COMPUTATIONAL FLUID DYNAMICS

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JOHN WILEY & SONS
New York Chichester Brisbane Toronto Singapore

First Published in 1988
WILLEY EASTERN LIMITED
4835/24 Ansari Road, Daryaganj
New Delhi 110 002. India

Distributors:

Australia and New Zealand:
Jacaranda Wiley Ltd., Jacaranda Press
JOHN WILEY & SONS, INC.
GPO Box 859, Brisbane, Queensland 4001, Australia

Canada:
JOHN WILEY & SONS CANADA LIMITED
22 Worcester Road, Rexdale, Ontario, Canada

Europe and Africa:
JOHN WILEY & SONS LIMITED
Baffins Lane, Chichester, West Sussex, England

South East Asia:
JOHN WILEY & SONS, INC.
05-05, Block B, Union Industrial Building
37 Jalan Pemimpin Singopore 2057

Africa and South Asia:
WILEY EASTERN LIMITED
4835/24, Ansari Road, Daryaganj
New Delhi 110 002, India

North and South America and rest of the world:
JOHN WILEY & SONS, INC.
605 Third Avenue, New York, NY 10158 USA

Library of Congress Cataloging in Publication Data

Bose, T.K. (Tarit Kumar), 1939—
Computational Fluid Dynamics.

Bibliography: p.
1. Aerodynamics—Mathematics. 2. Aerodynamics—Data processing. I. Title.
TL573.B59 1988 629.132'3 87-25308

ISBN 0-470-20953-4 John Wiley & Sons, Inc.
ISBN 0-85226-039-3 Wiley Eastern Limited

Printed in India at Prabhat Press, Meerut.

Computational Fluid Dynamics

Foreword

There has been a revolutionary development in the methodology of design and analysis of engineering systems over the past 15 years, mainly as a result of the digital computer, which possesses capabilities for calculation at break-neck speeds, for storing information, and for making decisions according to pre-programmed criteria. In the field of fluid dynamics, the computer has been posing a serious challenge to the wind tunnel in providing an understanding of fluid flow phenomena.

Whether a computer can render experimental measurements unnecessary has been the subject of an interesting controversy. On the one hand, it is to be remembered that all our descriptions of the physical world, including the equations of motion, rest entirely on observation. All a computer can do is to rearrange the information fed into it, and the information does not acquire extra merit or accuracy by being subjected to a few million arithmetic operations. The value of the computer is that it can handle more complicated descriptions of the physical world than can be handled by analytic methods. While the experimenter has new techniques of conditional sampling, laser anemometry and measurement of pressure fluctuations available to him, advances in CFD, in terms of computing power, have been occurring at such a tremendous pace that a 'fact gap' has arisen, with 'too many computers chasing too few facts'! Bradshaw believes that experiments are the foundation of our understanding and should be the foundation of the prediction methods.

On the other hand, useful research results can be obtained from computer solution of intelligently simplified versions of the time-dependent equations. There are several quantities which are difficult, if not impossible, to measure directly, and 'computer experiments' offer a possible path to understanding.

Concurrent with the increase in the complexity of computational techniques, the role of the user of the computer codes has undergone a tremendous change. No longer it is possible for every user to program the computation procedure himself, and he is forced to accept a program package from the originator. This places alternative responsibilities on the user, who will have to bear the consequences of inadequate prediction. The user must keep in touch with the advances in physical understanding on which the prediction methods are based, so that he can interpret the results and more readily recognize errors. He must recognize that even with the best of codes, the output accuracy is only as good as the input accuracy. Too often the codes are not balanced, in that they have sophisticated numerics and poor models. At the other extreme, an advanced code with all the best physics in it may not be useful if only one calculation can be performed. Thus, as in all other aspects of engineering, CFD involves a compromise between conflicting factors and demands user judgement for optimal solutions.

In order to familiarize the teachers and students of mechanical, aeronautical and chemical engineering with the latest developments in CFD, Professor TARIT BOSE has written this Monograph. He has been active in this field for several years and has utilized all his rich, diverse and direct experience to provide a thorough and lucid presentation. It is hoped that this Monograph will enable the mechanical engineering community to increasingly and effectively utilize CFD techniques in their design and analysis tasks.

