COMPUTATIONAL FLUID DYNAMICS

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by

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PREFACE

At the time of this writing, it is obvious that the general area of computer simulation of physical processes, and the particular area of computational fluid dynamics, is rapidly expanding. One need only glance through the titles in any of the scientific abstracting indexes to see a disproportionate number of doctoral dissertations in computational fluid dynamics. Everyone with a computer is computing.

Unfortunately, research progress has been hindered by a widely scattered literature source. Scarcely a month goes by without someone rediscovering upwind differencing or expounding with the intensity of a religious convert on the aesthetic satisfaction of the asymptotic unsteady-flow approach to steady-flow problems. But these ideas have been around for a long time. It is hoped that this book will contribute to starting next year's crop of researchers off from approximately the same point, so that research may proceed.

Several excellent texts, covering numerical solutions of partial differential equations, are available, notably those of Forsythe and Wasow (1960), Richtmyer (1957), Richtmyer and Morton (1967), Ames (1965, 1969), and Mitchell (1969).* The present book differs from these in the material covered and in the approach used.

As for the material covered, the reader is advised that this is not a mathematics book (see Forsythe, 1970; "Pitfalls in Computation, or Why a Math Book Isn't Enough"). The basic interior point-differencing methods are presented in a direct and hopefully intelligible manner. Also, the importance of numerical boundary conditions is discussed. This topic has heretofore received no attention in texts and little in research papers, although there is a growing awareness of its dominant importance. This book also treats the equally important and neglected topics of special finite-difference mesh systems, specialized forms of the differential equations, the problems of initial conditions and convergence criteria, plotting methods and other information-processing techniques, and even some specific suggestions on programming practices. In short, this text addresses the messy problems associated with actually obtaining numerical solutions to the fluid dynamics problems, rather than nice mathematical propositions associated with merely related problems.

As for the approach used, the reader is again advised that this is not a mathematics book. Even the mathematics books admit the necessity of physical intuition, heuristic reasoning, and numerical experimentation in this area, although they do not often use the intuitive, heuristic, or experimental approaches. Some of the mathematical research is certainly valuable, but our interest is the primary interest of the engineers, physicists, and chemists; i.e., our first interest is in the physical phenomena, and in the mathematics only as it relates to the physics. This difference in approach is not merely of subjective value, but often has led to entirely different problem formulations, especially in regard to boundary conditions. Generally, the physical simulation approach has been more successful.

In this regard, it is interesting to note that most practitioners of computational fluid dynamics are converted theoreticians who still regard themselves as such. The present author's background has been largely experimental. It is hoped that my biases will combine with those of previous authors to produce something new. For it is this author's contention that computational fluid dynamics is a separate discipline, distinct from experimental fluid dynamics and from theoretical fluid dynamics, with its own techniques, its own difficulties, and its own utility.

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*A list of references, arranged alphabetically by the first author and by the year, will be found at the end of this book. For additional texts and a concise evaluation of each, see the literature compilation by Price (1966).

ACKNOWLEDGMENTS

When you work on a book, off and on, for four years, you acquire an impressive indebtedness. As all those authors claim, it really does become impossible to acknowledge everyone who has contributed to the book. But I must acknowledge several people in particular.

Most of the creative (and pleasant) part of this work was done at the University of Kentucky. My good friend, Dr. Charles Knapp, suggested this project to me in 1968, and in 1970 he arranged for my visit to the University. He and Ann arranged housing for my family and provided moral support and friendship to us during our stay. More than any other person except my wife, Dr. Knapp is responsible for the completion of this work.

My stay at Kentucky was made possible by the Chairman of the Mechanical Engineering Department, Dr. Roger Eichhorn. My sincere thanks go to him, to the students in my course, and to those many kind people who gave furniture, dishes, and friendship, particularly Dr. Cliff Cremers, Dr. John Lienhard, Dr. Shiva Singh, Dr. Frank Saggendorf, and Delores Black. My stay at Kentucky was also made possible by my management at Sandia Laboratories, who allowed my leave of absence and who have patiently encouraged the completion of this work; my thanks to Dr. Fred Blottner, Dr. Ken Touryan, and Alan Pope.

In 1967, when this subject was in its infancy, I had the rare good luck to be taught a course in it at Notre Dame by Dr. Steve Piacsek; he has remained a source of enlightenment and inspiration. Also, I would never have become involved in this fascinating area had it not been for the guidance of Dr. T.J. Mueller.

Professor William Oberkampf of the University of Texas at Austin taught a one-semester course from the first three chapters of the manuscript. He found an embarrassing number of manuscript errors and gave many valuable suggestions for improving the textual clarity. I only regret that the remainder of the book has not benefited from the thorough scrutiny of him and his students.

