H K Versteeg
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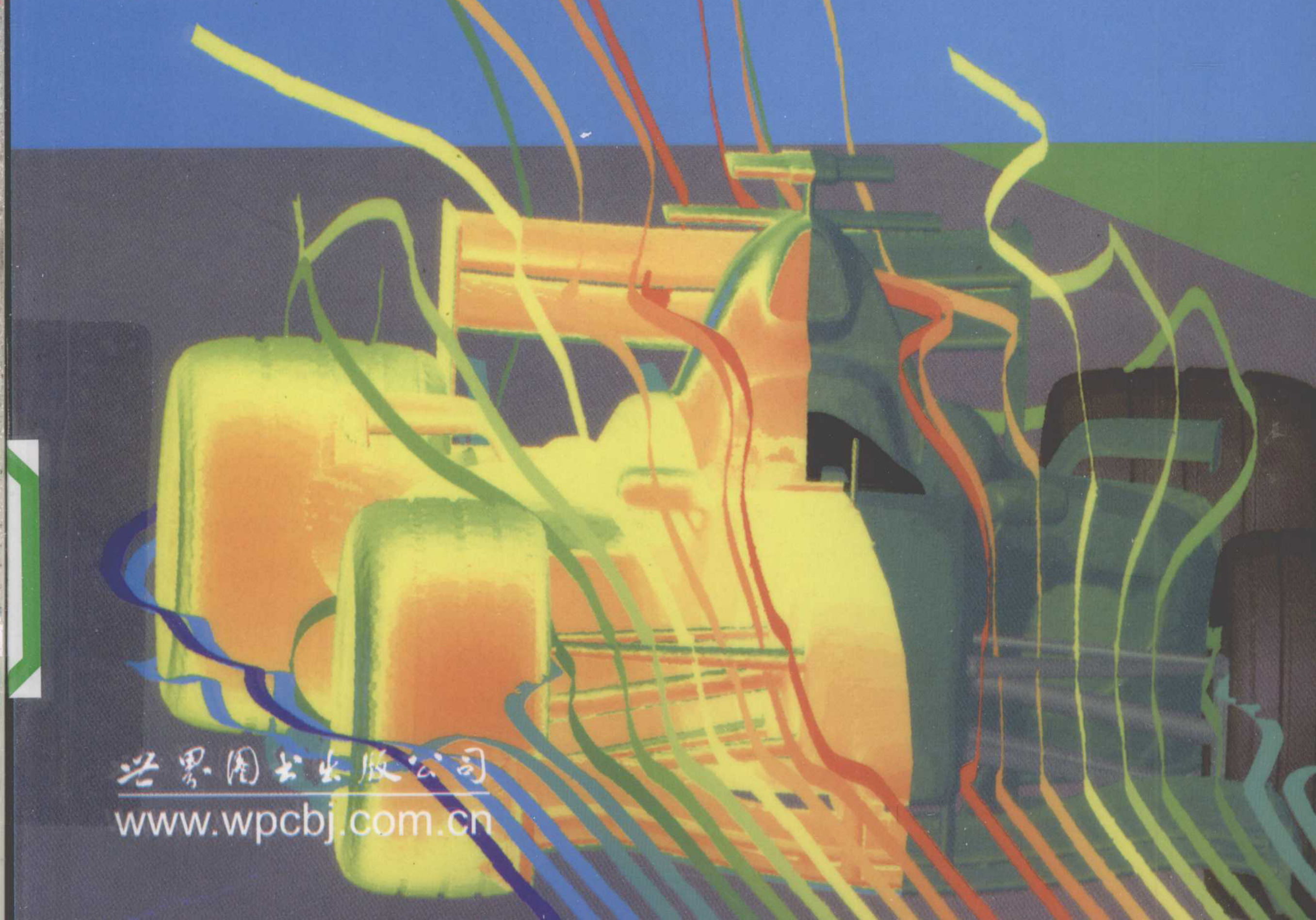
An Introduction to COMPUTATIONAL FLUID DYNAMICS
The Finite Volume Method

second edition

计算流体动力学导论：有限体积法

第2版



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An Introduction to Computational Fluid Dynamics

THE FINITE VOLUME METHOD

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Preface

We were pleasantly surprised by the ready acceptance of the first edition of our book by the CFD community and by the amount of positive feedback received over a period of 10 years. To us this has provided justification of our original plan, which was to provide an accessible introduction to this fast-growing topic to support teaching at senior undergraduate level, post-graduate research and new industrial users of commercial CFD codes. Our second edition seeks to enhance and update. The structure and didactic approach of the first edition have been retained without change, but augmented by a selection of the most important developments in CFD.

In our treatment of the physics of fluid flows we have added a summary of the basic ideas underpinning large-eddy simulation (LES) and direct numerical simulation (DNS). These resource-intensive turbulence prediction techniques are likely to have a major impact in the medium term on CFD due to the increased availability of high-end computing capability.

Over the last decade a number of new discretisation techniques and solution approaches have come to the fore in commercial CFD codes. To reflect these developments we have included summaries of TVD techniques, which give stable, higher-order accurate solutions of convection–diffusion problems, and of iterative techniques and multi-grid accelerators that are now commonly used for the solution of systems of discretised equations. We have also added examples of the SIMPLE algorithm for pressure–velocity coupling to illustrate its workings.

At the time of writing our first edition, CFD was firmly established in the aerospace, automotive and power generation sectors. Subsequently, it has spread throughout engineering industry. This has gone hand in hand with major improvements in the treatment of complex geometries. We have devoted a new chapter to describing key aspects of unstructured meshing techniques that have made this possible.

Application of CFD results in industrial research and design crucially hinges on confidence in its outcomes. We have included a new chapter on uncertainty in CFD results. Given the rapid growth in CFD applications it is difficult to cover, within the space of a single introductory volume, even a small part of the submodelling methodology that is now included in many general-purpose CFD codes. Our selection of advanced application material covers combustion and radiation algorithms, which reflects our local perspective as mechanical engineers with interest in internal flow and combustion.

Finally, we thank colleagues in UK and overseas universities who have encouraged us with positive responses and constructive comments on our first edition and our proposals for a second edition. We are also grateful to several colleagues and postgraduate researchers who have given help in the

development of material, particularly Dr Jonathan Henson, Dr Mamdud Hossain, Dr Naminda Kandamby, Dr Andreas Haselbacher, Murthy Ravikanti-Veera and Anand Odedra.

August 2006
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Chapter one 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 internal combustion 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 with 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 has entered into the wider industrial community since the 1990s.

We estimate the minimum cost of suitable hardware to be between £5,000 and £10,000 (plus annual maintenance costs). The perpetual licence fee for commercial software typically ranges from £10,000 to £50,000 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 person-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.

Below we look at the overall structure of a CFD code and discuss the role of the individual building blocks. 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. We shall be solely concerned with the finite volume method, a special finite difference formulation that is central to the most well-established CFD codes: CFX/ANSYS, FLUENT, PHOENICS and STAR-CD. In outline the numerical algorithm consists of the following steps:

- Integration of the governing equations of fluid flow over all the (finite) control volumes of the domain
- Discretisation – conversion of the resulting 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 the finite element and spectral methods. The conservation of a general flow variable ϕ, e.g. 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:

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

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 by the TDMA (tri-diagonal matrix algorithm) 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 Gauss–Seidel point iterative techniques with multigrid accelerators 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. Due 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 at 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 be aware of all the assumptions, clear-cut and tacit ones, that have been made.

Performing the computation itself requires operator skills of a different kind. Specification of the domain geometry and grid design are the main tasks at the input stage and subsequently the user needs to obtain a successful simulation result. The two aspects that characterise such a result are convergence and grid independence. The solution algorithm is iterative in nature, and in a converged solution the so-called residuals – measures of the overall conservation of the flow properties – are very small. Progress towards a converged solution can be greatly assisted by careful selection of the settings of various relaxation factors and acceleration devices. There are no straightforward guidelines for making these choices since they are problem dependent. Optimisation of the solution speed requires considerable experience with the code itself, which can only be acquired by extensive use. There is no formal way of estimating the errors introduced by inadequate grid design for a general flow. Good initial grid design relies largely on an insight into the expected properties of the flow. A background in the fluid dynamics of the particular problem certainly helps, and experience with gridding of similar problems is also invaluable. The only way to eliminate errors due to coarseness of a grid is to perform a grid dependence study, which is a procedure of successive refinement of an initially coarse grid until certain key results do not change. Then the simulation is grid independent. A systematic search for grid-independent results forms an essential part of all high-quality CFD studies.

Every numerical algorithm has its own characteristic error patterns. Well-known CFD euphemisms for the word 'error' are terms such as numerical diffusion, false diffusion or even numerical flow. The likely error patterns can only be guessed on the basis of a thorough knowledge of the algorithms. At the end of a simulation the user must make a judgement whether the results are 'good enough'. It is impossible to assess the validity of the models of physics and chemistry embedded in a program as complex as a CFD code or the accuracy of its final results by any means other than comparison with experimental test work. Anyone wishing to use CFD in a serious way must realise that it is no substitute for experimentation, but a very powerful additional problem solving tool. Validation of a CFD code requires highly detailed information concerning the boundary conditions of a problem, and generates a large volume of results. To validate these in a meaningful way it is necessary to produce experimental data of similar scope. This may involve a programme of flow velocity measurements with hot-wire anemometry, laser Doppler anemometry or particle image velocimetry. However, if the environment is too hostile for such delicate laboratory equipment or if it is simply not available, static pressure and temperature measurements complemented by pitot-static tube traverses can also be useful to validate some aspects of a flow field.

Sometimes the facilities to perform experimental work may not (yet) exist, in which case the CFD user must rely on (i) previous experience,