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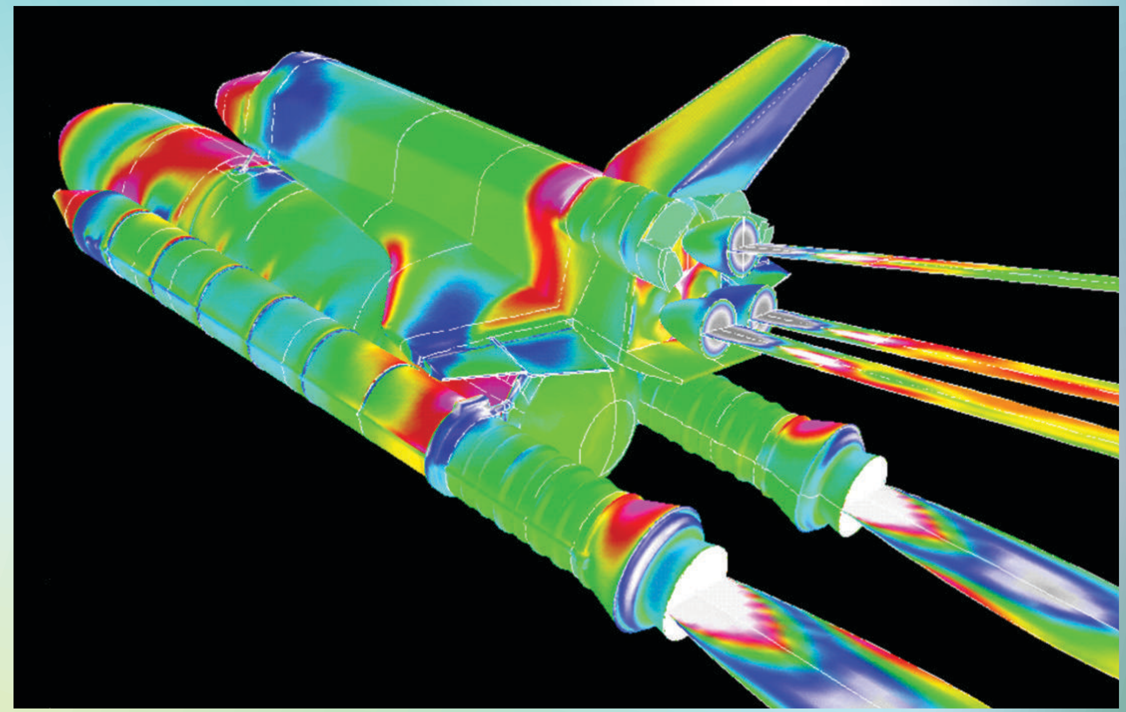

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John C. Tannehill
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Computational Fluid Mechanics and Heat Transfer

Fourth Edition

Dale A. Anderson, John C. Tannehill,
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and Vijaya Shankar

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Preface to the Fourth Edition

It has been another 7 years since the third edition of this textbook was published. In that time, application of numerical methods to engineering problems has been substantially expanded. This expansion has been supported by increases in computational power and speed as well as improvements in available algorithms. Perhaps the largest increase in capability has been provided by the advent of multicore processors and recent use of graphics processors as computational engines. These improvements have encouraged application of digital simulation methods to solve more complex problems on a much larger scale. More detailed computations of flows using complex models for realistic configurations have evolved where advanced turbulence models or, in some cases, direct simulation of turbulence is now within the realm of possibility. Multiphase and multifluid flow problems are now solved on a routine basis and include methods for tracking moving boundaries.

The trend of using commercial software for computational fluid dynamics (CFD) applications has continued. Companies find it financially more prudent to use commercial codes rather than invest in developing new software. This trend will continue with applications being the largest share of effort using digital simulation involving CFD. Organizations usually have a suite of codes that are considered to be their standard resource base for solving certain classes of problems. Engineers are charged with the responsibility of altering these resource codes to solve new problems and extend their use beyond their original range of applicability. There is also a large research effort targeting applications of numerical techniques to new problems. The goal of the present text is to prepare those working in the area of CFD to be able to modify existing codes, write new codes, and interpret results produced by digital simulation.

The format of the fourth edition of the text retains the same two-part division of the previous editions. The first four chapters concentrate on introducing fundamental ideas, while the last seven chapters are primarily focused on applications. No commercial software is employed in the text. Students are expected to write code to solve numerous homework problems in order to gain an understanding of how code is written and to interpret results produced by that code. This experience will assist in understanding if results are physically reasonable and also to identify possible errors that are introduced due to inadequacies in engineering models or its discrete representation. The numerous homework problems included in this text provide the necessary experience to achieve this end. It is essential that students spend significant time writing code and interpreting results in order to better understand the application of CFD in solving problems. This is a field where there is no substitute for experience.

Modifications to the previous edition have been made in both the fundamental and application sections of the text. Chapter 1 has been expanded to include recent developments in CFD methods. A comprehensive list of recommended references on a variety of physical problems encountered in digital simulation in heat transfer and fluid mechanics has been added. Chapter 2 remains as printed in the third edition. Chapter 3 now includes introductory material on finite-element methods. Selection of basis functions and error estimates are discussed, and the Galerkin and discontinuous Galerkin methods are presented. Additional details on heat and mass transfer across interfaces when multiple materials are encountered have been added to Chapter 4, and applications using finite-element schemes are included. Governing equations are presented in Chapter 5, where additional material has been included on flows with real gas chemistry. Basic ideas applied to free-surface flows, front tracking methods, and free convection have been added. Chapters 6 through 8 remain as presented in the third edition. Chapter 9 now includes expanded calculations for several classical problems in fluid mechanics. These include the driven cavity, cavity with free convection, and channel flow. Examples of free-surface flows including the broken dam problem are also included. Additions to Chapter 10 are mainly focused on generating higher-order meshing strategies that may contribute to a reduction of error in large-scale simulations. Chapter 11 has been added and addresses the impact of modern computer architecture on CFD. A review of recent progress in computer hardware and evolving computer languages is included. Appendix C from the third edition has been retained, while Appendices A and B, tridiagonal algorithms, have been eliminated. These packages are readily available as open source programs, or they can be found on the website associated with this text at https://www.routledge.com/9780815357124.

Additional material has been included in this edition, but rather little has been eliminated. There are two reasons for retaining the original form and substance of the previous edition. As time has progressed, students encountered in CFD courses appear to have a weaker foundation in classical fluid mechanics, heat transfer, and aerodynamics. For this reason, fundamental material on these areas has been retained. In the area of numerical methods, classical schemes that reveal the historical development of CFD are used as teaching aids in helping students learn code preparation and interpretation of results produced by computer simulations. For this reason, the historically important methods and ideas have also been retained.

In this edition, two new authors have been added. Dr. Vijaya Shankar and Dr. Ramakanth Munipalli both share the same CFD legacy as the original team. They bring perspectives from present-day developments and industrial applications to the material in the text. The additions to the present text are consistent with the goals of the previous editions and provide students with background in areas that are of current interest. As in the past editions, it is hoped that the ideas and concepts included in this book are fundamental and will continue to form a basic framework for students studying CFD.

This textbook is dedicated to Richard (Dick) Pletcher. Dick passed away unexpectedly in 2015 after the publication of the third edition and prior to the start of work on the present edition. The remaining original authors, Dale Anderson and John Tannehill, worked closely with Dick beginning in the 1970s in creating and teaching a two-semester sequence of courses in CFD at Iowa State University. The class notes that resulted from this sequence of courses formed the basis for the first edition of this textbook published in 1984. During his professional career, Dick was a major influence in shaping the lives of many of his students. He mentored them through advanced degree programs and instilled in them his carefully disciplined approach to research and teaching. He was an accomplished researcher, teacher, and a prolific author and lecturer. We remember Dick as our friend and colleague whose presence in the lives of others was always a positive factor. He was a kind, creative, hard-working man whose life was an inspiration to all who knew him.

Dale A. Anderson
John C. Tannehill
Ramakanth Munipalli
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Preface to the Third Edition

Another 15 years have gone by since the second edition of this text appeared. During this period, the rate of development in algorithms has slowed compared to any earlier period, but the increase in computational power has been astounding and shows no sign of slowing. Desktop computers can outperform the supercomputers of the early 1990s. The rate of improvement of computing power is such that a problem that required a year of computing time to solve 10 years ago can now be solved overnight. The increase in computing power has enabled engineers to solve more complete equations and complex geometries for aerodynamic flows, i.e., use less physical modeling and fewer approximations. It has also motivated efforts to compute more complex physical phenomena such as turbulence and multiphase flows.

Another clear trend is the increasing use of commercial software for computational fluid dynamics (CFD) applications. In the early days, CFD was mostly a do-it-yourself enterprise. It is more likely now that a CFD code is thought of as representing a large investment, and companies do not launch into writing a new one without considerable thought. It is more likely that CFD engineers will become involved in modifying or extending an existing code than in writing a new code from "scratch." However, even making modifications to CFD codes requires knowledge of algorithms, general numerical strategies, and programming skills. The text promotes programming skills by explaining algorithm details and including homework problems that require programming. Even those engineers that will utilize commercial codes and be responsible for interpreting the results will be better prepared as a result of the knowledge and insight gained from developing codes themselves. It is very important for engineers to know the limitations of codes and to recognize when the results are not plausible. This will not change in the future. The experience gained by writing and debugging codes will contribute toward the maturity needed to wisely use and interpret results from CFD codes.

It is essential that courses evolve as technology advances and new knowledge comes forth. However, not every new twist will have a permanent impact on the discipline. Fads die out, and some numerical approaches will become obsolete as computing power relentlessly advances. The authors have included a number of new developments in this edition while preserving the fundamental elements of the discipline covered in earlier editions. A number of ideas and algorithms that are now less frequently utilized due to advances in computer hardware or numerical algorithms are retained so that students and instructors can gain a historical perspective of the discipline. Such material can be utilized at the discretion of the instructor. Thirty-four new homework problems have been added bringing the total number of homework problems to 376.

We have retained the two-part, ten-chapter format of the text. Additions and clarifications have been made in all chapters. Part I, consisting of Chapters 1 through 4, deals with the basic concepts and fundamentals of the finite-difference and finite-volume methods. The historical perspective in Chapter 1 has been expanded. The sections on the finite-volume method in Chapter 3 have been revised and expanded. The conjugate gradient and generalized minimal residual (GMRES) methods are now discussed in the section on Laplace's equation in Chapter 4. Part II, consisting of Chapters 5 through 10, covers applications to the equations of fluid mechanics and heat transfer. The governing equations are presented in Chapter 5. The equations for magnetohydrodynamic (MHD) flows and the quasi-one-dimensional form of the Euler equations are now included. Turbulence modeling has been updated. The coverage of large-eddy simulation (LES) has been expanded, and detached eddy simulation (DES) has been introduced. In Chapter 8, the material on the parabolized Navier–Stokes (PNS) equations has been expanded to include methods for handling flow fields with significant upstream influences, including large streamwise separated regions. A number of updates and additions are found in Chapter 9. Coverage of Runge–Kutta schemes, residual smoothing, and the lower–upper symmetric Gauss–Seidel (LU-SGS) scheme has been expanded. Some recent variations in time-accurate implicit schemes are also included.

