# 1 Introduction and Background

## 1.1 Introduction

During the last few decades, computational fluid dynamics (CFD) has emerged as an indispensable tool for aerodynamic analysis and design. Recently, however, it has been on a plateau where attached smooth flows can be very accurately predicted, but simulations of separated and turbulent flows continue to be subject to a significant level of uncertainty. In the context of aircraft design, we can now rely on CFD to predict the performance of a commercial aircraft at its design condition for long range cruise but not to predict its behavior at off design conditions such as stall, nor to accurately predict the performance of its high lift system. The very rapid strides currently being made in high performance computing systems are now presenting us with the opportunity to move CFD to an entirely new level within the near future. It will soon be feasible to perform large eddy simulations (LES) in the proper Reynolds number range for hitherto intractable problems of turbulent flows over realistic configurations.

Looming further downstream is the prospect of using direct numerical simulation (DNS) to resolve the full range of turbulent scales in industrial applications. This book aims to expose the kind of thinking that has brought CFD to its present level and will be needed to advance it to the new levels of fidelity that are now within reach.

The main focus of the book is the design and analysis of numerical algorithms for computational aerodynamics. Applications in aeronautical sciences, in particular the need to predict transonic and supersonic flows over complex configurations, have played a key role in driving the emergence of CFD as a distinct discipline during the past 50 years. The importance of transonic flow stems from two reasons. First, it is the most efficient regime for long range flight of jet aircraft. Second, due to its inherent nonlinearity, it has proved intractable to solution by analytical methods. Accordingly, once sufficiently powerful computers became available around 1970–1980, a resort to numerical solution offered the only route forward. It was soon discovered, however, that classical numerical methods were unable to produce acceptable results for flows with shock waves, generally exhibiting spurious oscillations of large amplitude. These difficulties were resolved through the development of a variety of high resolution shock capturing algorithms, which are a major subject of this text. While these techniques had their birth in aeronautical science, they are applicable to systems of nonlinear conservation laws in general, and they have successfully

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transferred to other branches of computational science, most notably to numerical simulations in astrophysics.

## 1.2 Focus and Historical Background

### 1.2.1 Classical Aerodynamics

This chapter surveys some of the principal developments of computational aerodynamics, with a focus on aeronautical applications. It is written with the perspective that computational mathematics is a natural extension of classical methods of applied mathematics, which has enabled the treatment of more complex, in particular nonlinear, mathematical models, and also the calculation of solutions in very complex geometric domains not amenable to classical techniques such as the separation of variables.

This is particularly true for aerodynamics. Efficient flight can be achieved only by establishing highly coherent flows. Consequently there are many important applications where it is not necessary to solve the full Navier–Stokes equations in order to gain an insight into the nature of the flow, and useful predictions can be made with simplified mathematical models. It was already recognized by Prandtl in 1904 (Prandtl 1904, Schlichting & Gersten 1999), essentially contemporaneous with the first successful flights of the Wright brothers, that in flows at the large Reynolds numbers typical of powered flight, viscous effects are important chiefly in thin shear layers adjacent to the surface. While these boundary layers play a critical role in determining whether the flow will separate and how much circulation will be generated around a lifting surface, the equations of inviscid flow are a good approximation in the bulk of the flow field external to the boundary layer. In the absence of separation, a first estimate of the effect of the boundary layer is provided by regarding it as increasing the effective thickness of the body. This procedure can be justified by asymptotic analysis (Van Dyke 1964, Ashley & Landahl 1985).

The classical treatment of the external inviscid flow is based on Kelvin's theorem that in the absence of discontinuities, the circulation around a material loop remains constant. Consequently an initially irrotational flow remains irrotational. This allows us to simplify the equations further by representing the velocity as the gradient of a potential. If the flow is also regarded as incompressible, the governing equation reduces to Laplace's equation. These simplifications provided the basis for the classical airfoil theory of Joukowsky (Glauert 1926) and Prandtl's wing theory (Prandtl & Tietjens 1957, Ashley & Landahl 1985). Supersonic flow over slender bodies at Mach numbers greater than two is also well represented by the linearized equations. Techniques for the solution of linearized flow were perfected in the period 1935–1950, particularly by W.D. Hayes, who derived the supersonic area rule (Hayes 1947).