Eva Marie Franks typed most of the difficult manuscript in both the rough-draft and final forms. Bettye Hollingsworth also provided some excellent typing. Rosemary Teasdale edited the manuscript, and Ruth Barth prepared the line drawings.

My wife, Catharine, and our children have been very good sports about this whole thing. Needless to say, it would have been impossible without their support.

I gratefully acknowledge those many friends, colleagues, and acquaintances who encouraged this undertaking. Their support meant a lot.

Finally, my sincere thanks go to Tommy Potter, who found Chapter VI.

P.J.R.

This book is dedicated to Mary and to her University, Notre Dame du Lac.

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CHAPTER I

INTRODUCTION

"Fluid mechanics is especially rich in nonlinearities," (Ames, 1965), as every student of the subject well knows. It is also "rich" in mixed hyperbolic and elliptic partial differential equations, in mathematical singularities of various orders, and in problems with boundary conditions at infinity. In previous years, fluid dynamics has provided a major impetus to the development of partial differential equation theory, complex variable theory, vector and tensor analysis, and nonlinear methods. It is not surprising that, today, fluid dynamics is benefiting from and greatly contributing to the current developments in finite-difference numerical analysis.

However, this book is not concerned with all branches of numerical analysis as applied to fluid dynamics problems. We do not treat the interesting two-point boundary-value problem of ordinary differential equations, which are so fundamental to the calculation of similarity solutions in boundary-layer theory, nor even the important method of characteristics. Rather, we are concerned with that new, and yet emerging, discipline which is perhaps best described by the expression "numerical simulation" of fluid dynamics. The label "computational fluid dynamics" is now coming into use, to vaguely distinguish it from the broader area of "numerical fluid dynamics."

I-A. The Realm of Computational Fluid Dynamics

In earlier days, fluid dynamics, like other physical sciences, was divided into theoretical and experimental branches. The question is, where does computational fluid dynamics stand in relation to these older branches? The answer is that it is separate from each, although it has aspects of both, and that it supplements rather than replaces them.

Computational fluid dynamics is certainly not pure theoretical analysis -- if anything, it is closer to the experimental branch. The existing mathematical theory for numerical solutions of nonlinear partial differential equations is still inadequate. There are no rigorous stability analyses, error estimates, or convergence proofs. Some progress has been made in the questions of existence and uniqueness, but not enough to provide unequivocal answers to specific problems of interest. In computational fluid dynamics, it is still necessary to rely heavily on rigorous mathematical analysis of simpler, linearized, more or less related problems, and on heuristic reasoning, physical intuition, wind tunnel experience, and trial-and-error procedures.

The applied mathematician Biot once made some remarks (Biot, 1956) about applied mathematics in general which seem especially applicable today to computational fluid dynamics. After quoting H. Bateman, who characterized the applied mathematician as a "mathematician without mathematical conscience," Biot went on to discuss the relationship between the applied mathematician and the rigorous science of mathematics. "One could understand the feelings of the artist who undoubtedly benefits from the scientific study of colors but who would be constantly reminded of proceeding with rigorous conformity to the dictates of physics and psychology." The newcomer to computational fluid dynamics is forewarned: In this field, there is at least as much artistry as science.

The numerical simulation of fluid dynamics is then closer to experimental than to theoretical fluid dynamics. The performance of each particular calculation on a computer closely resembles the performance of a physical experiment, in that the analyst "turns on" the equations and waits to see what happens, just as the physical experimenter does. Actual discovery of physical phenomena is possible; thus, Campbell and Mueller (1968) discovered the phenomenon of subsonic ramp-induced separation in a numerical experiment before they verified it in the wind tunnel. But the numerical experimenter has advantages. He has complete control over fluid properties such as density, viscosity, etc. His experimental probe does not disturb the flow. He can run a truly two-dimensional experiment, something virtually impossible in the laboratory. He has enormous flexibility in the choice of flow parameters, e.g., he can arbitrarily select an initial boundary-layer thickness and velocity profile, independent of the Reynolds number per foot and the Mach number, which would be impossible in a wind tunnel. Perhaps most importantly, the numerical experimenter can do what neither the theoretician nor the physical experimenter can do -- he can test the sensitivity of phenomena to independent

theoretical approximations, such as constant viscosity coefficient, neglect of buoyancy forces, unit Prandtl number, the boundary-layer approximations, etc. (One is reminded about the old gag of the novice wind tunnel experimentalist who ordered a railroad tank car full of inviscid, nonconducting, ideal gas.) He can also test the adequacy of the basic constitutive equations, e.g., for a new non-Newtonian fluid model.

