1
Introduction

This monograph deals with the *generalized Riemann problem* (GRP) of mathematical fluid dynamics and its application to computational fluid dynamics. It shows how the solution to this problem serves as a basic tool in the construction of a robust numerical scheme that can be successfully implemented in a wide variety of fluid dynamical topics. The flows covered by this exposition may be quite different in nature, yet they share some common features; they all belong to the class of compressible, inviscid, time-dependent flows. Fluid dynamical phenomena of this type often contain a number of smooth flow regions separated by singularities such as shock fronts, detonation waves, interfaces, and centered rarefaction waves. One must then address various computational issues related to this class of fluid dynamical problems, notably the "capturing" of discontinuities such as shock fronts, detonation waves, or interfaces; resolution of centered rarefaction waves where flow gradients are unbounded; and evaluation of flow variables in irregular computational cells at the intersection of a moving boundary surface with an underlying mesh.

From the mathematical point of view, the various systems of equations governing compressible, inviscid, time-dependent flow phenomena may all be characterized as systems of "(nonlinear) hyperbolic conservation laws."

Hyperbolic conservation laws (in one space variable) are systems of time-dependent partial differential equations. The most common problem associated with such systems is the *initial value problem* (henceforth IVP), which is the following: Given the values of the unknown functions at time $t = 0$ (as functions of the space variable $x \in \mathbb{R}$), use the equations to determine the evolution in time of those functions. When the unknown functions are defined over the whole real line $\mathbb{R}$, one often refers to the IVP as the "Cauchy Problem." In contrast, when the unknown functions are defined only over a finite interval $\mathcal{D} \subseteq \mathbb{R}$, suitable "boundary conditions" must be imposed at the endpoints of $\mathcal{D}$. From the physical point of view the latter is clearly the more realistic case. Thus, for example, $\mathcal{D}$ can represent a pipe of finite length, in which one studies the evolution (in time) of flow variables subject to the system of fluid dynamical equations. In this case, the boundary conditions consist of influx and outflux requirements imposed on the pressure, velocity, etc. at the edges of the pipe.

The solutions to the problems considered here possess one common fundamental property, that of "finite propagation speed"; that is, the waves travel at finite speeds. Mathematically speaking, when a change in the initial data is confined to the neighborhood of some point A, it is "felt" by the solution at any other point B only after a certain amount of time, an amount that depends on the distance between the points. It is precisely this feature that allows the construction of "conservation law schemes" for the (numerical) approximation of the solutions.

Although this monograph focuses on the resolution of compressible, inviscid flow problems, and the construction of suitable conservation law schemes, an effort is made to place the treatment in the broader (theoretical and numerical) perspective of hyperbolic conservation laws. However, the necessary background material from physics is also included. We refer the reader to the classical book by R. Courant and K. O. Friedrichs [30] for a thorough discussion of the mathematical aspects of compressible flow. This book also discusses in detail the derivation of the flow equations from the underlying physical conservation laws. For mathematical treatments of hyperbolic conservation laws, we refer to the books by Courant and Hilbert [31], Evans [36], Hörmander [63], Lax [75], and Smoller [103].

To simplify the discussion, we consider primarily the associated Cauchy problem, thus avoiding the further mathematical complications introduced by boundary conditions. Naturally, when dealing with real flow examples, boundary conditions will be needed, and the ways in which they are introduced into the numerical scheme will be explained.

The origin of the subject matter of this monograph can be traced back some forty years, to the early days of computational fluid dynamics. It can best be described by the opening sentence to Section 12.15 of the book by Richtmyer and Morton [96]: "In 1959, Godunov described an ingenious method for one-dimensional problems with shocks."

Godunov's method, as much as it was recognized for its novelty and robustness, suffered from some significant drawbacks. It was Bram van Leer, some twenty years later, who, in an important breakthrough [112], has shown how to modify Godunov's original construction and, indeed, has made it possible to implement the method as the most efficient tool (to date) in this area of computational fluid dynamics. In the simpler case of a scalar conservation law, these ideas will be explained in Chapter 3.