Classical aerodynamic theory provided engineers with a good insight into the nature of the flow phenomena and a fairly good estimate of the force on simple configurations such as an isolated wing, but could not predict the details of the flow over the complex configuration of a complete aircraft. Consequently, the primary tool for the development of aerodynamic configurations was the wind tunnel. Shapes were tested and modifications selected in the light of pressure and force measurements together with flow visualization techniques. In much the same way that Michelangelo, della Porta, and Fontana could design the dome of St. Peter's through a good physical understanding of stress paths, so could experienced aerodynamicists arrive at efficient shapes through testing guided by good physical insight. Notable examples of the power of this method include the achievement of the Wright brothers in leaving the ground (after first building a wind tunnel) and more recently Whitcomb's discovery of the area rule for transonic flow, followed by his development of aft-loaded supercritical airfoils and winglets (Whitcomb 1956, 1974, 1976). The process was expensive. More than 20,000 hours of wind tunnel testing were expended in the development of some modern designs, such as the Boeing 747.

### 1.2.2 The Emergence of Computational Aerodynamics and its Application to Transonic Flow

Prior to 1960, computational methods were hardly used in aerodynamic analysis, although they were already widely used for structural analysis. The NACA 6 series of airfoils had been developed during the forties, using hand computation to implement the Theodorsen method for conformal mapping (Theodorsen 1931). The first major success in computational aerodynamics was the introduction of boundary integral methods by Hess and Smith (1962) to calculate potential flow over an arbitrary configuration. Generally known in the aeronautical community as panel methods, these continue to be used to the present day to make initial predictions of low speed aerodynamic characteristics of preliminary designs. It was the compelling need, however, both to predict transonic flow and to gain a better understanding of its properties and character, that was a driving force for the development of computational aerodynamics through the period 1970–1990.

In the case of military aircraft capable of supersonic flight, the high drag associated with high $g$ maneuvers forces them to be performed in the transonic regime. In the case of commercial aircraft, the importance of transonic flow stems from the Breguet range equation. This provides a good first estimate of range as

$$R = \frac{V}{sfc}\frac{L}{D}\log\frac{W_0 + W_f}{W_0}.$$

Here $V$ is the speed, $L/D$ is the lift to drag ratio, $sfc$ is the specific fuel consumption of the engines, $W_0$ is the landing weight, and $W_f$ is the weight of the fuel burnt. The Breguet equation clearly exposes the multi-disciplinary nature of the design problem. A lightweight structure is needed to minimize $W_0$. The specific fuel consumption is mainly the province of the engine manufacturers, and in fact the largest advances during the last thirty years have been in engine efficiency. The aerodynamic designer should try to maximize $VL/D$. This means that the cruising speed should be increased until the onset of drag-rise due to the formation of shock waves. Consequently the best

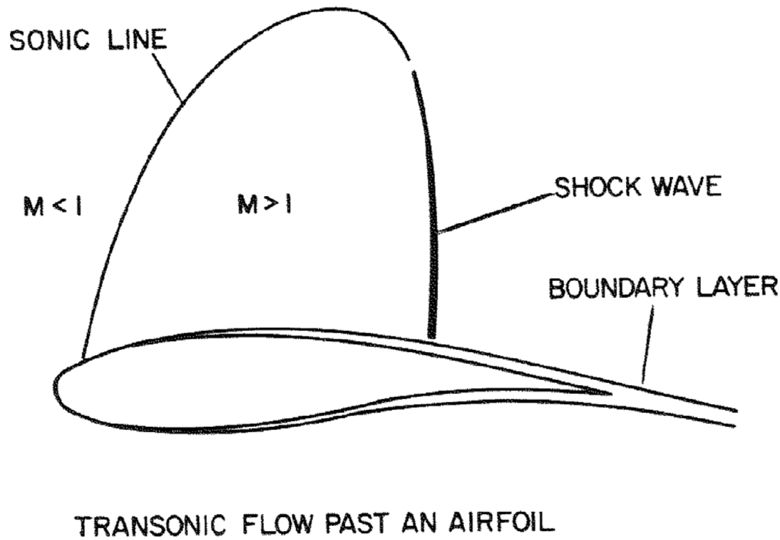


**Figure 1.1** Transonic flow past an airfoil.

cruising speed is in the transonic regime. The typical pattern of transonic flow over a wing section is illustrated in Figure 1.1.

Transonic flow had proved essentially intractable to analytic methods. Garabedian and Korn had demonstrated the feasibility of designing airfoils for shock-free flow in the transonic regime numerically by the method of complex characteristics (Bauer, Garabedian, & Korn 1972). Their method was formulated in the hodograph plane, and it required great skill to obtain solutions corresponding to physically realizable shapes. It was also known from Morawetz's theorem (Morawetz 1956) that shock free transonic solutions are isolated points.