But in no sense can numerical experimentation ever replace physical experimentation or theoretical analysis. For one obvious reason, the constitutive continuum equations can never hope to be called exact. For another, the numerical experimenter does not work with the continuum equations. It does not matter that the analogy becomes exact in some limiting case of vanishing mesh size, since we never attain this limit. The act of discretization changes not only the quantitative accuracy, but often changes the qualitative behavior of the equations. Thus, certain forms of the discrete analogs will introduce a kind of viscous behavior, even though the numerical experimenter intended to be using inviscid equations. Another very important limitation is the inability of the numerical experiment to properly account for turbulence or, more generally, any physical phenomenon such as turbulence, slip lines, corner eddies, etc., which are on too small a scale to be accurately resolved in the finite-difference mesh, but which may influence the larger features of the flow. An example of this would be the effect of turbulence in a boundary layer on the separation point. Also, there are examples of physical flows which appear to be two-dimensional but in practice are not, e.g., the reattachment line following "planar" flow separation, and planar flow over a cavity. In such cases, the apparent advantage of true two-dimensionality of the numerical experiment could be deceptive.

Finally, it should be noted that the numerical experiment is as limited as the physical experiment, in that it only gives discrete data for a particular parametric combination. It does not provide any functional relationships, beyond those obtained by dimensional analysis of the governing equations. It is therefore no substitute for even the simplest of theories.

Computational fluid dynamics is, then, a separate discipline, distinct from and supplementing both experimental and theoretical fluid dynamics, with its own techniques, its own difficulties, and its own realm of utility, offering new perspectives in the study of physical processes.

I-B. Historical Outline of Computational Fluid Dynamics

In 1910, L. F. Richardson presented to the Royal Society a 50-page paper which must be considered the cornerstone of modern numerical analysis of partial differential equations. Sheppard had done some previous groundwork in finite-difference operators, but Richardson's contributions overshadow the previous work. He treated the iterative solution of Laplace's equation, the biharmonic equation, and others. He distinguished between steady-state problems "according as the integral can or cannot be stepped out from a part of the boundary," i.e., between hyperbolic and elliptic problems, in modern terminology. He carefully treated numerical boundary conditions, including those at a sharp corner and those at infinity. He obtained error estimates and gave an accurate method of extrapolating answers toward the zero grid space limit, and further suggested checking the accuracy of numerical methods with exact solutions of simple geometries such as a cylinder. Finally, he was the first to actually apply these methods to a large-scale practical problem, that of determining stresses in a masonry dam.*

In Richardson's iteration method for elliptic equations, each point in the mesh in turn at the n-th iteration is made to satisfy the finite-difference equation, which involves "old"

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*Richardson also presented what, in modern vocabulary, must be called a "cost-effectiveness" study of the method, using human computers.

"So far I have paid piece rates for the operation (Laplacian) of about $\frac{n}{18}$ pence per coordinate point, n being the number of digits. The chief trouble to the computers has been the intermixture of plus and minus signs. As to the rate of working, one of the quickest boys averaged 2,000 operations (Laplacian) per week, for numbers of three digits, those done wrong being discounted." (Richardson, 1910, p. 325)

We may all be thankful that social conditions have changed since 1910. Many a computational fluid dynamicist would end up in the poorhouse if he were paid a certain fee per calculation, with "those done wrong being discounted."

values from the (n-1)-th iteration at neighboring points. In 1918, Liebmann showed how to greatly improve the convergence rate merely by using all "new" values as soon as they are available. In this "continuous substitution" scheme, each n-th iteration involves some neighboring point values at the old (n-1)-th iteration and some at the new n-th iteration. In each Liebmann iteration cycle, the most resistant errors are reduced as much as in two cycles of the Richardson procedure (Frankel, 1950).

This comparison exemplifies the tone of numerical analysis of partial differential equations. Seemingly minor modifications of finite-difference forms, iterative schemes, or boundary conditions can result in large improvements. The converse is also true -- plausible and apparently accurate techniques can result in numerical catastrophe. The classic historical example is Richardson's explicit method for the parabolic heat conduction equation. It involves accurate, centered finite-difference approximations for both space and time derivatives; it has been shown (O'Brien et al., 1950) to be unstable for all time steps.*

The emphasis in pre-electronic-computer days was on elliptic equations, or the so-called "jury problem." An early rigorous mathematical treatment of convergence and error bounds for iterative solutions of elliptic equations by Liebmann's method was given by Phillips and Wiener (1923). In 1928, the classic paper of Courant, Friedrichs, and Lewy appeared. The authors were primarily interested in using finite-difference formulations as a tool for pure mathematics (Lax, 1967). By first discretizing the continuum equations, then proving convergence of the discretized system to the continuum system, and finally using algebraic methods to establish the existence of finite-difference solutions, they proved existence and uniqueness theorems for continuum elliptic, parabolic, and hyperbolic systems.** Their work became the guide for practical finite difference solutions in later years.