The monograph is divided into two parts, Part I (Basic Theory) and Part II (Numerical Implementation). Part I (Chapters 2–6) deals with the more basic aspects (theoretical and numerical) of systems of conservation laws and the development of the GRP method. Part II (Chapters 7–10) is devoted to several extensions (physical and geometric) of the GRP method for computational fluid dynamics. A more detailed discussion of the contents will follow. The reader will also find a brief summary at the beginning of each chapter.

In writing this monograph we have aimed at a wide readership, consisting not only of graduate students and researchers in applied mathematics but also of those working in various areas of physics and engineering. Yet, we have attempted to maintain a solid level of mathematical rigor. Notions such as "weak solutions" and "convergence of a scheme" are carefully introduced (Chapter 2) in suitable functional settings. We believe that, given the current mathematical level of modern numerical analysis, such concepts ought to be familiar to anyone working in this field. In particular, theorems related to the convergence of the Godunov scheme (in the scalar case) are proved in all mathematical detail (Section 2.2 and Appendix B). In this context we introduce (and compare numerically) some of the "classical" discrete schemes of hyperbolic equations, such as the Lax–Friedrichs and the Lax–Wendroff schemes. At the same time, our main objective in Chapters 2 and 3 is the introduction of the "high-resolution GRP scheme," by way of the Riemann and generalized Riemann problems. We refer to LeVeque [81] for introductory material on finite-difference schemes for conservation laws and to Richtmyer and Morton [96] for the general theory of finite-difference methods (primarily linear theory). A comprehensive survey of the convergence properties of finite-difference schemes to scalar conservation laws can be found in Godlewski and Raviart [54].

In Chapter 4 we introduce systems of conservation laws. The first section outlines the general mathematical background and can be skipped on first reading, as it is of a more mathematical nature. The physical systems of interest, those representing the basic conservation laws of compressible, inviscid flow in the "quasi-one-dimensional" setting, are introduced in the second section. This section is self-contained; the analysis of centered rarefaction waves, as well as the Rankine–Hugoniot shock conditions and the solution to the Riemann problem, is discussed in detail.

Chapter 5 is devoted to the analysis of the GRP in the context of the systems considered in Section 4.2. In Section 5.1 we study the solution to the linear GRP, which is the core of the GRP method. Given linear initial distributions of the flow variables on the two sides of a jump discontinuity, we determine their instantaneous time derivatives (at that singularity). Van Leer's idea to use this solution for the refinement of Godunov's scheme is implemented in the development of the GRP scheme in Section 5.2.

Chapter 6 is devoted to an investigation of the GRP scheme for fluid dynamics. Numerical results are compared to analytical or asymptotic solutions for a variety of wave interaction problems.

In Chapter 7 we introduce, in rather general terms, the operator-splitting method of Strang. It enables us to extend the GRP algorithm to two-dimensional (2-D) settings, while retaining its second-order accuracy. Chapter 8 deals with further geometric extensions, such as (one-dimensional) "tracking" of singularities and (2-D) moving boundaries.

In Chapter 9 we consider a reacting flow system. The basic set of conservation laws is augmented by a chemical reaction-rate equation, thus providing a simple model of combustion. The GRP algorithm is applied to this extended system.

As a concluding (numerical) example for this monograph, we consider in Chapter 10 a case of wave interaction with a segment of decreasing cross-sectional area in a two-dimensional duct. The major (GRP) numerical approaches developed in Chapters 5, 7, and 8, namely the quasi-1-D approximation and the fully 2-D scheme, are applied to this case. A comparative study of the two solutions sheds light on the nature of the fluid dynamical interaction, as well as on the nature of the quasi-1-D approximation.

Finally, a comment about the numbering system in this book. For the reader's convenience, all theorems, remarks, definitions, claims, etc. within each chapter are sequentially numbered. Thus, for example, Remark 2.22 comes after Definition 2.21 and is followed by Example 2.23.