A major breakthrough was accomplished by Murman and Cole (1971) with their development of type-dependent differencing in 1970. They obtained stable solutions by simply switching from central differencing in the subsonic zone to upwind differencing in the supersonic zone and using a line-implicit relaxation scheme. Their discovery provided major impetus for the further development of CFD by demonstrating that solutions for steady transonic flows could be computed economically. Figure 1.2, taken from their landmark paper, illustrates the scaled pressure distribution on the surface of a symmetric airfoil. Efforts were soon underway to extend their ideas to more general transonic flows.

Numerical methods to solve transonic potential flow over complex configurations were essentially perfected during the period 1970–1982. The AIAA First Computational Fluid Dynamics Conference, held in Palm Springs in July 1973, signified the emergence of computational fluid dynamics (CFD) as an accepted tool for airplane design and seems to mark the first use of the name CFD. The rotated difference scheme for transonic potential flow, first introduced by the author at this conference,

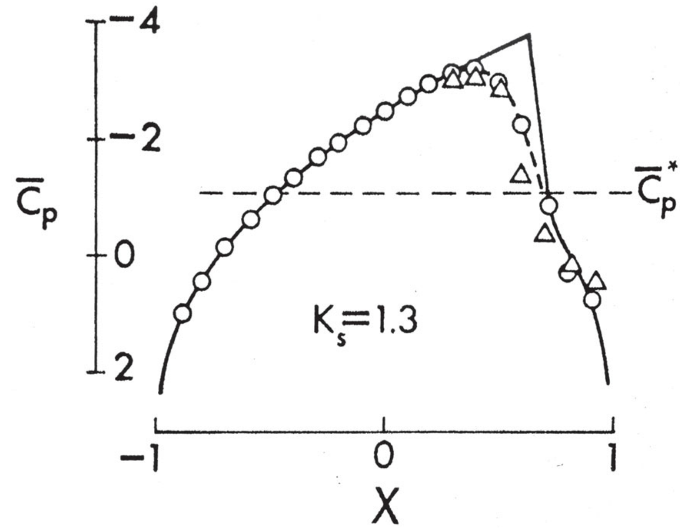


**Figure 1.2** Scaled pressure coefficient on surface of a thin, circular-arc airfoil in transonic flow, compared with experimental data; solid line represents computational result.

proved to be a very robust method, and it provided the basis for the computer program FLO22, developed with David Caughey during 1974–1975 to predict transonic flow past swept wings. At the time we were using the CDC 6600, which had been designed by Seymour Cray and was the world's fastest computer at its introduction, but it had only 131,000 words of memory. This forced the calculation to be performed one plane at a time, with multiple transfers from the disk. FLO22 was immediately put into use at McDonnell Douglas. A simplified in-core version of FLO22 is still in use at Boeing today. Figure 1.3, supplied by John Vassberg, shows the result of a recent calculation using FLO22 of transonic flow over the wing of a proposed aircraft to fly in the Martian atmosphere. The result was obtained with 100 iterations on a 192 × 32 × 32 mesh in 7 seconds, using a typical modern workstation. When FLO22 was first introduced at Long Beach, the calculations cost $3,000 for each run. Nevertheless, they found it worthwhile to use it extensively for the aerodynamic design of the C17 military cargo aircraft.

In order to treat complete configurations, it was necessary to develop discretization formulas for arbitrary grids. An approach that proved successful (Jameson & Caughey 1977) is to derive the discretization formulas from the Bateman variational principle that the integral of the pressure over the domain,

$$I = \int_D p d\xi,$$

is stationary (Jameson 1978). The resulting scheme is essentially a finite element scheme using trilinear isoparametric elements. It can be stabilized in the supersonic zone by the introduction of artificial viscosity to produce an upwind bias. The