The first numerical solution of the partial differential equations for a viscous fluid-dynamics problem was given by Thom in 1933. The most sophisticated version of what is still essentially Liebmann's method was presented in 1938 by Shortley and Weller. They developed block relaxation, the trial function method, error relaxation, methods for refining mesh spacings, and error extrapolation. They were also the first to precisely identify and analyze convergence rates.

Southwell (1946) developed a more efficient relaxation method for solving elliptic equations. In this residual relaxation*** method, each point of the mesh is not calculated in turn. Rather, the mesh is scanned for the larger "residuals", and new values are calculated at those points. (In the steady-state heat conduction equation, a "residual" is proportional to the rate of accumulation of energy in the finite-difference cell; hence, a steady-state solution is approached when all residuals approach zero.) An account of sophisticated variants of Southwell's residual relaxation method, including rules for over- and underrelaxation (in which the residual is not set exactly equal to zero), choosing the mesh point to be relaxed, and block relaxation, was given by Fox (1948).

Allen and Southwell (1955) applied Southwell's residual relaxation method by hand calculations in solving the viscous incompressible flow over a cylinder. This was an innovative work in numerical fluid dynamics, in several respects. The authors used a conformal transformation to represent the circular boundary in a regular rectangular mesh. They achieved a computationally stable solution at a Reynolds number of 1000, which is above the physically stable limit. In their hand calculations, they also gained "a distinct impression of instability" at a Reynolds number of 100, and linked this with a physical tendency toward

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*The instability did not manifest itself in Richardson's sample calculations only because of the small number of time-step calculations performed.

**Three companion articles discussing the significance of the 1928 Courant-Friedrichs-Lewy paper, plus an English translation of the paper, appear in the March 1967 IBM Journal (Lax, 1967; Parter, 1967; Widlund, 1967).

***Older papers reserve the term "relaxation" only for Southwell's residual relaxation method. We use the description "residual relaxation" to distinguish clearly from iterative methods such as Liebmann's, which today are also known as relaxation methods.

instability, thus foreshadowing the modern philosophy of numerical simulation. Their work must also stand as a model of resourcefulness in obtaining research funding, being supported by a grant made to London's Imperial College in 1945 by the Worshipful Company of Clothworkers!

Southwell's method is not so readily adaptable to electronic computers. The human computer can scan a matrix for the largest residual much faster than he can perform the arithmetic. For the electronic computer, the gain of scanning speed over arithmetic speed is not nearly as large, and it becomes more efficient to simply relax every mesh point residual in turn to zero, which is identically Liebmann's method.

Electronic computers thus gave motivation to the further development of a Liebmann-type procedure which might utilize the advantage of the overrelaxation concept of Southwell's residual relaxation. In 1950, Frankel (and independently Young, 1954) presented a method which he called the "extrapolated Liebmann method," which has since come to be known as the "successive overrelaxation" (Young, 1954), or "optimum overrelaxation" method. Frankel also noted the analogy between iterative solutions of elliptic equations and the time-step solution of parabolic equations, which was to have important consequences.

The development of electronic computers also focused attention on parabolic problems, since time-history solutions now became feasible. In Richtmyer's first book (1957), which contributed greatly to the development of one-dimensional fluid dynamics, he presented more than 10 numerical schemes. The first of the implicit methods which, for multidimensional problems, require iterative solutions at each time step, was the Crank-Nicolson method published in 1947. This method is still one of the most popular, and is the basis for the most widely used non-similar boundary-layer calculation method (Blottner, 1970).

Of undeterminable origin is the idea of using an asymptotic time solution of the unsteady flow equations to obtain a steady-state solution. It is doubtful that anyone could have seriously considered it before the age of electronic computers.

Much of the pioneering work in computational fluid dynamics was done at the Los Alamos Scientific Laboratory. It was at Los Alamos that J. von Neumann, during World War II, developed his criterion for stability of parabolic finite-difference equations and presented a method of analyzing a linearized system. His brief open-literature description of the method (Charney et al., 1950) did not appear until 1950.* This important paper also presented the first large-scale meteorological calculation of the nonlinear vorticity equations. The authors explained the advantage of stability of the vorticity equations over the primitive equations and presented heuristic arguments for their treatment of the mathematically incomplete problem of upstream and downstream boundary conditions for a nonsteady problem.