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Part I

Basic Theory

2
Scalar Conservation Laws

This chapter introduces the basic concepts of the present monograph. In Section 2.1 we review the general theory of (nonlinear) scalar conservation laws and introduce the fundamental notions of weak solutions and Rankine–Hugoniot jump conditions. In Section 2.2 we introduce the basic ideas of discrete approximations, such as accuracy and convergence.

2.1 Theoretical Background

In this chapter we overview the basic details concerning the simplified model of *scalar* conservation laws. This means that we are looking for the solution $u(x, t)$ of the Cauchy problem for a single partial differential equation of the type

$$\frac{\partial}{\partial t}u + \frac{\partial}{\partial x}f(u) = 0, \qquad x \in \mathbb{R}, \quad t > 0, \tag{2.1}$$

$$u(x, 0) = u_0(x), \qquad x \in \mathbb{R}. \tag{2.2}$$

The solution $u(x, t)$ as a function of the space variable $x \in \mathbb{R}$ is sought for all nonnegative time values. The function $f(u)$ is assumed to be smooth (namely, continuously differentiable at least as many times as needed in the analysis).

The term "conservation law" stems from the following argument. Integrating Equation (2.1) over a rectangle $0 \le t \le T$, $x_1 \le x \le x_2$, one gets

$$\int_{x_1}^{x_2} u(x, T)\,dx - \int_{x_1}^{x_2} u_0(x)\,dx = -\int_0^T f(u(x_2, t))\,dt + \int_0^T f(u(x_1, t))\,dt. \tag{2.3}$$

Thinking of $u(x, t)$ as "mass density" (per unit length) we see that the integral $\int_{x_1}^{x_2} u(x, t)dx$ expresses the total mass in $[x_1, x_2]$ at time t, whereas

$\int_0^T f(u(x,t))dt$, for any fixed x, can be interpreted as the "mass flux" to the right at the point x over the time interval $[0, T]$. Thus, Equation (2.3) may be viewed as a "balance equation," stating that the gain in total mass in $[x_1, x_2]$ equals the net flux into the interval through its boundary points x_1 and x_2. Accordingly, we call $f(u)$ the "flux function." In particular, if we let $[x_1, x_2]$ expand to $\mathbb{R} = (-\infty, \infty)$, and we assume that the fluxes diminish to zero [e.g., if $f(0) = 0$ and $u(x_1, t)$, $u(x_2, t)$ vanish as $x_1 \to -\infty$, $x_2 \to +\infty$], Equation (2.3) reduces to

$$\int_{-\infty}^{\infty} u(x,t)\,dx = \int_{-\infty}^{\infty} u_0(x)\,dx, \qquad 0 \le t \le T. \tag{2.4}$$

Clearly, this equation expresses the conservation (in time) of the total mass over the real axis. We refer the reader to LeVeque [81], where Equation (2.1) serves as a model for traffic flow.

A rigorous treatment of the problem (2.1), (2.2) should include a specification of the set of "admissible functions," i.e., the appropriate differentiability requirements needed to make sense out of the equation. In particular, it seems as if a "natural" requirement is that the partial derivatives u_t, u_x exist (and are continuous) at all points $(x, t) \in \mathbb{R} \times (0, \infty)$. However, this is not so, and indeed one of the basic features of conservation laws (both from the mathematical and the physical points of view) is the fundamental role played by discontinuous solutions. In the physical context, they manifest themselves as "shock waves" or "material interfaces." In this chapter we introduce the basic mathematical notions developed in the search for a systematic way in which such discontinuous functions can serve as solutions of (2.1), (2.2)–so-called weak solutions. The purpose here is to outline the main ideas and arguments of the theory, and the reader is referred to Evans [36] for more comprehensive presentations.

