how many species will there be? in most case air is taken as the studied fluid. That will ease the studied case. While if several species are taken into account will complicate the study more. Several species will lead us to two cases either a reactive or a non-reactive case.
5. Compressible or non compressible fluid case. Each case has a different approach to solve the major difference is in how to solve the pressure problem. In compressible flows you just use the ideal gas equation while in incompressible flows you will need to use a more complex approach for it.
6. Choosing the physical governing laws of importance. Will it be a Conservation of momentum or Conservation of mass or Conservation of energy or all at the same time?
7. Choosing thermodynamic reference parameters temperature, viscosity, pressure, this is essential, because at certain occasions due to that some parameters change in relation to other parameters , as an example viscosity is related to temperature using the Sutherland formula.
8. Now we are ready to Choose a Numerical Model. A quick survey on the available models their pros and cons. Usually you can find a researcher who had already done this in a recently published paper if your studied case is not that recent then look for a book that has summarised the models. At really advanced stages you might have to make your own model which is very hard not forgetting it's not easy to convince people to use your model except if it's something really outstanding.

9. None dimensionlizing process of the used equations where required, this always gives the written code a more dynamic characteristic to use the code on a wider spectrum of problems.

Equations Used (Numerical Method)

All the equations used in the study of flows are derived from Reynolds Transport Theory, it is recommended to memories this equation and from it derive all the forms you want to study. From it you can derive the continuity equation, the momentum equations, the species equation and finally the energy equation (in the case of working with compressible gases new quantities will be added to the study such as the adiabatic equation). You can add as many quantities to your studied case by using the Reynolds Transport Theory keeping in mind the computer resource that are available for the researcher.

The Navier-Stokes Equations are used, that's in general term, in detail the researcher can think of these equations as representing the motion of a particle in space. Using CFD the splitting of a predefined space into small cells and using the Navier-Stokes Equations for each studied cell. People usual feel scared from the term equations and once derivatives and lots of them are used that quickly lead to a quick decision i can't understand it i won't read it. Actually these set of equations represent the change of a vector quantity in 3D space, the vector quantity in the Stokes equation is the velocity vector. The Stokes equations represent the transfer of momentum in a studied flow.

$$\int \frac{d\rho\phi}{dt} dt dV + \int \text{div}(\rho\phi V) dt dV = \int D \text{div}(\text{grad}\phi) dt dV + \int S_\phi dt dV$$

simplifying the equation to a form that is related to a regular uniform mesh gives

$$\frac{d\rho\phi}{dt} + \text{div}(\rho\phi V) = D \text{div}(\text{grad}\phi) + S_\phi$$

applying would lead to the continuity equation

$$\frac{d\rho}{dt} + \text{div}(\rho V) = S$$

Once you write down the set of equations you will be using for your study, the next step is to see what forces are wanted to be taken into account and what factors will be neglected in the study. This will lead the researcher to the available models for his study which starts with DNS (Direct Numerical Analysis and finishes with simple models) the selection of the model depends on the studied case from one perspective and available recourses from another perspective.

so for a case of studying the transport of the scalar quantity of velocity in the y axis direction we would assign the value $\phi = v$ which results in the following formula:

$$\frac{d\rho v}{dt} + \text{div}(\rho v V) = D \text{div}(\text{grad}\phi) + S_v$$

while for a case of studying the transport of the scalar quantity of temperature in the studied domain we would assign the value $\phi = T$ which results in the following formula:

$$\frac{d\rho T}{dt} + \text{div}(\rho T V) = D_T \text{div}(\text{grad}\phi) + S_T$$

so for a case of studying the transport of the scalar quantity of species in the studied domain we would assign the value $\phi = Y_n$ which is called a volume fraction which results in the following formula.

$$\frac{d\rho Y_n}{dt} + \text{div}(\rho Y_n V) = D_n \text{div}(\text{grid} Y_n) + S_n$$

A CFD code consist of the following parts:

Just as a way to make things clear for the reader you can think of a CFD parts as a Human body where input parameters are food to be eaten, the time discretization section is the humans head, the space discretization section is the human body. While the computer compiler represents the heart.

1. Input Parameters:

This section holds the number of grid points in the domain, domain dimensions, initialization profile selection, and simulation time length. As a researcher you would be working most of the time on the input file changing different variables and then running a simulation. At more advanced stages of PhD you would have to write your own subroutines and add them to the code.

2. Time Discretization Section:

The two mostly liked methods that are used in CFD, are the Runge-Kutta and Crank Nicholson Method. If the code uses the Runge-Kutta method the time stepping section forms a mostly independent section of the code while using the crank Nicholson Method you will find there is a more strong coupling between the time and space discretization parts of the code. Codes usually have a criteria to run a simulation where after each calculated time step the code checks that the simulation stays stable. In such cases there are some formulas that are used to satisfy the condition in having the best discrete time to achieve a stable simulation.

3. Space Discretization Section:

Space discretization consist of the next four parts, these four parts are essential and cannot be neglect, because each one is related to the other and has a direct impact to the other.

a. Grid Generation.

A grid has to be generated and depending to the type of fluid it will be chosen. as an example the use of staggered grid in incompressible gases. Some people would say why is the grid so important. Once you start the analysis process you will need to see the values of the studied scalar at the generated points. This is done through plotting the vector fields or plotting contour plotetc. Some time you will need to see the value of velocity at a certain part of the domain. In such a case you will just give the coordinates of the point to extract its value

b. Initialization Profiles.

You can run a simulation without having an initialization profile but its side effects that you will need several thousand time steps till the flow develops into its predicted form depending on the simulation stop criteria. Explicit or implicit methods are also related to initialization for space discretization and time.

c. Boundary Conditions.

During a fluid flow simulation you always need to assign a certain surface some inflow parameters and another one at least to be outflow surface. You can specify that be assigning a source term a value of flow velocity .The choice of periodic condition or none periodic depends on your requirements. Periodic satisfies a condition where at each time step of the simulation the

amount of flow into the domain is the same as the amount of going out of the domain. Choosing surface roughness is also a requirement.

d. Discretization Methods.

There are various discretization schemes they start with very simple ones such as central differencing scheme which requires two points and can end with schemes that use more than 15 grid points.

4. Output Section:

This is the section usually the researcher is assigned to. The researcher has to read the output data into a visualization software such as Tecplot, MATLAB, Excel...etc. Usually the code generates a set of output files these files have the calculated sets of data like the grid reference number its coordinates the value of the velocity at the point its temperature its pressure ...etc.

Skills for Building a Code:

1. To build a working numerical model that gives you data output which is not necessarily correct is done using random number generators. This can also be accomplished using straight forward numbers such as 1.
2. Checking the physical units of the formula that they are homogenous.
3. Once you get the code working without bugs, next comes validation of data output. This is done by seeing experimental plots or published tables of the studied quantity.

What's an Equation?

An equation is a mathematical expression that represents a region of points in a certain space. The researcher has to choose the range of study to specify his data matrix dimensions. Once the known's are specified for the studied case then comes writing the mathematical formula into a way the programming language interprets it to the computer. This is done by taking the formula apart depending on the number of variables and assigning them suitable names. Then comes specifying the number of points required. This is mostly done based on computer resources and how much is the required accuracy.