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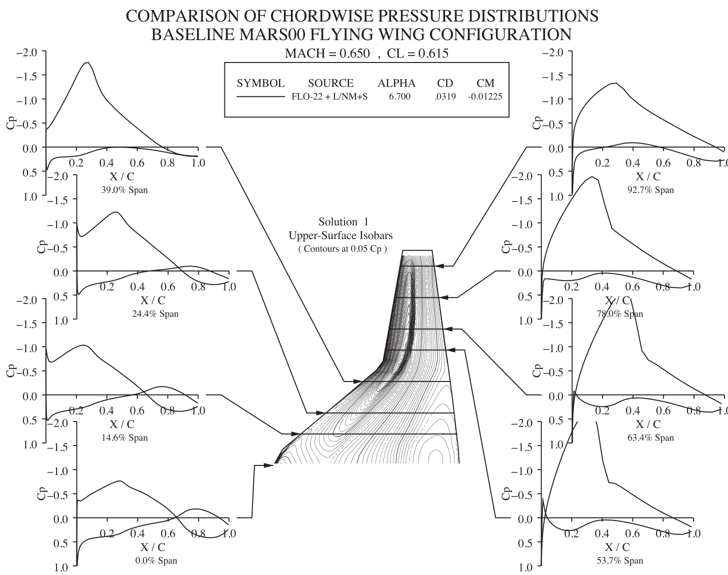


**Figure 1.3** Pressure distribution over the wing of a Mars Lander using FLO22.

"hour-glass" instability that results from the use of one point integration scheme is suppressed by the introduction of higher order coupling terms based on mixed derivatives. The flow solvers (FLO27-30) based on this approach were subsequently incorporated in Boeing's A488 software, which was used in the aerodynamic design of Boeing commercial aircraft throughout the 1980s (Rubbert 1998).

In the same period, Perrier was focusing the research efforts at Dassault on the development of finite element methods using triangular and tetrahedral meshes, because he believed that if CFD software was to be really useful for aircraft design, it must be able to treat complete configurations. Although finite element methods were more computationally expensive, and mesh generation continued to present difficulties, finite element methods offered a route toward the achievement of this goal. The Dassault/INRIA group was ultimately successful, and they performed transonic potential flow calculations for complete aircraft such as the Falcon 50 in the early eighties (Bristeau et al. 1985).

### 1.2.3 The Development of Methods for the Euler and Navier–Stokes Equations

By the 1980s, advances in computer hardware had made it feasible to solve the full Euler equations using software that could be cost-effective in industrial use. The idea of directly discretizing the conservation laws to produce a finite volume scheme had been introduced by MacCormack (MacCormack & Paullay 1972). Most of the early flow solvers tended to exhibit strong pre- or post-shock oscillations. Also, in a workshop held in Stockholm in 1979 (Rizzi & Viviand 1981), it was apparent that none

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of the existing schemes converged to a steady state. These difficulties were resolved during the following decade.

The Jameson–Schmidt–Turkel scheme (Jameson, Schmidt, & Turkel 1981), which used Runge–Kutta time stepping and a blend of second- and fourth-differences (both to control oscillations and to provide background dissipation), consistently demonstrated convergence to a steady state, with the consequence that it has remained one of the most widely used methods to the present day.

A fairly complete understanding of shock capturing algorithms was achieved, stemming from the ideas of Godunov, Van Leer, Harten, and Roe. The issue of oscillation control and positivity had already been addressed by Godunov (1959) in his pioneering work in the 1950s (translated into English in 1959). He had introduced the concept of representing the flow as piecewise constant in each computational cell and solving a Riemann problem at each interface, thus obtaining a first order accurate solution that avoids nonphysical features such as expansion shocks. When this work was eventually recognized in the West, it became very influential. It was also widely recognized that numerical schemes might benefit from distinguishing the various wave speeds, and this motivated the development of characteristics-based schemes.

The earliest higher order characteristics-based methods used flux vector splitting (Steger & Warming 1981) but suffered from oscillations near discontinuities similar to those of central difference schemes in the absence of numerical dissipation. The Monotone Upwind Scheme for Conservation Laws (MUSCL) of Van Leer (1974) extended the monotonicity-preserving behavior of Godunov's scheme to higher order through the use of limiters. The use of limiters dates back to the flux-corrected transport (FCT) scheme of Boris and Book (1973). A general framework for oscillation control in the solution of nonlinear problems was provided by Harten's concept of Total Variation Diminishing (TVD) schemes. It finally proved possible to give a rigorous justification of the JST scheme (Jameson 1995a, 1995b).

Roe's introduction of the concept of locally linearizing the equations through a mean value Jacobian (Roe 1981) had a major impact. It provided valuable insight into the nature of the wave motions and also enabled the efficient implementation of Godunov-type schemes using approximate Riemann solutions. Roe's flux-difference splitting scheme has the additional benefit that it yields a single-point numerical shock structure for stationary normal shocks. Roe's and other approximate Riemann solutions, such as that due to Osher, have been incorporated in a variety of schemes of Godunov type, including the Essentially Nonoscillatory (ENO) schemes of Harten, Engquist, Osher, and Chakravarthy (1987).