We start by looking at the simple case $f(u) = au$, where $a \neq 0$ is a real constant. Equation (2.1) takes now the form of the (constant-speed) advection equation,

$$u_t + au_x = 0, \tag{2.5}$$

for which the solution is easily seen to be the "traveling wave"

$$u(x,t) = u_0(x - at), \qquad x \in \mathbb{R}, \quad t \ge 0. \tag{2.6}$$

In this case the "initial profile" $u_0(x)$ propagates unmodified at a speed a. This "constant-speed propagation" can be seen even more clearly if we note that

Equation (2.5) can be reformulated as

$$\frac{D}{Dt}u(x,t) = 0 \qquad \text{along} \quad \frac{dx}{dt} = a. \tag{2.7}$$

The notation $\frac{D}{Dt}u(x,t)$ introduced in (2.7) designates the "total derivative" (also referred to as the "Lagrangian" or "convective" derivative), namely, the derivative $\frac{d}{dt}u\,(x(t),t)$, where $x = x(t)$ is any line in the family of straight lines satisfying the equation $\frac{d}{dt}x(t) = a$.

Definition 2.1 The lines satisfying

$$\frac{d}{dt}x(t) = a \tag{2.8}$$

are called the "characteristic lines" associated with Equation (2.5).

Thus we can rephrase the aforementioned observation by saying that the solution is constant along characteristic lines.

Remark 2.2 In the more general case where $a = a(x,t)$ in (2.5), one can still define the family of characteristic curves by (2.8), namely, $\frac{d}{dt}x(t) = a(x(t),t)$. Individual curves are uniquely determined by giving the initial point $x(0) = x_0$. As before, we verify the validity of Equation (2.7), where $\frac{D}{Dt}$ is now the derivative along the characteristic curve, implying that u is constant along such a curve. However, as is known from the theory of ordinary differential equations, the existence of the characteristic curves for all $t \geq 0$ is not guaranteed in this case. This is easily seen, for example, in the case $a(x,t) = x^2$ (try the curve passing through $x_0 = 1$, $t_0 = 0$).

Let us now go back to the nonlinear problem (2.1), (2.2). Assuming that u is a smooth (that is, in our case, continuously differentiable) solution, we can write the equation in the form

$$u_t + f'(u)u_x = 0. \tag{2.9}$$

We see that here $f'(u)$ plays the role of the coefficient a in (2.5), and as in (2.7) we get the invariance of the value of u along "characteristic curves," namely,

$$\frac{D}{Dt}u(x,t) = 0 \qquad \text{along} \quad \frac{dx}{dt} = f'(u). \tag{2.10}$$

However, there is a fundamental difference between the characteristic curves

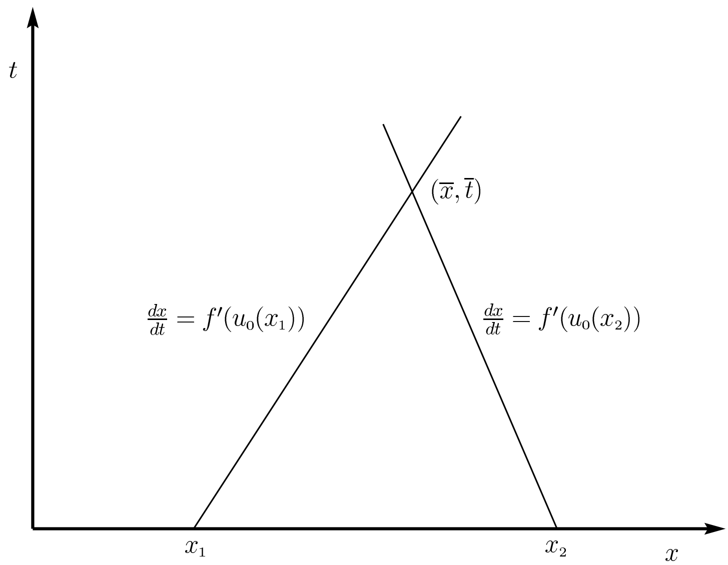

Figure 2.1. Characteristic curves in the nonlinear case.

in the linear case [$a = a(x, t)$] and those of the nonlinear case at hand. Indeed, in the linear case these curves are determined uniquely by $a(x, t)$ and do not depend on the solution function u. However, in the situation given in (2.10) the slopes $f'(u)$ of these curves depend on the solution u itself! Thus, referring to the notation in Figure 2.1, the characteristic curve passing through $(x_1, 0)$ initially has a slope $f'(u_0(x_1))$. Its slope at later times is given by $f'(u(x(t), t))$. However, it follows from (2.10) that $u = constant = u_0(x_1)$ along this curve, so that the slope is constant and equal to $f'(u_0(x_1))$.