In the mid-fifties, Peaceman and Rachford (1955) and Douglas and Rachford (1956) presented efficient methods for solving an implicit form of the parabolic equation which allowed for arbitrarily large time steps. Known as the "alternating direction-implicit" (or simply ADI) methods, they were also applied to the solution of elliptic problems, the transfer being based on the analogy of Frankel (1950) of the time step of a parabolic equation and the iteration number for an elliptic equation. ADI methods are probably the most popular methods used for incompressible flow problems using the vorticity transport equation.

In 1953, DuFort and Frankel presented their "leapfrog" method for parabolic equations, which, like ADI methods, allows for arbitrarily large time steps (in the absence of advection terms) and has the advantage of being fully explicit. This method was used by Harlow and Fromm (1963) in their well-known numerical solutions of the time-dependent vortex street.

Their *Scientific American* article (Harlow and Fromm, 1965) especially served to excite widespread interest among the U.S. scientific community in the potentialities of computational fluid dynamics. At almost the same time, a similar article by Macagno appeared in the French magazine *La Houille Blanche* (Macagno, 1965). In both these articles, the concept of numerical simulation, or computer experiment, was clearly stated for the first time. With the appearance of these two articles, we can date the emergence of computational fluid dynamics as a separate discipline.

All the time-dependent solutions mentioned so far had encountered an upper Reynolds-number limit to computational stability. (Fundamentally, the limit is on the Reynolds number of the

*A more complete elucidation was given in 1950 by O'Brien, Hyman, and Kaplan.

finite-difference cell spacing.) In 1966, Thoman and Szewczyk achieved apparently unlimited computational stability by the use of upwind differencing of advection terms and by careful attention to boundary conditions. Their calculations of flow over a cylinder extended to a Reynolds number of one million, and they were even able to "spin" the cylinder and obtain Magnus lift, with no computational instability developing. The agreement of their calculations with experimental values, in spite of the fact that the method has only first-order accuracy, forced a reappraisal of the importance of the formal truncation order in partial differential equations. In this regard, the work of Cheng (1968), which clarified the dominant effect of numerical boundary conditions, is of considerable importance.

The direct (noniterative) Fourier method for solving the elliptic Poisson equation had been known for some time (e.g., see Forsythe and Wasow, 1960) but had not been used in a fluid dynamics problem. Hockney (1965) used a related (but faster) method to solve large Poisson problems very efficiently. Since his paper, direct methods for the Poisson equation have been used more extensively.

The methods described so far have been applicable to subsonic incompressible fluid flow problems. Supersonic flow problems differ from the subsonic in several important aspects, most importantly in that shock waves (discontinuities in the solutions) may develop in supersonic flow.

The fundamental paper on the numerical treatment of hyperbolic equations was published by Courant, Friedrichs, and Lewy in 1928. The "characteristic" properties are discussed and the well-known method of characteristics is outlined. They also presented and explained the famous Courant-Friedrichs-Lewy necessary stability condition; that, in a numerical grid which does not follow the characteristic directions, the finite-difference domain of dependence must at least include the continuum domain of dependence. This CFL stability requirement (which, stated in modern vocabulary, simply requires that the "Courant number" be less than one) holds in both Lagrangian and in Eulerian systems.

Lagrangian methods which "follow the particles" were developed to a high sophistication by the Los Alamos group (Fromm, 1961). Eulerian methods are generally preferable for two-dimensional problems, but the problem of shock resolution is aggravated in the Eulerian system. If the mesh spacing is not smaller than the shock thickness, oscillations develop which destroy accuracy. These oscillations in a finite mesh are physically meaningful (Richtmyer, 1957) The ordered kinetic energy of the velocity defect across the shock is being converted to internal energy by random collisions of molecules, the computational molecules being the finite-difference cells.

The most common treatment of shock waves in an Eulerian mesh involves smearing out the shock over several cells by the introduction of an artificial dissipation, explicit or implicit, which does not destroy the solution away from the shock waves. In 1950, von Neumann and Richtmyer proposed their artificial dissipation scheme in which the "viscosity coefficient" is proportional to the square of the velocity gradient. Ludford, Polacheck, and Seeger (1953) simply used large values of physical viscosity in the viscous equations in a Lagrangian mesh, but unrealistically high values of viscosity are required in this method.

Instead of using explicit viscosities, the implicit dissipation of the finite differences may be enough to smear out the shock. This is used in the well-known Particle-in-Cell, or PIC, method of Evans, Harlow, and others at Los Alamos*, in Lax's method (Lax, 1954) and others.

The 1954 paper by Lax is far less important for the numerical scheme presented therein than for the form of the differential equations used -- the conservation form. Lax showed that, by recasting the usual equations which have velocities, density, and temperature as dependent variables, a set of equations which have momenta, density, and stagnation specific internal energy can be derived. This new set of equations shows the nature of the physical conservation laws involved and allows overall integral properties to be maintained identically in the finite-difference system. This system of equations is now in common use in calculations of shock development, regardless of the finite-difference methods used, since the exact planar shock speed will be produced by any stable method (see Longley, 1960, and Gary, 1964).