Solution methods for the Reynolds averaged Navier–Stokes (RANS) equations had been pioneered in the seventies by MacCormack and others, but at that time they were extremely expensive. By the 1990s, computer technology had progressed to the point where RANS simulations could be performed with manageable costs, and they began to be fairly widely used by the aircraft industry. The need for robust and reliable methods to predict hypersonic flows, which contain both very strong shock waves and near vacuum regions, gave a further impetus to the development of advanced shock capturing algorithms for compressible viscous flow.

## 1.3 Overview of the Simulation Process

The essential steps of developing a numerical simulation of a physical problem can be outlined as follows:

1. Formulate a mathematical model of the physical problem that captures the important aspects for the purpose in hand and can provide the desired accuracy. Here it should be noted that models of widely varying complexity and levels of fidelity can be useful. For example, potential flow models based on Laplace's equation can provide reasonably accurate predictions of low speed aerodynamic flows over streamlined shapes at a low computational cost, and this is very useful at an early stage in the design when rapid turnaround is crucial. At the final stage of the design, one would wish to confirm the expected performance using a model with the highest possible fidelity, typically the Reynolds averaged Navier–Stokes equations in actual practice.
2. Analyze the mathematical properties of the model, such as proper formulation of boundary conditions that ensure the existence and convergence of a solution.
3. Formulate a discrete numerical scheme to approximate the mathematical model that has been selected. Analyze the stability, accuracy, and convergence of the scheme. Can we prove, for example, that the error in the numerical approximation decreases as some power of the mesh spacing when the spacing is progressively reduced?
4. Implement the discrete scheme in software that makes efficient use of the available hardware. This is becoming harder with the emergence of parallel systems with multiple levels of parallelism down to multiple threads within each core of multi-core processing chips, which are in turn arranged in parallel clusters. This stage also requires the use of every possible procedure to assure that the software is actually correct.
5. Validate the software by showing that it produces trustworthy results in practice. Here we should distinguish between the questions of whether the software is correct and whether the selected mathematical model adequately represents the physics. To address the first question, we may test whether the results are correct for some limiting situations for which the true answer is known. For example, an arbitrary body has zero drag in inviscid flow. Or is the numerical solution symmetric for flow over a symmetric profile at zero angle of attack? We should also test the convergence of the numerical solution as the grid is refined. Does it exhibit the expected order of accuracy? We may also compare the results with those obtained by other software developed to solve the same problem. Workshops such as the AIAA Drag Prediction Workshops can play a useful role in this process. Finally, once a sufficiently high confidence level has been established for the software, comparisons with experimental data can be used to address the question of whether the mathematical model adequately represents the physical problem of interest.

While mathematical models of fluid flow and their properties are briefly reviewed in the text, it is mainly focused on the third step in the process, the formulation of discrete schemes that yield proper solutions with the desired accuracy and avoid spurious numerical artifacts.

A primary requirement in aeronautical science is the capability to predict steady flows, such as the flow over an airfoil or wing or the flow over a complete aircraft in cruising flight. Accordingly, the issues associated with the prediction of steady solutions are given a substantial emphasis in the text. Three requirements in particular are:

1. The numerical solution should be capable of converging to an exactly steady state within machine zero. This was not the case for any of the early Euler solvers, as reported in the Stockholm workshop of 1979. It is also not the case for some popular high resolution schemes, such as the ENO scheme, which may reach a limit cycle in which the stencil alternates in successive iterations.
2. If the steady state is approached by advancing in time, the final result should be independent of the time step. This is not true of schemes that are formulated using an integrated space and time discretization, such as the Lax–Wendroff scheme.
3. In simulations of inviscid gas dynamics, there should be constant total enthalpy in the steady state. This is not true of many of the standard high resolution shock capturing schemes.

The rate at which the scheme approaches the steady state is also crucial. This is measured both by the number of iterations required to reach a steady state within some tolerance and also the cost of each iteration. The most widely used methods in current use are actually based on advancing the unsteady flow equations in time with varyingly drastic modifications to accelerate convergence to a steady state. Multigrid schemes have proved particularly effective, and these will be examined in detail.

It turns out that there is a close interplay between steady state methods and implicit time stepping schemes, because the nonlinear equations that need to be solved in each implicit time step have a form that closely resembles the steady state problem. Accordingly, many of the techniques that have proved useful for steady state problems can be directly carried over to the formulation of implicit schemes for unsteady problems. For these reasons, steady state simulation techniques are the subject of careful analysis in this text.