We conclude that in the nonlinear case the characteristic curves must be straight lines, at least as long as the solution exists and is smooth. Observe that in the linear case characteristics are straight lines only if $a = constant$.

Consider now another point x_2, where the initial value is $u_0(x_2)$. The characteristic (straight) line through this point has slope $f'(u_0(x_2))$ and it carries the constant value $u = u_0(x_2)$. However, as we see from Figure 2.1, if $x_2 > x_1$ and $f'(u_0(x_2)) < f'(u_0(x_1))$, the two straight lines will intersect at some $t = \overline{t} > 0$. At the point of intersection $(\overline{x}, \overline{t})$ we cannot expect the existence of a smooth (in fact, even continuous) solution, as the two constant values, $u_0(x_1)$ and $u_0(x_2)$, carried by the characteristic curves to that point, are in conflict. Note that this "breakdown in finite time" of the smooth solution does not depend on the smoothness of the initial function $u_0(x)$. From the preceding discussion, we can even assume that $u_0(x)$ is infinitely differentiable and compactly supported (that is, vanishes outside of a finite interval) and still face the same situation [by assigning to two points $x_1 < x_2$ values $u_0(x_1), u_0(x_2)$ such that $f'(u_0(x_1)) > f'(u_0(x_2))$].

Weak Solutions and Jump Conditions

We are thus led to one of the most fundamental aspects of the theory (and its practical application), namely, the inclusion of "discontinuous solutions" as members of the family of admissible solutions. Although this is forced on us in the nonlinear case, there is a natural need for such an extension even in the linear case. For example, we would like to refer to the traveling wave (2.6) as solving Equation (2.5) ($a = constant$) even when $u_0(x)$ is a "step function" (say $u_0(x) = 1$ for $x < 0$ and $u_0(x) = 0$ for $x \geq 0$).

The basic clue to the method that will allow us to activate such a generalization of the concept of a solution may be found in the derivation of the "balance equation" (2.3). As explained there, this equation is obtained by integrating (2.1) over the rectangle $Q^T_{x_1,x_2} = [x_1, x_2] \times [0, T]$. This can also be written as

$$\int_{\mathbb{R}} \int_0^{\infty} (u_t + f(u)_x)\, \chi^T_{x_1,x_2}(x,t)\, dx\, dt = 0, \tag{2.11}$$

$$\chi^T_{x_1,x_2}(x,t) = \begin{cases} 1 & \text{if } (x,t) \in Q^T_{x_1,x_2}, \\ 0 & \text{if } (x,t) \notin Q^T_{x_1,x_2}. \end{cases}$$

The modern theory of partial differential equations has taken this integrated version of the equation one step further, replacing the discontinuous function $\chi^T_{x_1,x_2}(x,t)$ by a smooth "test function" $\phi(x,t)$. This is the well-established procedure of defining "solutions in the sense of distributions" (see Evans [36]). In our case the family of test functions is C^1_0, that is, the class of functions ϕ that are continuously differentiable and vanish outside of some rectangle $Q^T_{-N,N}$ (where T and N depend on ϕ). Assuming that u is a smooth solution of (2.1), multiplying the equation by a test function $\phi(x,t)$, and integrating by parts over $\mathbb{R} \times [0, \infty]$, we obtain

$$\int_{\mathbb{R}} \int_0^{\infty} (u\phi_t + f(u)\phi_x)\, dx\, dt + \int_{\mathbb{R}} \phi(x,0) u_0(x)\, dx = 0. \tag{2.12}$$

The crucial idea in the introduction of discontinuous (henceforth called "weak") solutions is to reverse the procedure leading up to (2.12), by viewing the latter as defining the solution. The rigorous definition is the following: