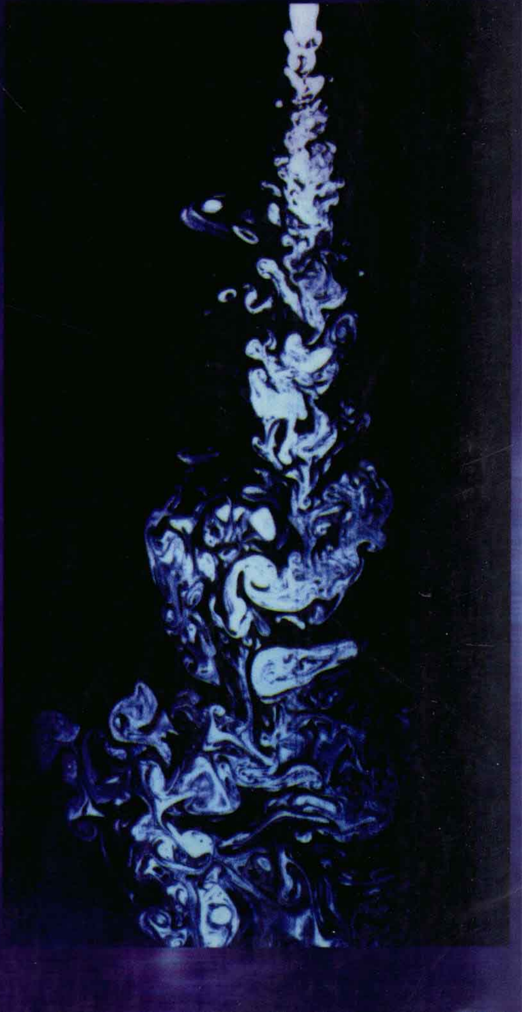
An introduction to Computational Fluid Dynamics

The Finite Volume Method



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The finite volume method

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Preface

The use of computational fluid dynamics (CFD) to predict internal and external flows has risen dramatically in the past decade. In the 1980s the solution of fluid flow problems by means of CFD was the domain of the academic, postdoctoral or postgraduate researcher or the similarity trained specialist with many years of grounding in the area. The widespread availability of engineering workstations together with efficient solution algorithms and sophisticated pre- and post-processing facilities enable the use of commercial CFD codes by graduate engineers for research, development and design tasks in industry. The codes that are now on the market may be extremely powerful, but their operation still requires a high level of skill and understanding from the operator to obtain meaningful results in complex situations. The long learning curve, previously including apprenticeships of up to four years – more widely known as MPhil and PhD studies – meant that the users of the 1980s were, through their own experiences, very conscious of the limitations of CFD. However, the pressure on engineers in industry to come up with solutions to problems implies that there is not always the time available for the new type of user of the 1990s to learn about the pitfalls of CFD by osmosis and frequent failure.

It is the purpose of this book to fill a gap in the available literature for novice CFD users who, whilst developing CFD skills by using commercially available software, need a reader that provides the fundamentals of the fluid dynamics behind complex engineering flows and of the numerical solution algorithms on which the CFD codes are based. Although the material has been developed from first principles wherever possible, the book will be of greatest benefit to those who are familiar with the ideas of calculus, elementary vector and matrix algebra and basic numerical methods. Furthermore, we assume a knowledge of the conservation laws for mass, momentum and energy and an awareness of their application to fluid flow problems.

Although commercial CFD codes based on the finite element method have more recently entered the fray, the market is currently dominated by four codes, PHOENICS, FLUENT, FLOW3D and STAR-CD, that are all based on the finite volume method. This book intends to provide the theoretical background required for the effective use of this type of commercial code and covers the following subject areas:

Fluid dynamics

- Governing equations of viscous fluid flows
- Boundary conditions
- Introduction to the physics of turbulence
- Turbulence modelling in CFD

The finite volume method and its implementation in CFD codes

- Finite volume discretisation for the key transport phenomena in fluid flows: diffusion, convection and sources
- Discretisation procedures for unsteady phenomena
- Iterative solution processes (SIMPLE and its derivatives) to ensure correct coupling between all the flow variables
- Solution algorithms for systems of discretised equations (TDMA)
- Implementation of boundary conditions

The basic numerical techniques have been developed around a series of worked examples, which can be easily programmed on a PC. However, it is impossible to get to grips with the art of CFD without running a good quality code to explore the issues raised in this book in greater detail. As an illustration of the power of CFD we have presented a set of industrially relevant applications ranging from a benchmark simulation to very complex fire modelling. Throughout, one of the key messages is that CFD cannot be professed adequately without continued reference to experimental validation. The early ideas of the computational laboratory to supersede experimentation have fortunately gone out of fashion. Not all industrial companies have the high cost experimental infrastructure in place to support CFD activities, but the scientific literature contains a huge resource to the user of commercial codes. A vast and ever-increasing number of journals cover all aspects of CFD ranging from mathematically abstruse to applied work firmly rooted in industry. In addition to the necessary theoretical grounding the book, therefore, provides a set of connection points with up-to-date research literature giving the reader access to source material for code validation and further study.

After starting to teach CFD at senior undergraduate level we became acutely aware of the absence of a 'suitable' text pitched at 'the right level'. Undeniably, this book, which was developed from our course notes, was conceived with our own students as a target audience so, first and foremost, we hope that the book will be valuable as a learning and teaching resource to support CFD courses at undergraduate and postgraduate level. Nevertheless, with its intent to bridge the gap between introductory mathematics and fluid dynamics concepts, the academic CFD literature and applied industrial practice, we believe that this book will also be of use to professional engineers in industry, involved in R&D and design, who require a thorough but user-friendly reference guide to all the background knowledge needed to operate commercial CFD codes successfully.

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Introduction

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 micro-circuits
- 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.

We estimate the minimum cost of suitable hardware to be between £5000 and £10000 (plus annual maintenance costs). The perpetual licence fee for commercial software typically ranges from £10000 to £50000 depending on the number of 'added extras' required. CFD software houses can usually arrange annual licences as an alternative. 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. We complete this otherwise upbeat section by wondering whether the next constraint to the further spread of CFD amongst the industrial community could be a scarcity of suitably trained personnel instead of availability and/or cost of hardware and software.

1.2 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. Optimal meshes are often non-uniform: finer in areas where large variations occur from point to point and coarser in regions with relatively little change. Efforts are under way to develop CFD codes with a (self-)adaptive meshing capability. Ultimately such programs will automatically refine the grid in areas of rapid variations. A substantial amount of basic development work still needs to be done before these techniques are robust enough to be incorporated into commercial CFD codes. At present it is still up to the skills of the CFD user to design a grid that is a suitable compromise between desired accuracy and solution cost.

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 ϕ 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 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 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. The governing equation is precisely satisfied by the exact solution ϕ. If the piecewise approximating functions for ϕ 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. A standard work for fluids applications is Zienkiewicz and Taylor (1991).

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. Further information on this specialised method can be found in Gottlieb and Orszag (1977).

The finite volume method. The finite volume method was originally developed as a special finite difference formulation. This book shall be solely concerned with this most well-established and thoroughly validated general purpose CFD technique. 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, for example a velocity component or enthalpy, within a finite control volume can be expressed as a balance between the various processes tending to increase or decrease it. In words we have:

$$\begin{bmatrix}\text{Rate of change}\\ \text{of } \phi \text{ in the the control}\\ \text{volume with}\\ \text{respect to time}\end{bmatrix} = \begin{bmatrix}\text{Net flux of}\\ \phi \text{ due to}\\ \text{convection into}\\ \text{the control volume}\end{bmatrix} + \begin{bmatrix}\text{Net flux of}\\ \phi \text{ due to}\\ \text{diffusion into the}\\ \text{control volume}\end{bmatrix} + \begin{bmatrix}\text{Net rate of creation}\\ \text{of } \phi \text{ inside the}\\ \text{control volume}\end{bmatrix}$$

CFD codes contain discretisation techniques suitable for the treatment of the key transport phenomena, convection (transport due to fluid flow) and diffusion (transport due to variations of ϕ from point to point) as well as for the source terms (associated with the creation or destruction of ϕ) and the rate of change with respect to time. The underlying physical phenomena are complex and non-linear so an iterative solution approach is required. The most popular solution procedures are the TDMA line-by-line solver of the algebraic equations and the SIMPLE algorithm to ensure correct linkage between pressure and velocity. Commercial codes may also give the user a selection of further, more recent, techniques such as Stone's algorithm and conjugate gradient methods.

Post-processor

As in pre-processing a huge amount of development work has recently taken place in the post-processing field. Owing to the increased popularity of engineering workstations, many of which have outstanding graphics capabilities, the leading CFD packages are now equipped with versatile data visualisation tools. These include:

- Domain geometry and grid display
- Vector plots
- Line and shaded contour plots
- 2D and 3D surface plots
- Particle tracking
- View manipulation (translation, rotation, scaling etc.)
- Colour postscript output

More recently these facilities may also include animation for dynamic result display and in addition to graphics all codes produce trusty alphanumeric output and have data export facilities for further manipulation external to the code. As in many other branches of CAE the graphics output capabilities of CFD codes have revolutionised the communication of ideas to the non-specialist.

1.3 Problem solving with CFD

In solving fluid flow problems we need to be aware that the underlying physics is complex and the results generated by a CFD code are at best as good as the physics (and chemistry) embedded in it and at worst as good as its operator. Elaborating on the latter issue first, the user of a code must have skills in a number of areas. Prior to setting up and running a CFD simulation there is a stage of identification and formulation of the flow problem in terms of the physical and chemical phenomena that need to be considered. Typical decisions that might be needed are whether to model a problem in two or three dimensions, to exclude the effects of ambient temperature or pressure variations on the density of an air flow, to choose to solve the turbulent flow equations or to neglect the effects of small air bubbles dissolved in tap water. To make the right choices requires good modelling skills, because in all but the simplest problems we need to make assumptions to reduce the complexity to a manageable level whilst preserving the salient features of the problem in hand. It is the appropriateness of the simplifications introduced at this stage that at least partly governs the quality of the information generated by CFD, so the user must continually stay aware of all the assumptions, clear-cut and tacit ones, that have been made.

A good understanding of the numerical solution algorithm is also crucial. Three mathematical concepts are useful in determining the success or otherwise of such algorithms: convergence, consistency and stability. **Convergence** is the property of a numerical method to produce a solution which approaches the exact solution as the grid spacing, control volume size or element size is reduced to zero. **Consistent** numerical schemes produce systems of algebraic equations which can be demonstrated to be equivalent to the original governing equation as the grid spacing tends to zero. **Stability** is associated with damping of errors as the numerical method proceeds. If a technique is not stable even roundoff errors in the initial data can cause wild oscillations or divergence.

Convergence is usually very difficult to establish theoretically and in practice we use Lax's equivalence theorem which states that for linear problems a necessary and sufficient condition for convergence is that the method is both consistent and stable. In CFD methods this theorem is of limited use since we shall see in Chapter 2 that the governing equations are non-linear. In such problems consistency and stability are necessary conditions for convergence, but not sufficient.

Our inability to prove conclusively that a numerical solution scheme is convergent is perhaps somewhat unsatisfying from a theoretical standpoint, but we need not be too concerned since the process of making the mesh spacing very close to zero is not feasible on computing machines with a finite representation of numbers (eight digits on Real*4). Roundoff errors would swamp the solution long before a grid spacing of zero is actually reached. Engineers need CFD codes that produce physically realistic results with good accuracy in simulations with finite (sometimes quite coarse) grids. Patankar (1980) has formulated rules which yield robust finite volume calculation schemes. These are discussed further in Chapter 5; here we highlight three crucial properties of robust methods: conservativeness, boundedness and transportiveness.

The finite volume approach guarantees local conservation of a fluid property ϕ for each control volume. Numerical schemes which possess the **conservativeness** property also ensure global conservation of the fluid property for the entire domain. This is clearly important physically and is achieved by means of consistent expressions for fluxes of ϕ through the cell faces of adjacent control volumes. The **boundedness** property is akin to stability and requires that in a linear problem without sources the solution is bounded by the maximum and minimum boundary values of the flow variable. Boundedness can be achieved by placing restrictions on