Shock smearing is also accomplished by implicit dissipation terms in several other methods. The Lax-Wendroff method (1960), or two-step versions of it such as Richtmyer's (1963), is now

*See Evans and Harlow (1957, 1958, 1959), Harlow et al., (1959), Evans et al., (1962), and Harlow (1963).

widely used. The PIC technique (see previous footnote) and the EIC (explosive-in-cell) variation by Mader (1964) attain smearing by the use of a finite number of computational particles. This concept also permits delineation of fluid interfaces (Harlow and Welch, 1965 and 1966; Daly, 1967). The PIC method, like the earlier Courant-Isaacson-Rees method (1952), uses one-sided differences for the first spatial derivatives, thus introducing a kind of numerical viscosity (see Chapter III); but these methods do retain the true characteristic sense of the differential equations. Although all these methods contain implicit shock-smearing dissipation terms, each does require additional explicit artificial dissipation terms to achieve stability for particular conditions.

As an alternate to smearing the shock over several computational cells, one may actually maintain the discontinuity. Moretti and Abbett (1966B) and Moretti and Bleich (1967) calculated the inviscid supersonic flows using shock fitting, and this approach has become very popular in the early 1970's.

For an excellent broad treatment of nonlinear numerical methods, the recent books by Ames (1965, 1969) are recommended. The books by Richtmyer (1957) and Richtmyer and Morton (1967) are recommended for the mathematical aspects of numerical treatment of parabolic and hyperbolic systems, including shock-wave problems and neutron diffusion. The rigorous mathematical text of Forsythe and Wasow (1960) is recommended for elliptic equations. A forthcoming Academic Press book by Moretti will give details of the shock-fitting method.

I-C. Existence and Uniqueness of Solutions

The mathematical problems of existence and uniqueness of solutions to the partial differential equations (PDE) of fluid flow are far from settled, for both the continuum equations (PDE) and for their analogous finite-difference equations (FDE). Ladyzhenskaya (1963) has devoted her monograph to these problems for steady viscous incompressible flow. A readable précis of her work is given by Ames (1965). Based on comparison of the incompressible Navier-Stokes equations with other problems, Ames (page 480) conjectures that a unique steady solution exists only below an undefined Reynolds-number limit, that several solutions exist for a range of Re above this limit, and that no solutions exist above a second undefined Reynolds number. (However, he also rightly questions the validity of the steady-state Navier-Stokes equations themselves above a certain Re, since turbulence then occurs.) Such problems may be aggravated in the finite-difference analog when boundary conditions are vague.

For the compressible-flow problem with completely hyperbolic equations (supersonic flow), the existence for the inviscid limit is easily shown. Foy (1964) has also shown that a continuous viscous solution exists between any two states which can be connected by a sufficiently weak shock. For more general states and for mixed-flow problems, it appears that nothing really helpful is known.*

Existence of solutions is somewhat less a problem if we compute the unsteady equations, the approach which has proved most generally successful for the complete viscous flow equations. Since we have some confidence in the time-dependent Navier-Stokes equations, we are inclined to believe that a numerical solution which proceeds from a physically reasonable initial condition has validity. If no steady-state solution exists, we may detect that fact with the time-dependent finite-difference simulation. It does occur, however, that a continuum flow which is unstable to small disturbances will remain stable in a computational simulation. This can arise in both large-scale instability such as vortex shedding, and in small-scale shear-layer turbulence. Further, any approximation made to the complete Navier-Stokes equations (e.g., a Bousinesq linearization) also degrades confidence in the existence of solutions. This is especially true if one is experimenting with unproved constitutive equations, or equations of state. Godunov and Semendyayev (1962) say that the numerical solution to gas-dynamics problems can be made nonunique by a certain class of equations of state.

The question of uniqueness of an attained numerical solution is even more worrisome, simply because there are many examples, physical and purely mathematical, of nonuniqueness of steady-state solutions. The most obvious examples of physically nonunique flow situations are provided by the bistable fluid flip-flop devices, and the bistable vortex filament orientation caused by flow over a spherical cavity (Snedeker and Donaldson, 1966). These involve a

*Current research papers which treat these questions may be found in the journal, *Archive for Rational Mechanics and Analysis*, edited by C. Truesdell and J. Serrin, and published by Springer-Verlag.

kind of mirror symmetry choice. A more significant nonunique flow is exemplified by the stall hysterisis of an airfoil -- with identical boundary conditions, the airfoil exhibits completely different flow patterns at angles of attack near stall, depending on whether that angle of attack was approached from the low (unstalled) side or the high (stalled) side. McGlaughlin and Greber(1967) give other examples where flow separation is nonunique. Piacsek (1968) has calculated nonunique patterns of steady-state natural convection vortex cells, which probably have physical counterparts. The present author has calculated examples of what resembles supersonic diffuser stall (see Chapter III, Section C-8). This is a particular example of the computational nonuniqueness arising from numerical treatment of boundary conditions, although the physical counterpart does exist.

Ames (1965) gives an example of a quasi-linear elliptic differential equation which does not possess uniqueness. Another simple mathematical example of nonuniqueness is provided by classical oblique shock-wave theory. For supersonic inviscid flow over a wedge, three solutions to Thompson's cubic equation (Anon., 1953) exist. One solution causes a decrease in entropy and is discarded.* Of the remaining two, the "weaker" solution is known to correspond to physical flow over a wedge, whereas the "stronger" solution applies to detached shock problems.

In all these examples, the pertinent question is this: Towards *which* solution, if any, would a numerical scheme converge? No answer is available. We must depend on physical experience, i.e., experiment and intuition, to check the reasonableness of the solutions. More rigorous criteria must await better mathematical groundwork, which appears far in the future.

I-D. Preliminary Remarks on Consistency, Convergence, and Stability of Solutions

The mathematical foundations for the questions of convergence and stability of numerical schemes are well-developed only for linear systems. The results from linear theory are used as guidelines to nonlinear problems, the justification depending on numerical experiments.

The essence of a finite-difference numerical scheme is the replacement of derivatives such as $\partial f/\partial x$ in the differential equations by ratios of finite differences such as $\Delta f/\Delta x$ in the finite-difference equation. A *convergent* finite-difference scheme is defined mathematically as one in which all values of the finite-difference solution approach the continuum differential-equation solution as the finite-difference mesh size approaches zero.

This concept is more subtle than it appears at first glance. It is not simply a restatement of Newton's limit definition of a derivative; the limit behavior here is the limit of the whole solution of the differential equation, not merely the individual terms (differentials) of the equation. This latter property is termed the "consistency" condition (Lax and Richtmyer, 1956). For example, a finite-difference analog to a differential equation may have *consistent* finite differences, but be unstable and therefore *not convergent*. Further, the problem of practical convergence *criteria* has been neglected.

Stability has been defined by O'Brien, Hyman, and Kaplan (1950) and by Eddy (1949) in terms of the growth or decay of roundoff errors. Lax and Richtmyer (1956) define stability more generally, by requiring a bounded extent to which any component of the initial data can be amplified in the numerical procedure.

The equivalence theorem of Lax is of fundamental importance. It states that, for a consistent finite-difference scheme, stability is a necessary and sufficient condition for convergence, for a linear system of equations.

Von Neumann's stability criterion (Charney et al., 1950; O'Brien et al., 1950) is that the largest eigenvalue of the amplification matrix of the iteration scheme be less than unity minus terms of the order of the truncation error. Lax and Richtmyer (1956) demonstrate that this is sufficient for stability for a linear system with constant coefficients and that, if the amplification matrix satisfies any of three sets of properties, it is also sufficient for stability. These and other stability questions are discussed in Chapter III, Section A, and in Richtmyer and Morton (1967).

At this stage, we point out that neither the linearized analysis nor even the stability definitions are completely satisfactory. Phillips (1959) has given an example of what he

*Discarding this solution of a rarefaction shock can be automatically satisfied in a finite-difference scheme (see Lax, 1954).

termed nonlinear stability; it occurs because of nonconstant coefficients (Lilly, 1965). Thommen (1966) has shown that the two-step Lax-Wendroff, or Lax-Wendroff-Richtmyer (Richtmyer, 1963) method develops a nonlinear instability near a stagnation point. These examples show that linearized analysis and constant-coefficient analysis can fail to predict instabilities. Even more fundamentally, the definition of stability appears inadequate. Lilly (1965) shows that the midpoint leapfrog rule applied to a model equation results in oscillations, not bounding the correct solution. The equation used corresponds to the infinite Reynolds-number limit of the incompressible vorticity equation. The present author has shown that the oscillation also persists at decreased amplitude, even at low Reynolds number, when a steady-state solution is approached. This oscillation is something we would like to call a numerical "instability," yet the results are "stable" by the commonly used definitions of error growth or boundedness. Also, since the results do not oscillate about the correct solution, we cannot say with certainty that the correct solution will be approached as $\Delta x, \Delta t \to 0$. Yet we do know that, as Re is decreased, the correct solution is approached, so that, at a low but nonzero Re, we may get "close enough" to the solution for practical purposes. Thus, the results may be nonconvergent in the mathematical sense, but convergent in a practical sense.

Further, none of the analyses to date have accounted for the effect of such mathematically untidy boundary conditions as the various schemes used at downstream boundaries. Eddy (1949) and a few more recent authors have considered the stability effect of gradient boundary conditions. The destabilizing effect of boundary treatments is very frequently of first importance.

It is clear, then, that elegant mathematical analyses and definitions of stability for numerical schemes should not be treated as an end in themselves, but only as rational supports and guidelines for the numerical experimentation. It is this approach that will be emphasized in this book.

CHAPTER II

INCOMPRESSIBLE FLOW EQUATIONS IN RECTANGULAR COORDINATES

In this chapter, the equations used in solving two-dimensional incompressible flow problems in rectangular coordinates will be presented. Following the statement of the "primitive" equations, the vorticity-stream function equations will be derived. The "conservation" form of the vorticity transport equation will then be presented, although its significance will not become clear until the next chapter, and different normalizing systems will be discussed. Finally, two one-dimensional model equations for vorticity transport, the Burgers equation and the linearized one-dimensional advection-diffusion equation, will be presented.

II-A. Primitive Equations

The fundamental equations for two-dimensional incompressible flow of a Newtonian fluid with no body forces and constant properties are the two momentum equations (Navier-Stokes) and the continuity equation (see, e.g., Lamb, 1945, or Schlichting, 1968).

$$\frac{\partial \bar{u}}{\partial \bar{t}} + \bar{u}\frac{\partial \bar{u}}{\partial \bar{x}} + \bar{v}\frac{\partial \bar{u}}{\partial \bar{y}} = -\frac{1}{\bar{\rho}}\frac{\partial \bar{P}}{\partial \bar{x}} + \bar{\nu}\left(\frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{u}}{\partial \bar{y}^2}\right) \tag{2-1}$$

$$\frac{\partial \bar{v}}{\partial \bar{t}} + \bar{u}\frac{\partial \bar{v}}{\partial \bar{x}} + \bar{v}\frac{\partial \bar{v}}{\partial \bar{y}} = -\frac{1}{\bar{\rho}}\frac{\partial \bar{P}}{\partial \bar{y}} + \bar{\nu}\left(\frac{\partial^2 \bar{v}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{v}}{\partial \bar{y}^2}\right) \tag{2-2}$$

$$\frac{\partial \bar{u}}{\partial \bar{x}} + \frac{\partial \bar{v}}{\partial \bar{y}} = 0 \tag{2-3}$$

The overbars represent dimensional quantities. These equations are written in the primitive variables of velocity components, u and v, and pressure, P, and the fluid properties of mass density, ρ, and kinematic viscosity, ν. They are based on the following physical laws: equations (2-1) and (2-2) are the vector components of Newton's second law of motion $\vec{F} = m\vec{a}$, with viscous forces related to rate of strain through a linear Newtonian shear stress law; equation (2-3) is a statement of conservation mass. The equations are written in an Eulerian frame of reference, i.e., a space-fixed reference through which the fluid flows. (The alternate Lagrangian description, in which the reference frame moves with the fluid, will not be used in this book, although some references will be given in Chapter VI.) Although it is possible to obtain numerical solutions from these equations (see Section III-G), most successful numerical solutions have utilized the vorticity-stream function approach. The advantages and disadvantages of the vorticity-stream function approach will be discussed in a later section; for now, we note the pedagogical advantage that only *one* transport equation need be treated.

II-B. Stream Function and Vorticity Transport Equations for Planar Flows

The pressure is eliminated from equations (2-1) and (2-2) by cross-differentiating equation (2-1) with respect to y and equation (2-2) with respect to x. Defining the vorticity as*

$$\bar{\zeta} = \frac{\partial \bar{u}}{\partial \bar{y}} - \frac{\partial \bar{v}}{\partial \bar{x}} \tag{2-4}$$

one obtains the parabolic vorticity transport equation

$$\frac{\partial \bar{\zeta}}{\partial \bar{t}} = -\bar{u}\frac{\partial \bar{\zeta}}{\partial \bar{x}} - \bar{v}\frac{\partial \bar{\zeta}}{\partial \bar{y}} + \bar{\nu}\left(\frac{\partial^2 \bar{\zeta}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{\zeta}}{\partial \bar{y}^2}\right) \equiv -\vec{\bar{V}}\cdot(\bar{\nabla}\bar{\zeta}) + \bar{\nu}\bar{\nabla}^2\bar{\zeta} \tag{2-5}$$

*In three dimensions, vorticity is customarily defined as $\nabla \times \vec{V}$, which, when reduced to two dimensions, gives the negative of the present definition.