DR. B. NATARAJAN
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Preface

In recent years, there has been a phenomenal growth in use of computers for research, design and development to the extent, that we can now dispense with experimental methods in many cases. For aerodynamicists, therefore, *Computational Fluid Dynamics* (CFD) has grown important as a subject, and has come to stay. With the growing popularity of the subject among the scientists, and with growing demand from the students for a good course in the subject, a need was felt for a good text-book encompassing the broad field of the CFD. The present book is, therefore, written to satisfy the need. This book is an outgrowth of lectures given by this author to the undergraduate and graduate students of Aeronautical and Mechanical Engineering and Mathematics at the Indian Institute of Technology, Madras, India. At this stage it is presumed, that the student has a fairly good command of inviscid and viscous flow theories, and he has already undergone courses in numerical mathematics and computer programming. Thus after a short introduction a brief review is presented on some of the important numerical methods, followed by a review of the basic fluiddynamic equations. The latter are rewritten in general orthogonal coordinate system and in body-fitted coordinate system. In Chapter 2, applications of the numerical methods are given for some fluid dynamical problems. Subsequent chapters deal with some of the most current topics of interest: relaxation techniques, time-dependent method, panel method, finite element method, particle-in-cell method, and fluid-in-cell method. For the particle-in-cell method, however, there is need for a good on-line graphic terminal. For both the panel method and the finite element method, one has to deal with very large number of equations, for which large storage requirements in the computer core memory may be a problem. In the case of the finite element method, however, large number of zeros in the coefficient matrix require special methods to handle sparse matrices, and suggestions are made for this.

While a very large number of topics is being discussed in this book, the idea is to expose the reader to a number of topics of current interest. While selecting the topics, there was, of course, the usual dilemma, whether it would not be better to write exhaustive treatise on each of the topics, on which a large number of publications exists, and their number is growing at an explosive rate. It was, however, felt, that within the limited scope of a text book, exposure to various methods will be very much useful, and the reader can always look into other literatures. It must, however, be emphasised at the outset, that these are not the only topics available in the area of *Computational Fluid Dynamics,* althougb these give probably a very good cross-section of problems of current interest. At the time of preparation of the book a number of computer programmes were prepared, but these were admittedly not optimum in terms of the required computation time and memory locations. Hence, it was felt too premature to publish the listings of these subroutines, although, it is suggested that the reader should try to write computer programmes based on description of methods given in this book and try to improve on them.

I would now like to acknowledge help from different people. First, my students had worked out some of the numerical problems in detail and some of their results are presented in this book. Secondly, I had always very fruitful discussions with two of my colleagues, S. Santhakumar and S.C. Rajan, and H.N.V. Dutt of the Hindustan Aeronautics Ltd., Bangalore. Thirdly, the Curriculum Development Centre in Mechanical Engineering Department of IIT Madras has helped in typing and preparation of the original manuscript. Fourthly, I owe graritude to large number of authors for providing reprints, as referred to. Fifthly, I owe my gratitude to the publisher for careful editing, printing and publishing, and accommodating all my wishes. Finally my wife, Preetishree, and children, Mohua, Mayukh and Manjul, had to put up with me during the writing of the book.

T.K. BOSE

Contents

I. Introduction

The subject *Computational Fluid Dynamics* needs both a high-speed computer and efficient computational methods. It will, therefore, not be out of place to review and discuss first the development that took place to bring the subject to the current status. This is said to be composed mainly of 'three elements: aerodynamic (fluid-dynamic) theory, applied mathematics, and computers' (Graves, Jr., 1982).

According to Graves, Jr. (1982), 'Newton gave us the first real insight and mathematical formulation of the basic laws of fluid motion', for example, concepts leading to modern hypersonic theory and speed of sound, and the concept of viscous shear stress proportional to the velocity gradient in the transverse direction. 'Mathematical modeling of ideal fluids progressed expansively after Newton under the intellects of such notables as D'Alembert, Euler, Lagrange, and Helmholtz'. The 20th century saw the invention of an aircraft forcing a rapid expansion of the theory of inviscid and viscous flows by such giants as Prandtl, Joukowski, Kutta, Blasius and Von Karman. While, under the boundary layer type flow, only the integral method of Karman-Pohlhausen was in existence during 1940s, in 1950s and 1960s differential methods to compute laminar boundary layers with large pressure gradient and variable thermophysical and transport properties across the boundary layer were developed. In the 1970s came differential methods to compute two-dimensional and axi-symmetric shear layers (Cebeci and Smith, 1975), which were extended to large free-stream to wall stagnation exthalpy ratios (Bose, 1979) and real gases in a rocket nozzle (Bose, 1978). Some of the models used then to calculate turbulent shear layers were 'zero-equation' but others used one-equation and two-equation models also. The 'zero-equation' model requires a minimum of three equations-continuity, momentum and energy equations—but no differential equation for turbulent terms, for which semi-empirical relations are provided. While, in the 'one-equation' model an additional equation is used for computation of some turbulence properties, the turbulence terms are calculated in the 'two-equation' model from two additional equations, namely, the turbulence kinetic energy and dissipation function equations, provided value of some constants are determined from a known shear layer (Jones and Launder, 1972; Rodi, 1970 and 1982).

For inviscid flows, the first real milestone in the development of modern numerical analysis was the 1928 paper by Courant, Friedrich and Levy, that presented the famous CFL criterion discussed extensively in this book. Later in 1940s, Von Neumann and Richtmeyer collaborated in the development of the artificial viscous method, leading to capturing of shock waves.

There has been an extraordinary development for computation of flow around bodies and channels during the last fifteen years. For introduction to some of the methods developed and being discussed in this book reference may be made to the books of Kuethe and Chow (1976), Chow (1979), Roe (1982), Wirz and Smolderen (1978), and Anderson, Tannehill and Pletcher (1984). However, development of relaxation techniques for steady, transonic flow started actually with the work of Murman and Cole (1971), when they prescribed separate schemes for subsonic and supersonic regions of flow. The method had however, certain deficiencies in maintaining conservation of mass, momentum and energy flux in the shock region, and also the shock region extended to about three or four mesh intervals. Therefore, fully conservative equations with 'shock-point operator' were developed to 'capture' the shock, and subsequently the 'shock-fitting technique' was introduced (Yu, Seebass and Ballhaus, 1978; Hafez and Cheng, 1975; Martin, 1983) to take care of the physically abnormally large shock region. Earlier work of Murman and Cole was further extended by Krupp and Murman (1972), Bailey and Steger (1973), Newman and Klunker (1972), Murman (1974), Bailey and Ballhaus (1975) and others to calculate transonic flows for slender lifting bodies and wings, although the method so far applied is confined basically to supersonic flows in regions near the airfoil, where the coordinate system is closely aligned. In cases, where the flow at infinity is supersonic, the misalignment of coordinates leads to problems, and rotated difference scheme based on the method of characteristics was evolved by Jameson.

In transonic flows, the flow is strongly influenced by the occurrence of shock induced separation. According to Finke (1976), 'the flow mechanism can be explained as follows: When the boundary layer on the rear part of the wing separates, it acts as a flat plate and unsteady pressure distributions are produced in the outer subsonic flow which propagates downstream and upstream. The upstream propagating disturbances meet the shock and force it to move upstream; thereby the region of separation is increased. Near the point of maximum thickness the shock wave degenerates to a Mach wave. The flow becomes subsonic, and shortly thereafter it is accelerated until near the trailing edge the shock wave occurs'. This repeats again, and this unsteady phenomenon called 'buffeting' is part of the unsteady transonic flow.

Investigations of the unsteady flow by the time dependent method have opened a broad new field for study of steady and unsteady flow problems. For steady flows, introduction of the method has made it possible to avoid the problem of matching the elliptic, parabolic and hyperbolic equations at interfaces between subsonic-sonic and sonic-supersonic regions, since the time-dependent equations are always hyperbolic in nature with time. It was, therefore, possible to study not only external flows around bodies, but also internal flows in convergent-divergent nozzles and internal combustion engines. For steady, transonic external flows, the shock is 'captured' in a natural way, although the number of time steps required, owing to the restriction in time step size for stability reasons can be quite large by this method, which further increases for unsteady phenomena, including periodic phenomena. The time step, can, however, be increased by factorization (Ballhaus et. al., 1975 and 1978; Catherall, 1982) and computation in multiple grids.

For steady external flows, both the methods, namely, the transonic relaxation method and the time-dependent method have been used successfully for two and three-dimensional slender bodies. For arbitrary bodies (both the slender and non-slender bodies), however, there are obvious difficulties in satisfying boundary conditions on the surface of the body and the Kutta condition at the trailing edge, which could be removed by such approximate methods like the 'panel method' and the 'finite element method', or by solving the differential equations in body-fitted coordinates. In the panel method linearised flow equations are used for 'pure' subsonic or supersonic flows for 'thickness', 'camber' and 'angle of attack' problems around a complete aircraft including stores and in the neighbourhood of another body. However, the requirement in the panel method to handle very large number of simultaneous equations makes the method somewhat limited since it is very expensive with respect to both time and computer memory requirements. On the other hand, the finite element method requires inversion of very sparse matrices, which are symmetric, and for which special provisions can be made fairly easily. However, the stringent continuity requirement at element boundaries leads to complexities in the use of this method for fluid mechanical problems, and thus, the use of the method for such problems is somewhat limited.

For a completely different class of two-dimensional problems, the particle-in-cell and fluid-in-cell methods are ideal and allow real time observation of simulated flows, provided an on-line plotter is available.

Although the CFD, as Computational Fluid dynamics is popularly called in short form, started developing in the late 1960s and early 1970s, it was made possible technically by development of computing machines. In 1642, Blaise Pascal invented an adding machine, which operated by counting of integers. In 1671, Gottfried Wilhelm Leibnitz invented a machine for multiplication by repeated adding with the help of a 'stepped wheel'. It is, however, noted (Graves, jr., 1982), that Charles Babbage designed his 'analytical machine' around 1820. Babbage is said to have designed a machine that had all the characteristics of a modern computer, including input-output functions, branching and looping of instructions, etc., although Babbage's analytical machine was too advanced for the technology of his time. During the last quarter of the 19th century, however, desk calculators were developed, which were compact, and could perform the four basic arithmetic functions, and which were replaced by electromechanical calculators later.

Electric computers, which were used first in the 1940s in a few research laboratories, have developed fast. In the 1950s, the computers had still vacuum tubes as basic components, and there were only a few special registers, where computations could be made. At this time, the main storage was magnetic drum, and a basic floating point arithmetic took about one-hundredth of a second. The milestone event in electronics, however, occurred in 1948 with the invention of transistors, which replaced vacuum tubes in late 1950s. The computation speed increased to microsecond range, the internal memory was ferrite-core memory, and the magnetic discs, drums and tapes became peripherals. With the development of integrated circuits, a further increase in computation speed and storage space were possible. In the 1980s, the computational speed is being increased further to the order of ten nano-seconds (Kutler, 1983) by having many processors working parallel, while it is expected that by 1990 computers with storage capacities of several hundred billion words and operational speeds of a trillion floating point operations per second may be available. There are also proposals for giant computers with conventional technology—one such proposed giant is NASA's 'National Aerodynamic Simulator' (NAS) with an operational speed of a billion operations per second and a high speed memory of 240 million words (Graves Jr., 1982). These extraordinary increases in the storage capacity and speed of computation has resulted in reduction of the relative computation cost by an order of magnitude in every eight years (Chapman, 1979).

While integrated circuits already place upwards of 260,000 transistors on a single chip, the silicon-based integrated circuit technology is likely to be replaced in near future by gallium-arsenide (GaAs) technology resulting in an order of magnitude increase in the speed. Even as attractive as GaAs technology appears, a new and different form of integrated circuit technology in the form of the superconducting Josephson-junction may increase the computation speed by another two orders of magnitude (Graves, Jr., 1982). In fact, it is reported that by exploiting both GaAs and Josephson-junction technology, Japan is expected to build a computer by 1990 capable of sustained speeds of several hundred billion operations per second.

Thus, according to Chapman (1979), there are several compelling reasons to vigourously develop computational fluid dynamics. Firstly, because of decrease in relative computation cost and better algorithms, there has been an extra-ordinary cost reduction, whereas the cost of experiments is increasing steadily. While at the beginning of the century only about 20 hours of experiment in wind tunnels was adequate, presently a new aircraft needs ten thousand to one-hundred thousand hours of windtunnel time. Thus windtunnel experimentation has become increasingly both expensive and time consuming. Secondly, even after very long hours of experimentation, the results are often doubtful, and for such cases, a computer provides with a powerful, independent research tool to gain new technological capabilities. For example in transonic speed range, the pressure distribution and the flow separation on a body are very much dependent on Reynolds number, and there is a large gap between the actual Reynolds number in flight and the Reynolds number capability of windtunnels. Similarly, the windtunnels have rarely been able to simulate Reynolds number of atmospheric flight, aerodynamics of probes entering planetary atmospheres, flow and temperature field around atmospheric entry vehicles, propulsion-external flow interaction in flight, flow fields between rotating blades, etc.

Thus, the subject *Computational Fluid Dynamics* has come to stay as one of the most important subjects.

1.1 Basic Fluid Dynamic Equations

Basic fluid dynamic equations, being introduced now, are the equations of continuity, momentum and energy. These equations and their derivation are given in all text books of fluid dynamics, and hence, only the summary of results are presented. The equations are written in Cartesian coordinate system, and the underlying assumptions are: (1) the gas is a single component gas, (2) there is no volume force acting on it, and (3) the gas is not radiating. Thus the basic equations are as follows:

(a) *Equation of continuity*

If $\mathbf{V} = \mathbf{V}\{u, v, w\}$ is the velocity vector with velocity components u, v, w in the Cartesian coordinate system $\{x, y, z\}$ and in time t, the equation of continuity is written as follows:

$$\rho_t + (\rho u)_x + (\rho v)_y + (\rho w)_z = 0 \tag{1.1}$$

In Eq. (1.1), ρ is the density, and the subscripts t, x, y and z denote partial derivatives with respect to these independent variables. It is obvious, that for the incompressible case (ρ = constant, $\rho_t = 0$), Eq. (1.1) becomes

$$u_x + v_y + w_z = 0 \tag{1.1a}$$

(b) *Equation of momentum*

Equation for x-component of momentum is

$$(\rho u)_t + (\rho u^2)_x + (\rho uv)_y + (\rho uw)_z = \text{div}\,\boldsymbol{\tau} \tag{1.2}$$

where

$$\tau^{rs} = (-p - 2/3\mu\,\text{div}\,\mathbf{V})\,\delta^{rs} + \mu(V_r^s + V_s^r) \tag{1.2a}$$

In Eq. (1.2a) subscripts refer to partial derivatives and superscripts refer to components in s and r directions. Further, p is the pressure, μ is the (dynamic) viscosity coefficient and δ^{rs} is the Kroneker delta with the following values; r = s: $\delta^{rr} = 1$, r $\neq$ s: $\delta^{rs} = 0$. Thus in Cartesian coordinate system Eq. (1.2) becomes

$$(\rho u)_t + (\rho u^2)_x + (\rho uv)_y + (\rho uw)_z = -p_x + 2(\mu u_x)_x + [\mu(u_y + v_x)]_y + [\mu(u_z + w_x)]_z - (2/3)[\mu(u_x + v_y + w_z)]_x \tag{1.3}$$

There are, of course, similar momentum equations for y- and z-components. For incompressible flow, the right hand side of Eq. (1.3) becomes

$$-p_x + \mu(u_{xx} + u_{yy} + u_{zz}) \tag{1.4a}$$

and further, the left hand side of Eq. (1.3) can be simplified with the help of Eq. (1.1) to become

$$\rho[u_t + uu_x + vu_y + wu_z] \tag{1.4b}$$

(c) *Equation of kinetic energy*

Multiplying the momentum equation with the respective velocity component, and adding over all components, we get

$$q_t + (uq)_x + (vq)_y + (wq)_z = u \operatorname{div} \tau^{xs} + v \operatorname{div} \tau^{ys} + w \operatorname{div} \tau^{zs} \tag{1.5}$$

where $q = \rho V^2/2$.

(d) *Equation of energy*

Equation of energy is written in terms of the total internal energy $e^0 = e + V^2/2$, where e is the internal energy, and is as follows:

$$(\rho e^0)_t + (\rho e^0 u)_x + (\rho e^0 v)_y + (\rho e^0 w)_z = (kT_x)_x + (kT_y)_y + (kT_z)_z + \operatorname{div}(u\tau^{xs}) + \operatorname{div}(v\tau^{ys}) + \operatorname{div}(w\tau^{zs}) \tag{1.6}$$

In the above equation k is the heat conductivity coefficient and T is the temperature.

Subtracting Eq. (1.5) from Eq. (1.6), we get

$$(\rho e)_t + (\rho ue)_x + (\rho ve)_y + (\rho we)_z = (kT_x)_x + (kT_y)_y + (kT_z)_z - p \operatorname{div} \mathbf{V} + \phi \tag{1.7}$$

in which the dissipation function ϕ is given by the relation

$$\phi = -(2/3)\mu(u_x + v_y + w_z)^2 + 2\mu(u_x^2 + v_y^2 + w_z^2) + \mu[(v_x + u_y)^2 + (w_x + u_z)^2 + (w_y + v_z)^2] \tag{1.7a}$$

Noting the relationship between the static enthalpy, h, the total enthalpy, h^0, and the respective internal energies

$$h = e + p/\rho;\ h^0 = e^0 + p/\rho$$

We can write

$$(\rho e)_t + (\rho ue)_x + (\rho ve)_y + (\rho we)_z = (\rho h)_t + (\rho uh)_x + (\rho vh)_y + (\rho wh)_z - (up)_x - (vp)_y - (wp)_z$$

and

$$(\rho e^0)_t + (\rho ue^0)_x + (\rho ve^0)_y + (\rho we^0)_z = (\rho h^0)_t + (\rho uh^0)_x + (\rho vh^0)_y + (\rho wh^0)_z - (up)_x - (vp)_y - (wp)_z$$

Further, defining a 'substantial derivative'

$$D(\ )/Dt = (\ )_t + u(\ )_x + v(\ )_y + w(\ )_z$$

Equations (1.6) and (1.7), in terms of static and total enthalpy, h and h^0, respectively, become