We continue to be grateful for the help received from many colleagues and past students while this material was developed and revised. We especially thank Zhaohui Qin for his help with several new figures and with updates to several appendices. Finally, we would like to thank our families for their patience and encouragement during the preparation of this third edition.

This text continues to be a collective work by the three of us. There is no junior or senior author. The order of the authors for the previous two editions was determined by coin flips. Anderson and Tannehill were named the first author on the previous two editions, and Pletcher is the first author on the current work.

Richard H. Pletcher
John C. Tannehill
Dale A. Anderson

Preface to the Second Edition

Almost 15 years have passed since the first edition of this book was written. During the intervening years, the literature in computational fluid dynamics (CFD) has expanded manyfold. Due, in part, to greatly enhanced computer power, the general understanding of the capabilities and limitations of algorithms has increased. A number of new ideas and methods have appeared. We have attempted to include new developments in this second edition while preserving those fundamental ideas covered in the first edition that remain important for mastery of the discipline. Ninety-five new homework problems have been added. The two-part, ten-chapter format of the book remains the same, although a shift in emphasis is evident in some of the chapters. The book is still intended to serve as an introductory text for advanced undergraduates and/or first-year graduate students. The major emphasis of the text is on finite-difference/finite-volume methods.

Part I, consisting of Chapters 1 through 4, presents basic concepts and introduces the reader to the fundamentals of finite-difference/finite-volume methods. Part II, consisting of Chapters 5 through 10, is devoted to applications involving the equations of fluid mechanics and heat transfer. Chapter 1 serves as an introduction and gives a historical perspective of the discipline. This chapter has been brought up to date by reflecting the many changes that have occurred since the introduction of the first edition. Chapter 2 presents a brief review of those aspects of partial differential equation theory that have important implications for numerical solution schemes. This chapter has been revised for improved clarity and completeness. Coverage of the basics of discretization methods begins in Chapter 3. The second edition provides a more thorough introduction to the finite-volume method in this chapter. Chapter 4 deals with the application of numerical methods to selected model equations. Several additions have been made to this chapter. Treatment of methods for solving the wave equation now includes a discussion of Runge–Kutta schemes. The Keller box and modified box methods for solving parabolic equations are now included in Chapter 4. The method of approximate factorization is explained and demonstrated. The material on solution strategies for Laplace's equation has been revised and now contains an introduction to the multigrid method for both linear and nonlinear equations. Coloring schemes that can take advantage of vectorization are introduced. The material on discretization methods for the inviscid Burgers equation has been substantially revised in order to reflect the many developments, particularly with regard to upwind methods, that have occurred since the material for the first edition was drafted. Schemes due to Godunov, Roe, and Engquist and Osher are introduced. Higher-order upwind and total variation diminishing (TVD) schemes are also discussed in the revised Chapter 4.

The governing equations of fluid mechanics and heat transfer are presented in Chapter 5. The coverage has been expanded in several ways. The equations necessary to treat chemically reacting flows are discussed. Introductory information on direct and large-eddy simulation of turbulent flows is included. The filtered equations used in large-eddy simulation as well as the Reynolds-averaged equations are presented. The material on turbulence modeling has been augmented and now includes more details on one- and two-equation and Reynolds stress models as well as an introduction to the subgrid-scale modeling required for large-eddy simulation. A section has been added on the finite-volume formulation, a discretization procedure that proceeds from conservation equations in integral form.

Chapter 6 on methods for the inviscid flow equations is probably the most extensively revised chapter in the second edition. The revised chapter contains major new sections on flux splitting schemes, flux difference splitting schemes, the multidimensional case in generalized coordinates, and boundary conditions for the Euler equations. The chapter includes a discussion on implementing the integral form of conservation statements for arbitrarily shaped control volumes, particularly triangular cells, for two-dimensional applications.

Chapter 7 on methods for solving the boundary-layer equations includes new example applications of the inverse method, new material on the use of generalized coordinates, and a useful coordinate transformation for internal flows. In Chapter 8, methods are presented for solving simplified forms of the Navier–Stokes equations including the thin-layer Navier–Stokes (TLNS) equations, the parabolized Navier–Stokes (PNS) equations, the reduced Navier–Stokes (RNS) equations, the partially parabolized Navier–Stokes (PPNS) equations, the viscous shock layer (VSL) equations, and the conical Navier–Stokes (CNS) equations. New material includes recent developments on pressure relaxation, upwind methods, coupled methods for solving the partially parabolized equations for subsonic flows, and applications.

Chapter 9 on methods for the "complete" Navier–Stokes equations has undergone substantial revision. This is appropriate because much of the research and development in CFD since the first edition appeared has been concentrated on solving these equations. Upwind methods that were first introduced in the context of model and Euler equations are described as they extend to the full Navier–Stokes equations. Methods to efficiently solve the compressible equations at very low Mach numbers through low Mach number preconditioning are described. New developments in methods based on derived variables, such as the dual potential method, are discussed. Modifications to the method of artificial compressibility required to achieve time accuracy are developed. The use of space-marching methods to solve the steady Navier–Stokes equations is described. Recent advances in pressure-correction (segregated) schemes for solving the Navier–Stokes equations such as the use of nonstaggered grids and the pressure-implicit with splitting of operators (PISO) method are included in the revised chapter.

Grid generation, addressed in Chapter 10, is another area in which much activity has occurred since the appearance of the first edition. The coverage has been broadened to include introductory material on both structured and unstructured approaches. Coverage now includes algebraic and differential equation methods for constructing structured grids and the point insertion and advancing front methods for obtaining unstructured grids composed of triangles. Concepts employed in constructing hybrid grids composed of both quadrilateral cells (structured) and triangles, solution adaptive grids, and domain decomposition schemes are discussed.

We are grateful for the help received from many colleagues, users of the first edition, and others while this revision was being developed. We especially thank our colleagues Ganesh Rajagopalan, Alric Rothmayer, and Ijaz Parpia. We also continue to be indebted to our students, both past and present, for their contributions. We would like to acknowledge the skillful preparation of several new figures by Lynn Ekblad. Finally, we would like to thank our families for their patience and continued encouragement during the preparation of this second edition.

This text continues to be a collective work by the three of us. There is no junior or senior author. A coin flip determined the order of authors for the first edition, and a new coin flip has determined the order of authors for this edition.

John C. Tannehill
Dale A. Anderson
Richard H. Pletcher

Preface to the First Edition

This book is intended to serve as a text for introductory courses in computational fluid mechanics and heat transfer (or, synonymously, computational fluid dynamics [CFD]) for advanced undergraduates and/or first-year graduate students. The text has been developed from notes prepared for a two-course sequence taught at Iowa State University for more than a decade. No pretense is made that every facet of the subject is covered, but it is hoped that this book will serve as an introduction to this field for the novice. The major emphasis of the text is on finite-difference methods.

The book has been divided into two parts. Part I, consisting of Chapters 1 through 4, presents basic concepts and introduces the reader to the fundamentals of finite-difference methods. Part II, consisting of Chapters 5 through 10, is devoted to applications involving the equations of fluid mechanics and heat transfer. Chapter 1 serves as an introduction, while a brief review of partial differential equations is given in Chapter 2. Finite-difference methods and the notions of stability, accuracy, and convergence are discussed in Chapter 3.

Chapter 4 contains what is perhaps the most important information in the book. Numerous finite-difference methods are applied to linear and nonlinear model partial differential equations. This provides a basis for understanding the results produced when different numerical methods are applied to the same problem with a known analytic solution.

Building on an assumed elementary background in fluid mechanics and heat transfer, Chapter 5 reviews the basic equations of these subjects, emphasizing forms most suitable for numerical formulations of problems. A section on turbulence modeling is included in this chapter. Methods for solving inviscid flows using both conservative and nonconservative forms are presented in Chapter 6. Techniques for solving the boundary-layer equations for both laminar and turbulent flows are discussed in Chapter 7. Chapter 8 deals with equations of a class known as the "parabolized" Navier–Stokes equations, which are useful for flows not adequately modeled by the boundary-layer equations, but not requiring the use of the full Navier–Stokes equations. Parabolized schemes for both subsonic and supersonic flows over external surfaces and in confined regions are included in this chapter. Chapter 9 is devoted to methods for the complete Navier–Stokes equations, including the Reynolds-averaged form. A brief introduction to methods for grid generation is presented in Chapter 10 to complete the text.

At Iowa State University, this material is taught to classes consisting primarily of aerospace and mechanical engineers, although the classes often include students from other branches of engineering and earth sciences. It is our experience that Part I (Chapters 1 through 4) can be adequately covered in a one-semester, three-credit-hour course. Part II contains more information than can be covered in great detail in most one-semester, three-credit-hour courses. This permits Part II to be used for courses with different objectives. Although we have found that the major thrust of each of Chapters 5 through 10 can be covered in one semester, it would also be possible to use only parts of this material for more specialized courses. Obvious modules would be Chapters 5, 6, and 10 for a course emphasizing inviscid flows or Chapters 5 and 7 through 9 (and perhaps 10) for a course emphasizing viscous flows. Other combinations are clearly possible. If only one course can be offered in the subject, choices also exist. Part I of the text can be covered in detail in the single course, or, alternatively, only selected material from Chapters 1 through 4 could be covered as well as some material on applications of particular interest from Part II. The material in the text is reasonably broad and should be appropriate for courses having a variety of objectives.

For background, students should have at least one basic course in fluid dynamics, one course in ordinary differential equations, and some familiarity with partial differential equations. Of course, some programming experience is also assumed.

The philosophy used throughout the CFD course sequence at Iowa State University and embodied in this text is to encourage students to construct their own computer programs. For this reason, "canned" programs for specific problems do not appear in the text. Use of such programs does not enhance basic understanding necessary for algorithm development. At the end of each chapter, numerous problems are listed that necessitate numerical implementation of the text material. It is assumed that students have access to a high-speed digital computer.

We wish to acknowledge the contributions of all of our students, both past and present. We are deeply indebted to F. Blottner, S. Chakravarthy, G. Christoph, J. Daywitt, T. Hoist, M. Hussaini, J. Ievalts, D. Jespersen, O. Kwon, M. Malik, J. Rakich, M. Salas, V. Shankar, R. Warming, and many others for helpful suggestions for improving the text. We would like to thank Pat Fox and her associates for skillfully preparing the illustrations. A special thanks to Shirley Riney for typing and editing the manuscript. Her efforts were a constant source of encouragement. To our wives and children, we owe a debt of gratitude for all of the hours stolen from them. Their forbearance is greatly appreciated.

Finally, a few words about the order in which the authors' names appear. This text is a collective work by the three of us. There is no junior or senior author. The final order was determined by a coin flip. Despite the emphasis of finite-difference methods in the text, we resorted to a "Monte Carlo" method for this determination.

Dale A. Anderson
John C. Tannehill
Richard H. Pletcher

Authors

Dale A. Anderson received his BS from Parks College of Saint Louis University, St. Louis, Missouri, and his MS and PhD from Iowa State University, Ames, Iowa. He is currently professor emeritus at The University of Texas at Arlington. Prior to joining The University of Texas at Arlington, he was a professor of aerospace engineering and director of the Computational Fluid Dynamics Institute at Iowa State University. While at The University of Texas at Arlington, he served in various capacities, including professor of aerospace engineering, associate dean of the College of Engineering, dean of graduate studies, and vice president for research. Professor Anderson has served as a consultant or has held full-time positions with Lockheed-Martin, The Boeing Company, Aerospace Corporation, General Dynamics, British Petroleum, U.S. Air Force, Union Carbide, FMC and the Viskase Corporation. He has served as principal investigator on numerous grants and contracts and has published papers in diverse areas, including numerical methods, fluid dynamics, grid generation, reservoir simulation, and biomedical applications. Professor Anderson is an associate fellow of the American Institute of Aeronautics and Astronautics and has received numerous awards for his contributions to teaching and research, including the Oliver L. Parks Award from Saint Louis University, the Professional Achievement Citation in Engineering from Iowa State University, the Haliburton Award for Excellence in Teaching, and the Haliburton Award for Outstanding Research from The University of Texas at Arlington.

John C. Tannehill began his career as an assistant professor of Aerospace Engineering at Iowa State University, Ames, Iowa, in 1969, was promoted to full professor in 1979, and is currently an emeritus professor. He is recognized as a pioneer in the field of computational fluid dynamics (CFD). Along with Dale Anderson and Richard Pletcher, he designed and implemented the first CFD courses at Iowa State University in 1972. These courses led to the first edition of this textbook in 1984. Professor Tannehill is internationally recognized for his research in computing high-speed flows using the complete or parabolized Navier–Stokes equations. He has been actively involved with NASA in developing CFD computer codes for many projects, including the Space Shuttle, the National Aerospace Plane (X-30), the High-Speed Civil Transport, and the Hyper-X Research Vehicle (X-43A). Professor Tannehill was the director of the CFD Center at Iowa State University from its establishment in 1984 to 2006. He is a fellow of the American Institute of Aeronautics and Astronautics and has received numerous other awards, including the Iowa General Assembly Excellence in Teaching Award and the Boylan Eminent Faculty Award for Research.

Richard H. Pletcher received his BS degree from Purdue University and his MS and PhD degrees from Cornell University and was a professor emeritus of mechanical engineering and the director of the Computational Fluid Dynamics Center at Iowa State University. Prior to joining Iowa State, he worked as a senior research engineer in the Propulsion Section at the United Aircraft Research Laboratories, East Hartford, Connecticut. While on the faculty at Iowa State University, Professor Pletcher received awards for both teaching and research. In 2009, he received the American Society of Mechanical Engineers Heat Transfer Memorial Award in Science. He served as associate editor of the *Journal of Heat Transfer* and was on the editorial advisory board for *Numerical Heat Transfer*. Professor Pletcher conducted basic and applied studies over a wide range of topics in fluid dynamics and heat transfer. He served as principal investigator for numerous research grants from sponsors such as NSF, NASA, the Army Research Office, Allison Gas Turbines, and the Air Force Office of Scientific Research and was a consultant to industry and government. He served as a major or co-major professor for 33 PhD and 17 MS students. He was a life fellow of the American Society of Mechanical Engineers and an associate fellow of the American Institute of Aeronautics and Astronautics. Professor Pletcher passed away in 2015.

Ramakanth Munipalli received his BTech from IIT Madras (India), MS and PhD from The University of Texas at Arlington, all in aerospace engineering. He is currently a senior aerospace research engineer at the U.S. Air Force Research Laboratory (Edwards AFB). Previously, he was a senior computational physicist at HyPerComp, Inc. in Westlake Village, California. At AFRL, his work is mainly in the application of model reduction and data science techniques to high-fidelity CFD in aerospace propulsion. At HyPerComp, Inc., he has worked on computational magnetohydrodynamics, simulations of turbulent combustion, and high-order accurate solver development. His research was supported by DoE, DoD, and various private companies and has included extensive collaboration with experts from academia.

Vijaya Shankar received his BTech from the Indian Institute of Technology in Kharagpur in 1972 and his PhD in aerospace engineering from Iowa State University in 1977. He started his career with Rockwell Science Center in 1976 and became the director of computational sciences in 1987. He left Rockwell in 1998 to form HyPerComp, a software company that specializes in high-performance computing in multidisciplinary technologies catering to defense and commercial markets. For his many significant contributions to computational fluid dynamics, electromagnetics, and other disciplines, Dr. Shankar received numerous awards, including the Lawrence Sperry award and the Dryden Research Lectureship from AIAA, the NASA Public Service award, and the Rockwell Engineer of the Year. For his work in time-domain modeling of electromagnetic wave propagation for stealth applications, Dr. Shankar received the Computerworld Smithsonian Award in Science in 1993. Dr. Shankar is a fellow of AIAA.

Part I

Fundamentals

1

Introduction

1.1 General Remarks

The development of the high-speed digital computer during the 20th century has had a great impact on the way principles from the sciences of fluid mechanics and heat transfer are applied to problems of design in modern engineering practice. Problems that would have taken years to work out with the computational methods and computers available 50 years ago can now be solved at very little cost in a few seconds of computer time. This does not mean that computer runs today only last a few seconds. Instead, many computer tasks today take days of CPU time as the scope of problems that can be tackled have increased immensely. We still need even more computer power to accurately simulate the many flows that require evaluation for the design of modern vehicles, engines, processing equipment, etc.

The ready availability of previously unimaginable computing power has stimulated many changes. These were first noticeable in industry and research laboratories, where the need to solve complex problems was the most urgent. More recently, changes brought about by the computer have become evident in nearly every facet of our daily lives. In particular, we find that computers are widely used in the educational process at all levels. Many a child has learned to recognize shapes and colors from mom and dad's computer screen before they could walk. To take advantage of the power of the computer, students must master certain fundamentals in each discipline that are unique to the simulation process. It is hoped that the present textbook will contribute to the organization and dissemination of some of this information in the fields of fluid mechanics and heat transfer.

The steady advances in computer technology over the past half century have resulted in the creation of a new methodology for attacking complex problems in fluid mechanics and heat transfer. This new methodology has become known as computational fluid dynamics (CFD). In this computational (or numerical) approach, the equations (usually in partial differential or integral form) that govern a process of interest are solved numerically. Some of the ideas are very old. First, there must be conservation principles and physical understanding. This goes back to pioneers such as Archimedes (287–312 BC), Newton (1643–1727), Bernoulli (1700–1782), Euler (1707–1783), Navier (1785–1836), and Stokes (1819–1903). Even work on numerical methods goes back at least to the time of Newton. The English mathematician Brook Taylor developed the calculus of finite differences in 1715. Work on the development and application of numerical methods, especially finite-difference methods for solving ordinary and partial differential equations, intensified starting approximately with the beginning of the 20th century. The automatic digital computer was invented by Atanasoff in the late 1930s (see Gardner, 1982; Mollenhoff, 1988) and was used from nearly the beginning to solve problems in fluid dynamics. Still, these events alone did not revolutionize engineering practice. The explosion in computational activity did not begin until a third ingredient, general availability of high-speed digital computers, occurred in the 1960s.

Traditionally, both experimental and theoretical methods have been used to develop designs for equipment and vehicles involving fluid flow and heat transfer. With the advent of the digital computer, a third method, the numerical approach, has become available. Although experimentation continues to be important, especially when the flows involved are very complex, the trend is clearly toward greater reliance on computer-based predictions in design.

This trend can be largely explained by economics (Chapman, 1979). Over the years, computer speed has increased much more rapidly than computer costs. The net effect has been a phenomenal decrease in the cost of performing a given calculation. This is illustrated in Figure 1.1, where it is seen that the cost of performing a given calculation was reduced by approximately a factor of 10 every 8 years up through 1995. (Compare this with the trend in the cost of peanut butter in the past 8 years.) This trend in the cost of computations was based on the use of the best serial or vector computers available. It is true not every user will have easy access to the most recent computers, but increased access to very capable computers is another trend that started with the introduction of personal computers and workstations in the 1980s. The cost of performing a calculation on desktop computers has dropped by a great deal more than a factor of 10 in the most recent 8-year period (2010–2018). This cost reduction is primarily due to the advent of multicore processors and graphics processing units that enable teraflop (10^{12} FLOPS) performance in personal computers. For example, the intel i9 processor (with 18 cores) is advertised as the first teraflop chip for desktop use (https://www.popsci.com/intel-teraflop-chip), easily outperforming the multimillion dollar Cray machines of the 1990s.

The trend of reduced cost over time continues in the same direction today with an even steeper slope. However, the supercomputer architecture based primarily on vector processing that was common up to about 1995 has been replaced by massively parallel computing systems utilizing hundreds or thousands of processors. As a result, performance is not tied to the speed of a single computer chip. In effect, computational effort is split among many processors operating more or less simultaneously. Every year since 1993, a listing

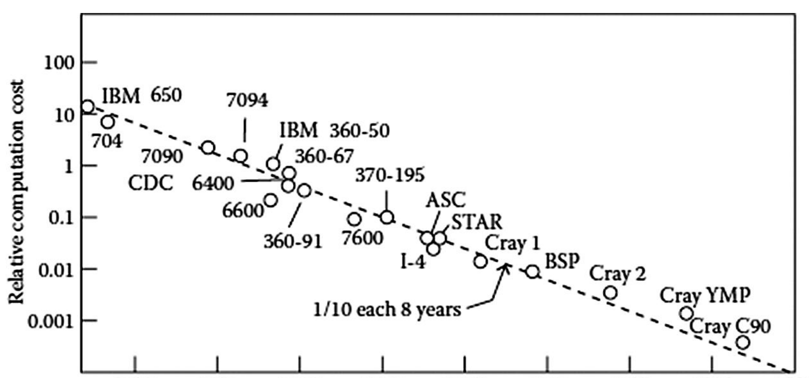

FIGURE 1.1
Trend of relative computation cost for a given flow and algorithm. (Based on Chapman, 1979; Kutler et al., 1987; Holst et al., 1992; Simon, 1995.)

of the 500 fastest computer systems has been prepared and is currently made available at the website www.top500.org sponsored by Prometeus GmbH, Waibstadt-Daisbach, Germany. Performance is measured by the LINPACK Benchmark (Dongarra et al., 2003), which requires the solution of a dense system of linear equations. Figure 1.2 illustrates the trend of performance with time in terms of floating point operations per second (FLOPS). Data is shown for the top performing computer for the date reported. In November 2019, the fastest system in the world was the 148.6 petaflops "Summit" computer built by IBM. For reference, a gigaflop (GFlop) is 10^9 FLOPS, a teraflop (TFlop) is 10^{12} FLOPS, a petaflop (PFlop) is 10^{15} FLOPS, exaflop is 10^{18} FLOPS, and zettaflop is 10^{21}. Notice that performance in terms of FLOPS has been increasing by a factor of 10 approximately every 3.3 years. This means that a computation that would require a full year to complete 10 years ago can now be run overnight (although that trend seems to have slowed down in recent years). The increase in computing power since the 1950s is almost incomprehensible. It is now possible to assign a homework problem in CFD, the solution of which would have represented a major breakthrough or could have formed the basis of a PhD dissertation in the 1950s or 1960s. On the other hand, the costs of performing experiments have been steadily increasing over the same period of time.

The suggestion here is not that computational methods will soon completely replace experimental testing as a means to gather information for design purposes. Rather, it is believed that computer methods will be used even more extensively in the future. In most fluid flow and heat transfer design situations, it will still be necessary to employ some experimental testing. However, computer studies can be used to reduce the range of conditions over which testing is required.

The need for experiments will probably remain for quite some time in applications involving turbulent flow, where it is presently not economically feasible to utilize computational

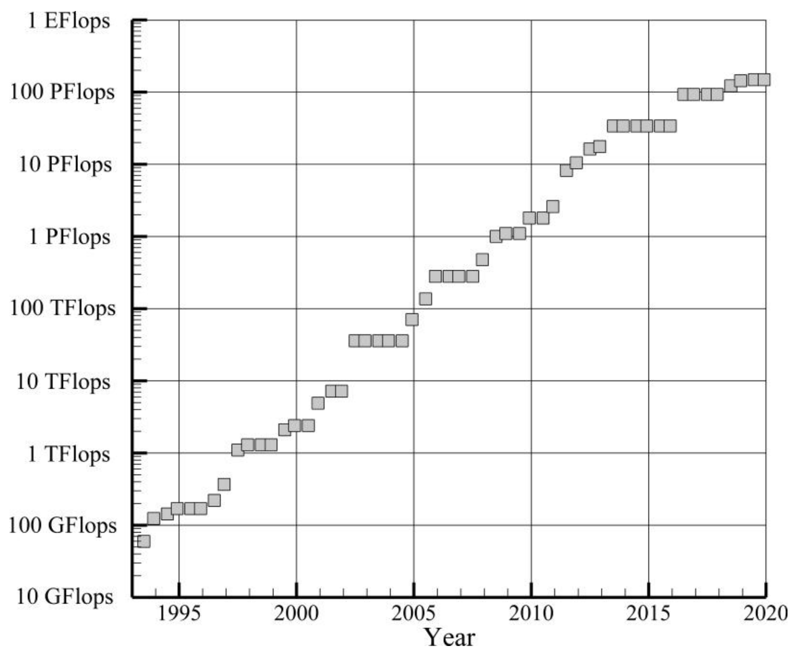

FIGURE 1.2
Growth of supercomputing power based on data from the TOP500 list (top500.org).

models that are free of empiricism for most practical configurations. This situation is destined to change eventually, since the time-dependent three-dimensional Navier–Stokes equations can be solved numerically to provide accurate details of turbulent flow. Thus, as computer hardware and algorithms improve, the frontier will be pushed back continuously allowing flows of increasing practical interest to be computed by direct numerical simulation. The prospects are also bright for the increased use of large eddy simulations, where modeling is required for only the smallest scales.

In applications involving multiphase flows, boiling, or condensation, especially in complex geometries, the experimental method remains the primary source of design information. Progress is being made in computational models for these flows, but the work remains in a relatively primitive state compared to the status of predictive methods for laminar single-phase flows over aerodynamic bodies.

1.2 Comparison of Experimental, Theoretical, and Computational Approaches

As mentioned in the previous section, there are basically three approaches or methods that can be used to solve a problem in fluid mechanics and heat transfer. These methods are

1. Experimental
2. Theoretical
3. Computational (CFD)

The theoretical method is often referred to as an analytical approach, while the terms computational and numerical are used interchangeably. In order to illustrate how these three methods would be used to solve a fluid flow problem, let us consider the classical problem of determining the pressure on the front surface of a circular cylinder in a uniform flow of air at a Mach number (M_∞) of 4 and a Reynolds number (based on the diameter of the cylinder) of 5×10^6.

In the experimental approach, a circular cylinder model would first need to be designed and constructed. This model must have provisions for measuring the wall pressures, and it should be compatible with an existing wind tunnel facility. The wind tunnel facility must be capable of producing the required free stream conditions in the test section. The problem of matching flow conditions in a wind tunnel can often prove to be quite troublesome, particularly for tests involving scale models of large aircraft and space vehicles. Once the model has been completed and a wind tunnel selected, the actual testing can proceed. Since high-speed wind tunnels require large amounts of energy for their operation, the wind tunnel test time must be kept to a minimum. The efficient use of wind tunnel time has become increasingly important in recent years with the escalation of energy costs. After the measurements have been completed, wind tunnel correction factors can be applied to the raw data to produce the final results. The experimental approach has the capability of producing the most realistic answers for many flow problems; however, the costs are becoming greater every day.

In the theoretical approach, simplifying assumptions are used in order to make the problem tractable. If possible, a closed-form solution is sought. For the present problem, a useful

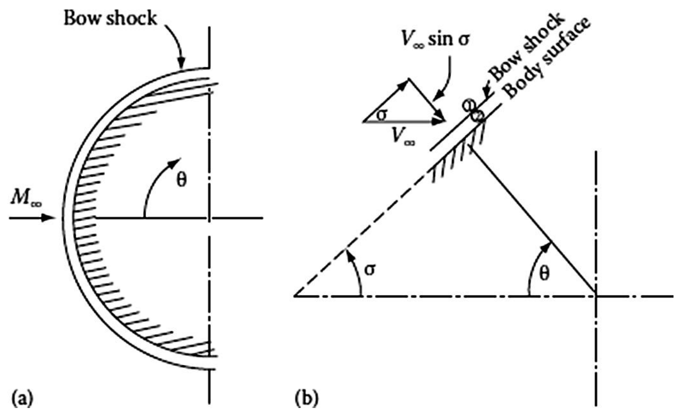

FIGURE 1.3
Theoretical approach. (a) Newtonian flow approximation. (b) Geometry at shock.

approximation is to assume a Newtonian flow (see Hayes and Probstein, 1966) of a perfect gas. With the Newtonian flow assumption, the shock layer (region between body and shock) is infinitesimally thin, and the bow shock lies adjacent to the surface of the body, as seen in Figure 1.3a. Thus, the normal component of the velocity vector becomes zero after passing through the shock wave, since it immediately impinges on the body surface. The normal momentum equation across a shock wave (see Chapter 5) can be written as

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \tag{1.1}$$

where

p is the pressure
ρ is the density
u is the normal component of velocity.

The subscripts 1 and 2 refer to the conditions immediately upstream and downstream of the shock wave, respectively.

For the present problem (see Figure 1.3b), Equation 1.1 becomes

$$p_\infty + \rho_\infty V_\infty^2 \sin^2 \sigma = p_{\text{wall}} + \rho_{\text{wall}}\, u_{\text{wall}}^{2\nearrow 0} \tag{1.2}$$

or

$$p_{\text{wall}} = p_\infty \left(1 + \frac{\rho_\infty}{p_\infty} V_\infty^2 \sin^2 \sigma \right) \tag{1.3}$$

For a perfect gas, the speed of sound in the free stream is

$$a_\infty = \sqrt{\frac{\gamma p_\infty}{\rho_\infty}} \tag{1.4}$$

where γ is the ratio of specific heats. Using the definition of Mach number

$$M_\infty = \frac{V_\infty}{a_\infty} \tag{1.5}$$

and the trigonometric identity

$$\cos\theta = \sin\sigma \tag{1.6}$$

Equation 1.3 can be rewritten as

$$p_{\text{wall}} = p_\infty\left(1+\gamma M_\infty^2 \cos^2\theta\right) \tag{1.7}$$

At the stagnation point, $\theta = 0°$, so that the wall pressure becomes

$$p_{\text{stag}} = p_\infty(1+\gamma M_\infty^2) \tag{1.8}$$

After inserting the stagnation pressure into Equation 1.7, the final form of the equation is

$$p_{\text{wall}} = p_\infty + \left(p_{\text{stag}} - p_\infty\right)\cos^2\theta \tag{1.9}$$

The accuracy of this theoretical approach can be greatly improved if, in place of Equation 1.8, the stagnation pressure is computed from Rayleigh's pitot formula (Shapiro, 1953):

$$p_{\text{stage}} = p_\infty\left[\frac{(\gamma+1)M_\infty^2}{2}\right]^{\gamma/\gamma+1}\left[\frac{\gamma+1}{2\gamma M_\infty^2 - (\gamma-1)}\right]^{1/(\gamma-1)} \tag{1.10}$$

which assumes an isentropic compression between the shock and body along the stagnation streamline. The use of Equation 1.9 in conjunction with Equation 1.10 is referred to as the modified Newtonian theory. The wall pressures predicted by this theory are compared in Figure 1.4 to the results obtained using the experimental approach (Beckwith and Gallagher, 1961). Note that the agreement with the experimental results is quite good up to about ±35°. The big advantage of the theoretical approach is that "clean," general information can be obtained, in many cases, from a simple formula, as in the present example.

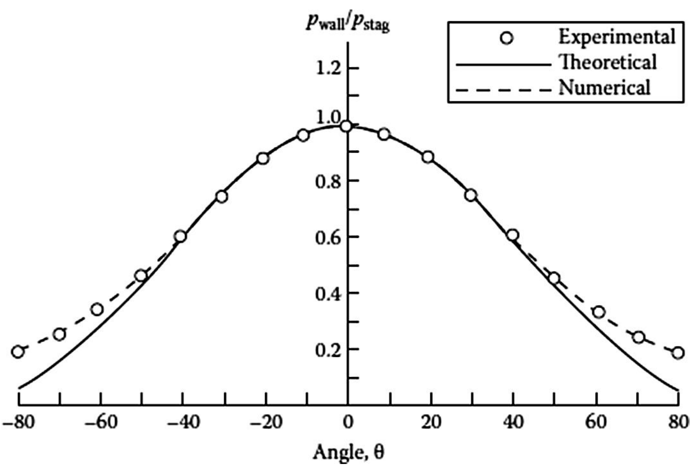

FIGURE 1.4
Surface pressure on circular cylinder.

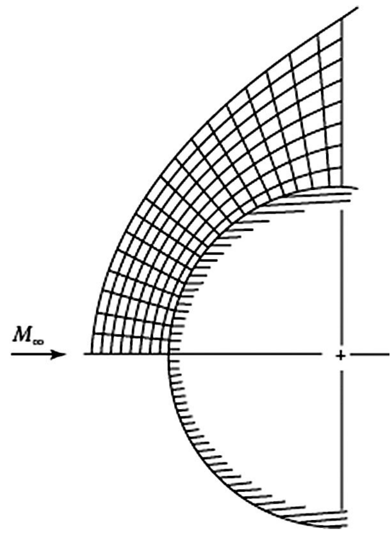

FIGURE 1.5
Computational grid.

This approach is quite useful in preliminary design work, since reasonable answers can be obtained in a minimum amount of time.

In the computational approach, a limited number of assumptions are made, and a high-speed digital computer is used to solve the resulting governing fluid dynamic equations. For the present high Reynolds number problem, inviscid flow can be assumed, since we are only interested in determining wall pressures on the forward portion of the cylinder. Hence, the Euler equations are the appropriate governing fluid dynamic equations. In order to solve these equations, the region between the bow shock and body must first be subdivided into a computational grid, as seen in Figure 1.5. The partial derivatives appearing in the unsteady Euler equations can be replaced by appropriate finite differences at each grid point. The resulting equations are then integrated forward in time until a steady-state solution is obtained asymptotically after a sufficient number of time steps. The details of this approach will be discussed in forthcoming chapters. The results of this technique (Daywitt and Anderson, 1974) are shown in Figure 1.4. Note the excellent agreement with experiment.

In comparing the methods, we note that a computer simulation is free of some of the constraints imposed on the experimental method for obtaining information upon which to base a design. This represents a major advantage of the computational method, which should be increasingly important in the future. The idea of experimental testing is to evaluate the performance of a relatively inexpensive small-scale version of the prototype device. In performing such tests, it is not always possible to simulate the true operating conditions of the prototype. For example, it is very difficult to simulate the large Reynolds numbers of aircraft in flight, atmospheric reentry conditions, or the severe operating conditions of some turbo machines in existing test facilities. This suggests that the computational method, which has no such restrictions, has the potential of providing information not available by other means. On the other hand, computational methods also have limitations; among these are computer storage and speed. Other limitations arise owing to our inability to understand and mathematically model certain complex phenomena. None of these limitations of the computational method are insurmountable in principle, and

TABLE 1.1

Comparison of Approaches

Approach	Advantages	Disadvantages
Experimental	1. Capable of being most realistic	1. Equipment required 2. Scaling problems 3. Tunnel corrections 4. Measurement difficulties 5. Operating costs
Theoretical	1. Clean, general information, which is usually in formula form	1. Restricted to simple geometry and physics 2. Usually restricted to linear problems
Computational	1. No restriction to linearity 2. Complicated physics can be treated 3. Time evolution of flow can be obtained	1. Truncation errors 2. Boundary condition problems 3. Computer costs 4. Model inadequacies (turbulence, chemical kinetics, etc.)

current trends show reason for optimism about the role of the computational method in the future. As seen in Figures 1.1 and 1.2, the relative cost of computing a given flow field has decreased by approximately five orders of magnitude during the past 20 years, and this trend is expected to continue in the near future. As a consequence, wind tunnels have begun to play a secondary role to the computer for many aerodynamic problems, much in the same manner as ballistic ranges perform secondary roles to computers in trajectory mechanics (Chapman, 1975). There are, however, many flow problems involving complex physical processes that still require experimental facilities for their solution.

Some of the advantages and disadvantages of the three approaches are summarized in Table 1.1. It should be mentioned that it is sometimes difficult to distinguish between the different methods. For example, when numerically computing turbulent flows, the eddy viscosity models that are frequently used are obtained from experiments. Likewise, many theoretical techniques that employ numerical calculations could be classified as computational approaches.

1.3 Historical Perspective

As one might expect, the history of CFD is closely tied to the development of the digital computer. Most problems were solved using methods that were either analytical or empirical in nature until the end of World War II. Prior to this time, there were a few pioneers using numerical methods to solve problems. Of course, the calculations were performed by hand, and a single solution represented a monumental amount of work. Since that time, the digital computer has been developed, and the routine calculations required in obtaining a numerical solution are carried out with ease.

The actual beginning of CFD or the development of methods crucial to CFD is a matter of conjecture. Most people attribute the first definitive work of importance to Richardson (1910), who introduced point iterative schemes for numerically solving Laplace's equation and the biharmonic equation in an address to the Royal Society of London. He actually carried out calculations for the stress distribution in a masonry dam. In addition, he clearly defined the difference between problems that must be solved by a relaxation scheme and those that we refer to as marching problems.

Richardson developed a relaxation technique for solving Laplace's equation. His scheme used data available from the previous iteration to update each value of the unknown. In 1918, Liebmann presented an improved version of Richardson's method. Liebmann's method used values of the dependent variable both at the new and old iteration levels in each sweep through the computational grid. This simple procedure of updating the dependent variable immediately reduced the convergence times for solving Laplace's equation. Both Richardson's method and Liebmann's scheme are usually used in elementary heat transfer courses to demonstrate how apparently simple changes in a technique greatly improve efficiency.

Sometimes the beginning of modern numerical analysis is attributed to a famous paper by Courant et al. (1928). The acronym CFL, frequently seen in the literature, stands for these three authors. In this paper, uniqueness and existence questions were addressed for the numerical solutions of partial differential equations. Testimony to the importance of this paper is evidenced in its republication in 1967 in the *IBM Journal of Research and Development.* This paper is the original source for the CFL stability requirement for the numerical solution of hyperbolic partial differential equations.

Thom (1933) published the first numerical solution for flow past a cylinder. Kawaguti (1953) obtained a similar solution for flow around a cylinder in 1953 by using a mechanical desk calculator, working 20 hours per week for 18 months. Allen and Southwell (1955) published another solution for viscous flow over a cylinder using the Southwell (1940) relaxation scheme. The Southwell relaxation method was extensively used in solving both structural and fluid flow problems. The method was tailored for hand calculations in that point residuals were computed, and these were scanned for the largest value, which was then relaxed as the next step in the technique. This numerical technique for hand calculations was generally taught to engineering students in the 1940s, 1950s, and even into the 1960s until programmable computers became widely available.

During World War II and immediately following, a large amount of research was performed on the use of numerical methods for solving problems in fluid dynamics. It was during this time that Professor John von Neumann developed his method for evaluating the stability of numerical methods for solving time-marching problems. It is interesting that Professor von Neumann did not publish a comprehensive description of his methods. However, O'Brien et al. (1950) later presented a detailed description of the von Neumann method. This paper is significant because it presents a practical way of evaluating stability that can be understood and used reliably by scientists and engineers. The von Newman method is the most widely used technique in CFD for determining stability. Another of the important contributions appearing at about the same time was due to Lax (1954). Lax developed a technique for computing fluid flows including shock waves that represent discontinuities in the flow variables. No special treatment was required for computing the shocks. This special feature developed by Lax was due to the use of the conservation-law form of the governing equations and is referred to as shock capturing.

At the same time, progress was being made on the development of methods for both elliptic and parabolic problems. Frankel (1950) presented the first version of the successive overrelaxation (SOR) scheme for solving Laplace's equation. This provided a significant improvement in the convergence rate. Peaceman and Rachford (1955) and Douglas and Rachford (1956) developed a new family of implicit methods for parabolic and elliptic equations in which sweep directions were alternated and the allowed step size was unrestricted. These methods are referred to as alternating direction implicit (ADI) schemes and were later extended to the equations of fluid mechanics by Briley and McDonald (1974) and Beam and Warming (1976, 1978). This implementation provided fast efficient solvers for the solution of the Euler and Navier–Stokes equations.

Research in CFD continued at a rapid pace during the 1960s. Early efforts at solving flows with shock waves used either the Lax approach or an artificial viscosity scheme introduced by von Neumann and Richtmyer (1950). Early work at Los Alamos included the development of schemes like the particle-in-cell (PIC), marker-and-cell (MAC), vorticity–stream function, and arbitrary Lagrangian–Eulerian (ALE) methods. The early work at the Los Alamos National Laboratory has been documented by Johnson (1996).

Lax and Wendroff (1960) introduced a method for computing flows with shocks that was second-order accurate and avoided the excessive smearing of the earlier approaches. The MacCormack (1969) version of this technique became one of the most widely used numerical schemes. Gary (1962) presented early work demonstrating techniques for fitting moving shocks, thus avoiding the smearing associated with the previous shock-capturing schemes. Moretti and Abbett (1966) and Moretti and Bleich (1968) applied shock-fitting procedures to multidimensional supersonic flow over various configurations. Even today, we see either shock-capturing or shock-fitting methods used to solve problems with shock waves.

Godunov (1959) proposed solving multidimensional compressible fluid dynamics problems by using a solution to a Riemann problem for flux calculations at cell faces. This approach was not vigorously pursued until van Leer (1974, 1979) showed how higher-order schemes could be constructed using the same idea. The intensive computational effort necessary with this approach led Roe (1980) to suggest using an approximate solution to the Riemann problem (flux-difference splitting) in order to improve the efficiency. This substantially reduced the work required to solve multidimensional problems and represents the current trend of practical schemes employed on convection-dominated flows. The concept of flux splitting was also introduced as a technique for treating convection-dominated flows. Steger and Warming (1979) introduced splitting where fluxes were determined using an upwind approach. Van Leer (1982) also proposed a new flux splitting technique to improve on the existing methods. These original ideas are used in many of the modern production codes, and improvements continue to be made on the basic concept.

In the 1970s, a group at Imperial College, London, developed a number of algorithms for low-speed (essentially incompressible) flows including parabolic flows (Patankar and Spalding, 1972) and the SIMPLE algorithm (Caretto et al., 1972), which inspired a number of related schemes for solving the incompressible Navier–Stokes equations.

As part of the development of modern numerical methods for computing flows with rapid variations such as those occurring through shock waves, the concept of limiters was introduced. Boris and Book (1973) first suggested this approach, and it has formed the basis for the nonlinear limiting subsequently used in most codes. Harten (1983) introduced the idea of total variation diminishing (TVD) schemes. This generalized the limiting concept and has led to substantial advances in the way the nonlinear limiting of fluxes is implemented. Others that also made substantial contributions to the development of robust methods for computing convection-dominated flows with shocks include Enquist and Osher (1980, 1981), Osher (1984), Osher and Chakravarthy (1983), Yee (1985a, 1985b), and Yee and Harten (1985). While this is not an all-inclusive list, the contributions of these and others have led to the addition of nonlinear dissipation with limiting as a major factor in state-of-the-art schemes in use today.

Other contributions were made in algorithm development dealing with the efficiency of the numerical techniques. Both multigrid and preconditioning techniques were introduced to improve the convergence rate of iterative calculations. The multigrid approach was first applied to elliptic equations by Fedorenko (1962, 1964) and was later extended to the equations of fluid mechanics by Brandt (1972, 1977). At the same time, strides in applying reduced forms of the Euler and Navier–Stokes equations were being made. Murman and Cole (1971) made a major contribution in solving the transonic small-disturbance equation by applying type-dependent differencing to the subsonic and supersonic portions of the flow field. The thin-layer Navier–Stokes equations have been extensively applied to many problems of interest, and the paper by Pulliam and Steger (1978) is representative of these applications. Also, the parabolized Navier–Stokes (PNS) equations were introduced by Rudman and Rubin (1968), and this approximate form of the Navier–Stokes equations has been used to solve many supersonic viscous flow fields. The correct treatment of the streamwise pressure gradient when solving the PNS equations was examined in detail by Vigneron et al. (1978a), and a new method of limiting the streamwise pressure gradient in subsonic regions was developed and is in prominent use today.

In addition to the changes in treating convection terms, the control-volume or finite-volume point of view as opposed to the finite-difference approach has been applied to the construction of difference methods for the fluid dynamic equations. The finite-volume approach provides an easy way to apply numerical techniques to unstructured grids, and many codes presently in use are based on unstructured grids. With the development of methods that are robust for general problems, large-scale simulations of complete vehicles are now a common occurrence. Among the many researchers who have made significant contributions in this effort are Jameson and Baker (1983), Shang and Scherr (1985), Jameson et al. (1986), Flores et al. (1987), Obayashi et al. (1987), Yu et al. (1987), and Buning et al. (1988). Until recently, most of the serious design work in the aircraft industry has been done with the aid of full potential/coupled boundary-layer and Euler/coupled boundary-layer methods (Johnson et al., 2005). This includes the design of aircraft such as the Boeing 777. Recently, Navier–Stokes and thin-layer Navier–Stokes codes have been used, particularly for regions of strong viscous interaction and for the analysis of high-speed and high-lift configurations. "The rapid development of parallel computing hardware and software, as well as PC clusters with large numbers of CPUs, have made the use of Navier-Stokes technology in practical airplane design and analysis a reality" (Johnson et al., 2005).

Finite-Element Methods (FEM) emerged from very different roots in computational physics and are extremely popular in fluid mechanics and heat transfer simulations. The name "Finite-Element Method" appears to have been coined by R.W. Clough (1960), following several years of research in structural dynamics at Boeing under the supervision of M.J. Turner. Indeed, the paper by Turner et al. (1956) is considered to be the pioneering publication in the engineering applications of FEM. Mathematical concepts underlying FEM date as far back as Leibnitz and Euler (17th and 18th centuries, respectively) in developing discretized formulations to solve problems in the calculus of variations. In the late 19th to early 20th centuries, Rayleigh (1877) and Ritz (1909) applied variational methods to solve elliptic differential equations and developed formal proofs for existence and convergence of solutions. Galerkin (1915) published a formulation that contains an expansion of the unknown quantity in terms of a set of basis functions which can be thought of as coordinate directions in a space of functions, where the error in solving a given differential equation is driven to zero. This method bears his name and continues to be the cornerstone of FEM-related formulations. There are two somewhat related ways by which FEM procedures have been derived in the literature. One, the Ritz method (after Walter Ritz, 1878–1909), follows a variational approach (Ritz, 1909; Finlayson, 1972), where the minimum of a certain functional is sought subject to a given set of constraints. The other, the Galerkin method (after Boris Galerkin, 1871–1945), seeks to derive algebraic equations which result in driving the error in a certain integral form of the governing equations to zero. These result in the same numerical procedure for several cases but are in general not the same. The Galerkin method is more readily generalized and presents several variants many of which are actively used in research and commercial CFD and heat transfer codes. In the appendix to his 1943 paper, Courant (1943) developed a method in which he numerically solved a variational problem on a triangular mesh using a piecewise linear approximation. This is often considered the origin of the present-day mathematical interpretation of the FEM, though some related ideas were developed earlier by other authors (see, e.g., Oden 1990).

Recently, a class of methods named "discontinuous Galerkin" methods [see, e.g., Cockburn and Shu, (2001); Hesthaven and Warburton, (2008)] have become extremely successful and are well suited to newer computer hardware such as the Grahics Processing Units (GPUs)(Klockner et al. 2009). Here, the test and basis functions are local to each element and discontinuous at element boundaries. This is in contrast to the conventional (continuous) Galerkin method where basis functions are assumed to be continuous. The burden of assembling a single large matrix due to the implicit nature of the FEM is relieved and replaced by algebraic expressions that connect a given cell with its immediate neighbors, thus improving parallel performance for large problems.

Historically, the discontinuous Galerkin (DG) method was first used to solve the steady advection equation for neutron transport by Reed and Hill (1973). In the 1990s, DG was made popular in CFD-related problems in large parts due to the efforts of Cockburn and Shu (2001) and has matured rapidly since then. DG offers all of the flexibility present in finite-volume methods and better performance in convection-dominated problems, particularly those involving discontinuous solutions such as shock waves.

The progress in CFD over the past 50 years has been enormous. For this reason, it is impossible, with the short history given here, to give credit to all who have contributed. A number of review and history papers that provide a more precise state of the art may be cited and include those by Hall (1981), Krause (1985), Diewert and Green (1986), Jameson (1987), Kutler (1993), Rubin and Tannehill (1992), MacCormack (1993), Johnson (1996), and Johnson et al. (2005). In addition, the Focus 92 issues of *Aerospace America* are dedicated to a review of the state of the art. The appearance of text materials for the study of CFD should also be mentioned in any brief history. The development of any field is closely paralleled by the appearance of books dealing with the subject. Early texts dealing with CFD include books by Roache (1972), Holt (1977), Chung (1978), Chow (1979), Patankar (1980), Baker (1983), Peyret and Taylor (1983), and Anderson et al. (1984). More recent books include those by Sod (1985), Thompson et al. (1985), Oran and Boris (1987), Hirsch (1988), Fletcher (1988), Hoffmann (1989), Anderson (1995), Tannehill et al. (1997), Laney (1998), Roache (1998), Ferziger and Peric (1999), Wesseling (2000), Lomax et al. (2001), Date (2005), Hirsch (2007), Versteeg and Malalsekera (2007), and Pletcher et al. (2013). The interested reader will also note that occasional writings appear in the popular literature that discuss the application of digital simulation to engineering problems. These applications include CFD but do not usually restrict the range of interest to this single discipline.

The past few decades have seen not only tremendous progress in the science of CFD but also a spectacular diversity in the fields where it is being applied. A few selected references from the recent literature are suggested below. These are textbook-style references, providing detailed and modern presentations of their respective subject areas.

General mathematical foundations of numerical methods used in CFD are dealt with extensively in the books by Gustafsson et al. (2013) and Quarteroni (2017). CFD applications of high-order accurate spectral and finite-element methods have gained much prominence in recent years. Relevant textbooks include the works by Canuto et al. (2007), Hesthaven and Warburton (2008), and Karniadakis and Sherwin (2005). Recent developments in compressible flow simulation are covered in the books by Leveque (2002), Toro (2009), Pulliam and Zingg (2014), Lomax et al. (2001), Wendt (2009), MacCormack (2014), and Hirsch (2007). Incompressible flows are treated in Ferziger and Peric (2001), Kwak and Kiris (2011), Versteeg and Malalasekera (2007), and Gresho and Sani (2000). The *Handbook of Numerical Methods* (Abgrall and Shu 2017) contains important summaries of the mathematical and implementation aspects.

Numerical heat transfer methods are well summarized in the *Handbook of Numerical Heat Transfer* (Minkowycz et al. 2006), Reddy and Gartling (2010), Ozisik et al. (2017) and the review by Murthy and Mathur (2012). Modeling of multiphase flows has advanced tremendously in the past two decades. The textbooks by Tryggvason et al. (2011) cover front tracking and volume of fluid methods, while the texts by Osher and Fedkiw (2003) and Sethian (1999) have become standard references for the level set method. Ozisik et al. (2017) present an elementary numerical treatment of phase change, while a multi-faceted discussion of related physical phenomena can be found in Shyy (2006).

More advanced topics in applied CFD that have gained a great deal of momentum in recent times include Large Eddy Simulations [Sagaut (2005)], Combustion [Oran and Boris {2005}; Poinsot and Veynante {2012)], micro-flows [Karniadakis et al. {2005)], weather and climate modeling (Warner 2011), computational acoustics [Tam (2012); Wagner et al., (2007)], and flow-structure interaction [Lohner (2008); Bazilevs et al., (2013)]. CFD methods are being applied with great success in plasma dynamics and magnetohydrodynamics (see the textbooks by Jardin (2010) and Shang (2016)).

Notable successes in all of these fields have led to the need to stretch the limits of computing resources and attempt increasingly larger problems (in turbulent flows and other flows dominated by multiscale phenomena), thus gaining higher model fidelity. Methods have been devised to reduce the computational cost in high-fidelity simulations and gainfully deployed in problems involving acoustics, heat transfer, incompressible flow, and some simple compressible flow situations. These methods bear promise and, when coupled with the achievements in massively parallel high-performance computing, can enable large-scale multi-parameter studies which have previously been impractical. Recent texts covering these developments include the books by Quarteroni et al. (2016), Benner et al. (2017), and the introductory text by Kutz (2013) dealing with data-driven models.

A number of interesting review articles covering historical aspects of CFD have been published [Anderson,(2010); Lax, (2007); Roe, (2005); Shang, (2004); van Leer, (2009)], and conferences are being held specifically to piece together the many ideas, ideologies, and events that have led to the growth of CFD (e.g., "Four decades of CFD", 2013; "Future directions" 2012). The state of the art of some challenging areas in CFD (nearly always containing some aspects of turbulent flow) have periodically been assessed at workshops held with the purpose of code verification and validation. In the aerospace industry, an important instance of this is the drag prediction workshop [Roy and Tinoco, (2017); Tinoco et al., (2017)]. General discussion of aeronautical applications of CFD in recent times may be found in the papers by Tinoco et al. (2005), Piomelli (2013), and Spalart and Venkatakrishnan (2016). Recently, a study, "CFD Vision 2030," was initiated by NASA where a team of experts from the industry and academia brought forth a roadmap for future developments and needs within the field (specifically for aerospace applications). These have been published in the report by Slotnick et al. (2014).

A testimony to the progress made in CFD has been its widespread use in animated motion pictures. The emphasis here is on a realistic animated rendering of fluid flows for cinematic depiction rather than on performing accurate technical predictions. However, several innovations introduced here have a general applicability and may grow to involve more traditional fluid dynamicists in the coming years. The highly engaging textbooks by Stam (2016) and Bridson (2016) summarize the methods used and the current state of practice in this area. Various such works with a strong CFD component have received academy awards (scientific and technical) for motion picture animations (e.g., the Industrial Light & Magic (ILM) Fluid Simulation System (2007), Autodesk Maya Fluid Effects System (2003, 2005, and 2008)).

2

Partial Differential Equations

2.1 Introduction

Many important physical processes in nature are governed by partial differential equations (PDEs). For this reason, it is important to understand the physical behavior of the model represented by the PDE. In addition, knowledge of the mathematical character, properties, and solution of the governing equations is required. In this chapter, we will discuss the physical significance and the mathematical behavior of the most common types of PDEs encountered in fluid mechanics and heat transfer. Examples are included to illustrate important properties of the solutions of these equations. In the last sections, we extend our discussion to systems of PDEs and present a number of model equations, many of which are used in Chapter 4 to demonstrate the application of various discretization methods.

2.1.1 Partial Differential Equations

PDEs are distinguished by the fact that they contain derivatives with respect to more than one independent variable. On the other hand, ordinary differential equations (ODEs) contain derivatives with respect to just one independent variable. Some examples of PDEs include

$$\phi_x + \phi_y + y\phi = 0 \tag{2.1}$$

$$(\phi_{xx})^2 + \phi_{xy} + \phi\phi_{yy} = 0 \tag{2.2}$$

$$\phi\phi_{xx} + \phi\phi_x + x\phi_y = 0 \tag{2.3}$$

In these equations, ϕ is the dependent variable and x and y are the independent variables. Differentiation is denoted by using a subscript so that $\phi_x = \partial\phi/\partial x$ and $\phi_{xy} = \partial^2\phi/\partial y\,\partial x = \partial/\partial y(\phi_x)$. The *order* of a PDE is defined by the highest-order derivative in the equation. Equation 2.1 is referred to as a first-order, *linear* PDE since the highest derivatives are first order and is linear because the coefficients of the derivatives do not contain the dependent variable or its derivatives. Equation 2.2 is a second-order, *nonlinear* PDE since the highest derivative is second order and is nonlinear because of the coefficients ϕ_{xx} and ϕ. Equation 2.3 is also a second-order nonlinear PDE and is often referred to as a second-order *quasi-linear* PDE since the equation is linear in the highest partial derivative, ϕ_{xx}.

Problems governed by PDEs fall into one of the three physical categories:

1. Equilibrium problems
2. Eigenvalue problems
3. Marching (propagation) problems

These are discussed in the next section. In addition, PDEs can be classified in a mathematical sense and can be put into three categories:

1. Elliptic PDEs
2. Parabolic PDEs
3. Hyperbolic PDEs

These mathematical categories are discussed in Section 2.3.

2.2 Physical Classification

2.2.1 Equilibrium Problems

Equilibrium problems are problems in which a solution of a given PDE is desired in a closed domain subject to a prescribed set of boundary conditions (see Figure 2.1). Equilibrium problems are boundary value problems. Examples of such problems include steady-state temperature distributions, incompressible inviscid flows, and equilibrium stress distributions in solids.

Sometimes equilibrium problems are referred to as jury problems. This is an apt name, since the solution of the PDE at every point in the domain depends upon the prescribed boundary condition at every point on B. In this sense, the boundary conditions are certainly the jury for the solution in D. Mathematically, equilibrium problems are governed by elliptic PDEs.

Example 2.1

The steady-state temperature distribution in a conducting medium is governed by Laplace's equation. A typical problem requiring the steady-state temperature distribution in a two-dimensional (2-D) solid with the boundaries held at constant temperatures is defined by the equation

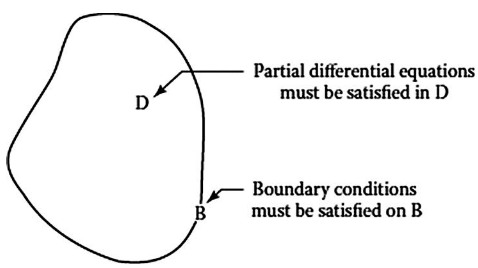

FIGURE 2.1
Domain for an equilibrium problem.

$$\nabla^2 T = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \quad 0 \le x \le 1 \quad 0 \le y \le 1 \tag{2.4}$$

with boundary conditions

$$T(0,y) = 0$$
$$T(1,y) = 0$$
$$T(x,0) = T_0$$
$$T(x,1) = 0$$

The 2-D configuration is shown in Figure 2.2.

Solution

One of the standard techniques used to solve a linear PDE is separation of variables (Greenspan, 1961). This technique assumes that the unknown temperature can be written as the product of a function of x and a function of y, that is,

$$T(x,y) = X(x)Y(y)$$

If a solution of this form can be found that satisfies both the PDE and the boundary conditions, then it can be shown (Weinberger, 1965) that this is the one and only solution to the problem. After this form of the temperature is substituted into Laplace's equation, two ODEs are obtained. The resulting equations and homogeneous boundary conditions are

$$\begin{aligned} X'' + \alpha^2 X &= 0 & Y'' - \alpha^2 Y &= 0 \\ X(0) &= 0 & & \\ X(1) &= 0 & Y(1) &= 0 \end{aligned} \tag{2.5}$$

The prime denotes differentiation, and the factor α^2 arises from the separation process and must be determined as part of the solution to the problem. The solutions of the two differential equations given in Equation 2.5 may be written as

$$X(x) = A\sin(n\pi x) \quad Y(y) = C\sinh[n\pi(y-1)]$$

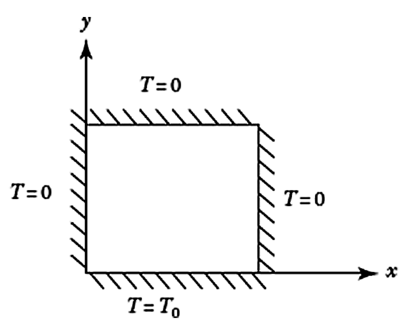

FIGURE 2.2
Unit square with fixed boundary temperatures.

with the boundary conditions entering the solution in the following way:

1. $T(0, y) = 0 \quad \rightarrow \quad X(0) = 0$
   $T(x, 1) = 0 \quad \rightarrow \quad Y(1) = 0$
   These two conditions determine the kinds of functions allowed in the expression for $T(x, y)$. The boundary condition $T(0, y) = 0$ is satisfied if the solution of the separated ODE satisfies $X(0) = 0$. Since the solution in general contains sine and cosine terms, this boundary condition eliminates the cosine terms. A similar behavior is observed by satisfying $T(x, 1) = 0$ through $Y(1) = 0$ for the separated equation.
2. $T(1, y) = 0 \rightarrow X(1) = 0$
   This condition identifies the eigenvalues, that is, the particular values of α that generate eigenfunctions satisfying this required boundary condition. Since the solution of the first separated equation, Equation 2.5, was
   $$X(x) = A\sin(\alpha x)$$
   a nontrivial solution for $X(x)$ exists that satisfies $X(1) = 0$ only if $\alpha = n\pi$, where $n = 1, 2, \ldots$.
3. $T(x, 0) = T_0$
   The prescribed temperature on the x-axis determines the manner in which the eigenfunctions are combined to yield the correct solution to the problem.

The solution of the present problem is written as

$$T(x,y) = \sum_{n=1}^{\infty} A_n \sin(n\pi x)\sinh\left[n\pi(y-1)\right] \tag{2.6}$$

In this case, functions of the form $\sin(n\pi x)\sinh[n\pi(y-1)]$ satisfy the PDE and three of the boundary conditions. In general, an infinite series composed of products of trigonometric sines and cosines and hyperbolic sines and cosines is required to satisfy the boundary conditions. For this problem, the fourth boundary condition along the lower boundary of the domain is given as

$$T(x,0) = T_0$$

We use this to determine the coefficients A_n of Equation 2.6. Thus, we find (see Problem 2.1)

$$A_n = \frac{2T_0\left[(-1)^n - 1\right]}{n\pi \quad \sinh(n\pi)}$$

The solution $T(x, y)$ provides the steady temperature distribution in the solid. It is clear that the solution at any point interior to the domain of interest depends upon the specified conditions at all points on the boundary. This idea is fundamental to all equilibrium problems.

Example 2.2

The irrotational flow of an incompressible inviscid fluid is governed by Laplace's equation. Determine the velocity distribution around the 2-D cylinder shown in Figure 2.3 in an incompressible inviscid fluid flow. The flow is governed by

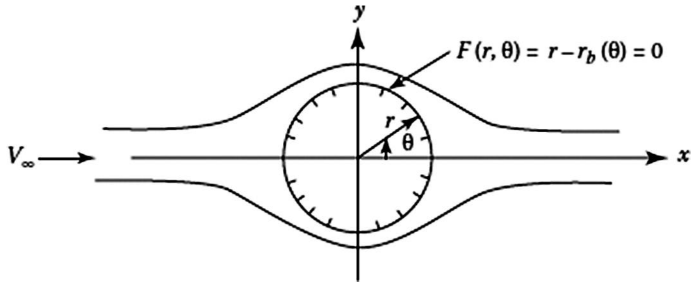

FIGURE 2.3
Two-dimensional flow around a cylinder.

$$\nabla^2\phi = 0$$

where ϕ is defined as the velocity potential, that is, $\nabla\phi = \mathbf{V}$ = velocity vector. The boundary condition on the surface of the cylinder is

$$\mathbf{V}\cdot\nabla F = 0 \tag{2.7}$$

where $F(r, \theta) = 0$ is the equation of the surface of the cylinder. In addition, the *velocity must* approach the free stream value as distance from the body becomes large, that is, as $(x, y) \to \infty$,

$$\nabla\phi = \mathbf{V}_\infty \tag{2.8}$$

Solution

This problem is solved by combining two elementary solutions of Laplace's equation that satisfy the boundary conditions. This superposition of two elementary solutions is an acceptable way of obtaining a third solution only because Laplace's equation is linear. For a linear PDE, any linear combination of solutions is also a solution (Churchill, 1941). In this case, the flow around a cylinder can be simulated by adding the velocity potential for a uniform flow to that for a doublet (Karamcheti, 1966). The resulting solution becomes

$$\phi = V_\infty x + \frac{K\cos\theta}{\sqrt{x^2+y^2}} = V_\infty x + \frac{Kx}{x^2+y^2} \tag{2.9}$$

where the first term is the uniform oncoming flow, and the second term is a solution for a doublet of strength $2\pi K$.

2.2.2 Eigenvalue Problems

An eigenvalue problem can be considered as an extension of an equilibrium problem, the difference being that the solution exists only for some discrete value of a parameter λ_i, called the eigenvalue. Typical examples of eigenvalue problems are the buckling and stability of structures, resonance in electric circuits, and natural frequencies in vibrations. Since eigenvalue problems occur infrequently in fluid mechanics and heat transfer, they are not discussed further in this chapter.

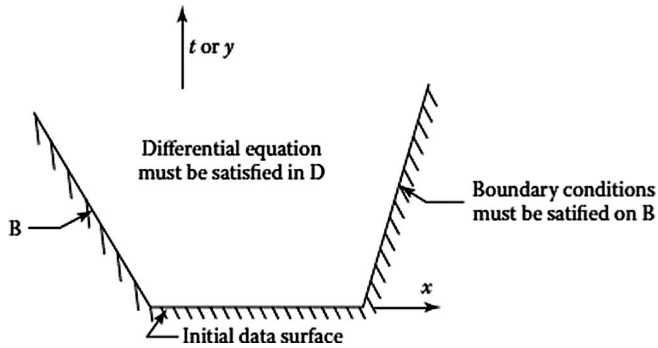

FIGURE 2.4
Domain for a marching problem.

2.2.3 Marching Problems

Marching or propagation problems are transient or transient-like problems where the solution of a PDE is required on an open domain subject to a set of initial conditions and a set of boundary conditions. Figure 2.4 illustrates the domain and marching direction for this case. Problems in this category are initial value or initial boundary value problems. The solution must be computed by marching outward from the initial data surface while satisfying the boundary conditions. Mathematically, these problems are governed by either hyperbolic or parabolic PDEs.

Example 2.3

Determine the transient temperature distribution in a one-dimensional (1-D) solid (Figure 2.5) with a thermal diffusivity α if the initial temperature in the solid is 0° and if at all subsequent times, the temperature of the left side is held at 0° while the right side is held at T_0.

Solution

The governing differential equation is the 1-D heat equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{2.10}$$

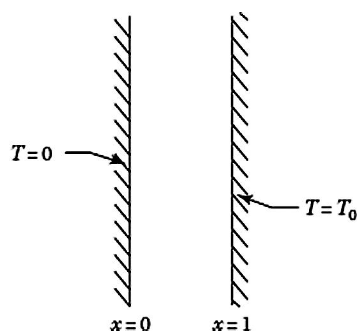

FIGURE 2.5
One-dimensional solid.

with boundary conditions

$$T(0,t)=0 \quad T(1,t)=T_0$$

and initial condition

$$T(x,0)=0$$

Again, for this linear equation, separation of variables will lead to a solution. Because of the nonhomogeneous boundary conditions in this problem, it is helpful to use the principle of superposition to determine the solution as the sum of the solution to the steady problem that results as the time becomes very large and a transient solution that dies out at large times. Thus, we let $T(x, t) = u(x) + v(x, t)$. Since u is independent of time, substituting this decomposition into the governing PDE results in the ODE

$$\frac{d^2u}{dx^2}=0 \tag{2.11}$$

with boundary conditions

$$u(0)=0 \quad u(1)=T_0$$

The solution for the steady problem is thus $u(x) = T_0\,x$. We also find that the transient solution must satisfy

$$\frac{\partial v}{\partial t}=\alpha\frac{\partial^2 v}{\partial x^2} \tag{2.12}$$

with associated boundary conditions

$$v(0,t)=v(1,t)=0$$

and initial condition

$$v(x,0)=-T_0x$$

The initial condition for v is required in order that the sum of u and v satisfy the initial conditions of the problem. Separation of variables may be used to solve Equation 2.12, and the solution is written in the form

$$v(x,t)=V(t)X(x)$$

If we denote the separation constant by $-\beta^2$, it is necessary to solve the ODEs

$$V'+\alpha\beta^2V=0 \quad X''+\beta^2X=0$$

$$X(0)=X(1)=0$$

with the initial distribution on v as noted earlier. The general solution for V is readily obtained as

$$V(t)=e^{-\alpha\beta^2 t}$$

A solution for X that satisfies the boundary conditions is of the form

$$X(x) = \sin \beta x$$

where β must equal $n\pi(n = 1,2, \ldots)$, so that the boundary conditions on X are met. The general solution that satisfies the PDE for v and the boundary conditions is then of the form

$$v(x,t) = e^{-\alpha n^2 \pi^2 t} \sin(n\pi x)$$

The orthogonality properties of the trigonometric functions (Weinberger, 1965) are used to meet the initial conditions as a Fourier sine series. This leads to the final solution for T, obtained by adding the solutions for u and v together

$$T = T_0 x + \sum_{n=1}^{\infty} \frac{2T_0(-1)^n}{n\pi} e^{-n^2\pi^2\alpha t} \sin(n\pi x) \tag{2.13}$$

Example 2.4

Find the displacement $y(x, t)$ of a string of length l stretched between $x = 0$ and $x = l$ if it is displaced initially into position $y(x, 0) = \sin(\pi x/l)$ and released from rest. Assume no external forces act on the string.

Solution

In this case, the motion of the string is governed by the wave equation

$$\frac{\partial^2 y}{\partial t^2} = \mathrm{a}^2 \frac{\partial^2 y}{\partial x^2} \tag{2.14}$$

where a is a positive constant. The boundary conditions are

$$y(0,t) = y(l,t) = 0 \tag{2.15}$$

and initial conditions

$$y(x,0) = \sin\frac{\pi x}{l} \quad \frac{\partial}{\partial t} y(x,t)|_{t=0} = 0 \tag{2.16}$$

The solution for this particular example is

$$y(x,t) = \sin\left(\pi \frac{x}{l}\right) \cos\left(a\pi \frac{t}{l}\right) \tag{2.17}$$

Solutions for problems of this type usually require an infinite series to correctly approximate the initial data. In this case, only one term of this series survives because the initial displacement requirement is exactly satisfied by one term.

The physical phenomena governed by the heat equation and the wave equation are different, but both are classified as marching problems. The behavior of the solutions to these equations and methods used to obtain these solutions are also quite different. This will become clear as the mathematical character of these equations is studied.

Typical examples of marching problems include unsteady inviscid flow, steady supersonic inviscid flow, transient heat conduction, and boundary-layer flow.

2.3 Mathematical Classification

The classification of PDEs is based on the mathematical concept of characteristics that are lines (in two dimensions) or surfaces (in three dimensions) along which certain properties remain constant or certain derivatives may be discontinuous. Such *characteristic* lines or surfaces are related to the directions in which "information" can be transmitted in physical problems governed by PDEs. Equations (single or system) that admit wavelike solutions are known as hyperbolic. If the equations admit solutions that correspond to damped waves, they are designated parabolic. If solutions are not wavelike, the equation or system is designated as elliptic. Although first-order equations or a system of first-order equations can be classified as indicated previously, it is instructive at this point to develop classification concepts through consideration of the following general second-order PDE:

$$a\phi_{xx} + b\phi_{xy} + c\phi_{yy} + d\phi_x + e\phi_y + f\phi = g(x, y) \tag{2.18a}$$

where a, b, c, d, e, and f are functions of (x, y), that is, we consider a linear equation. While this restriction is not essential, this form is convenient to use. Frequently, consideration is given to quasi-linear equations, which are defined as equations that are linear in the highest derivative. In terms of Equation 2.18a, this means that a, b, and c could be functions of x, y, ϕ, ϕ_x, and ϕ_y. For our discussion, however, we assume that Equation 2.18a is linear and the coefficients depend only upon x and y.

We will indicate how equations having the general form of Equation 2.18a can be classified as hyperbolic, parabolic, or elliptic and how a standard or canonical form can be identified for each class by making use of the characteristic curves associated with the PDE. This will be discussed for equations with two independent variables, but the concepts can be extended to equations involving more independent variables, such as would be encountered in three-dimensional (3-D) unsteady physical problems.

The classification of a second-order PDE depends only on the second-derivative terms of the equation, so we may rearrange Equation 2.18a as

$$a\phi_{xx} + b\phi_{xy} + c\phi_{yy} = -(d\phi_x + e\phi_y + f\phi - g) = H \tag{2.18b}$$

The characteristics of this equation, if they exist and are real curves within the solution domain, represent the locus of points along which the second derivatives may not be continuous. Along such curves, discontinuities in the solution, such as shock waves in supersonic flow, may appear. To identify such curves, we proceed as follows. For the general second-order PDE under consideration, the initial and boundary conditions are specified in terms of the function ϕ and first derivatives of ϕ. Assuming that ϕ and first derivatives of ϕ are continuous, we inquire if there may be any locations where this information would not uniquely determine the solution. In other words, are there locations where the second derivatives are discontinuous?

Let τ be a parameter that varies along a curve C in the x–y plane. That is, on C, $x = x(\tau)$ and $y = y(\tau)$. The curve C may be on the boundary. For convenience, on C, we define

$$\begin{aligned} \phi_x &= p(\tau) \qquad & \phi_{xx} &= u(\tau) \\ \phi_y &= q(\tau) \qquad & \phi_{xy} &= v(\tau) \\ & & \phi_{yy} &= w(\tau) \end{aligned}$$

We suppose that ϕ, p, and q are given along C, as they might be given as boundary or initial conditions. With these definitions, Equation 2.18b becomes

$$au(\tau) + bv(\tau) + cw(\tau) = H \tag{2.18c}$$

Using the chain rule, we observe that

$$\frac{dp}{d\tau} = u\frac{dx}{d\tau} + v\frac{dy}{d\tau} \tag{2.18d}$$

$$\frac{dq}{d\tau} = v\frac{dx}{d\tau} + w\frac{dy}{d\tau} \tag{2.18e}$$

Equations 2.18c through 2.18e can be considered a system of three equations from which the second derivatives (u, v, and w) might be determined from the specified values of ϕ and the first derivatives of ϕ along C. These can be written in matrix form ($[A]\mathrm{x} = \mathrm{c}$) as

$$\begin{bmatrix} a & b & c \\ \frac{dx}{d\tau} & \frac{dy}{d\tau} & 0 \\ 0 & \frac{dx}{d\tau} & \frac{dy}{d\tau} \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} H \\ \frac{dp}{d\tau} \\ \frac{dq}{d\tau} \end{bmatrix}$$

If the determinant of the coefficient matrix is zero, then there may be no unique solution for the second derivatives u, v, and w along C for the given values of ϕ and its first derivatives. By setting the determinant of the coefficient matrix to zero, we find the condition for discontinuity (or nonuniqueness) in the highest-order derivatives as

$$a\left(\frac{dy}{d\tau}\right)^2 - b\left(\frac{dx}{d\tau}\right)\left(\frac{dy}{d\tau}\right) + c\left(\frac{dx}{d\tau}\right)^2 = 0$$

or

$$a(dy)^2 - b\,dx\,dy + c(dx)^2 = 0 \tag{2.19}$$

Letting $h = dy/dx$, we can write Equation 2.19 as

$$a(h)^2(dx)^2 - bh(dx)^2 + c(dx)^2 = 0$$

which, after division by $(dx)^2$, reduces to a quadratic equation in h:

$$ah^2 - bh + c = 0 \tag{2.20}$$

Solving for $h = dy/dx$ gives

$$h = \frac{dy}{dx} = \frac{b \pm \sqrt{b^2 - 4ac}}{2a} \tag{2.21}$$