1

Introduction to Partial Differential Equations

Partial differential equations arise in a number of physical problems, such as fluid flow, heat transfer, solid mechanics and biological processes. These equations often fall into one of three types. **Hyperbolic equations** are most commonly associated with advection, and **parabolic equations** are most commonly associated with diffusion. **Elliptic equations** are most commonly associated with steady states of either parabolic or hyperbolic problems.

Not all problems fall easily into one of these three types. Advection–diffusion problems involve important aspects of both hyperbolic and parabolic problems. Almost all advection problems involve a small amount of diffusion.

It is reasonably straightforward to determine the type of a general second-order partial differential equation. Consider the equation

$$\sum_{j=1}^{d}\sum_{i=1}^{d}\mathbf{A}_{ij}\frac{\partial^2 u}{\partial \mathbf{x}_i\partial \mathbf{x}_j}+\sum_{i=1}^{d}b_i\frac{\partial u}{\partial \mathbf{x}_i}+cu=0.$$

Without loss of generality, we can assume that $\mathbf{A}$ is symmetric, by averaging the coefficients of the $i,\ j$ and j,i derivative terms. By performing a linear coordinate transformation

$$\xi=\mathbf{F}\mathbf{x}$$

we hope to transformation the equation into a simpler form. We will find a way to choose the transformation matrix $\mathbf{F}$ below.

Note that

$$\frac{\partial \xi_i}{\partial \mathbf{x}_j}=\mathbf{F}_{ij}$$

$$\frac{\partial u}{\partial \mathbf{x}_i}=\sum_{j=1}^{d}\frac{\partial u}{\partial \xi_j}\frac{\partial \xi_j}{\partial \mathbf{x}_i}=\sum_{j=1}^{d}\frac{\partial u}{\partial \xi_j}\mathbf{F}_{ji}$$

$$\frac{\partial^2 u}{\partial \mathbf{x}_i\mathbf{x}_j}=\sum_{\ell=1}^{d}\sum_{k=1}^{d}\frac{\partial \xi_k}{\partial \mathbf{x}_i}\frac{\partial^2 u}{\partial \xi_k\partial \xi_\ell}\frac{\partial \xi_\ell}{\partial \mathbf{x}_j}=\sum_{\ell=1}^{d}\sum_{k=1}^{d}\mathbf{F}_{ki}\frac{\partial^2 u}{\partial \xi_k\partial \xi_\ell}\mathbf{F}_{\ell j}$$

After the coordinate transformation, the differential equation takes the form

$$0 = \sum_{j=1}^{d}\sum_{i=1}^{d} \mathbf{A}_{ij}\left[\sum_{\ell=1}^{d}\sum_{k=1}^{d} \mathbf{F}_{ki}\frac{\partial^2 u}{\partial\xi_k\partial\xi_\ell}\mathbf{F}_{\ell j}\right] + \sum_{i=1}^{d} b_i\left[\sum_{j=1}^{d}\frac{\partial u}{\partial\xi_j}\mathbf{F}_{ji}\right] + cu$$
$$= \sum_{\ell=1}^{d}\sum_{k=1}^{d}\left[\sum_{j=1}^{d}\sum_{i=1}^{d}\mathbf{F}_{ki}\mathbf{A}_{ij}\mathbf{F}_{\ell j}\right]\frac{\partial^2 u}{\partial\xi_k\partial\xi_\ell} + \sum_{j=1}^{d}\left[\sum_{i=1}^{d}\mathbf{F}_{ji}b_i\right]\frac{\partial u}{\partial\xi_j} + cu.$$

We would like to choose the matrix $\mathbf{F}$ so that $\mathbf{D} = \mathbf{F}\mathbf{A}\mathbf{F}^\top$ is diagonal. Recall that we can diagonalize a symmetric matrix by means of an orthogonal change of variables. In other words, we can choose $\mathbf{F}$ to be an orthogonal matrix.

If $\mathbf{D}$ has nonzero diagonal entries all of the same sign, the differential equation is **elliptic**. The canonical example of an elliptic equation is the Laplace equation $\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{x}}u = 0$. If $\mathbf{D}$ has nonzero diagonal entries with one entry of different sign from the others, then the differential equation is **hyperbolic**. The canonical example of a hyperbolic equation is the wave equation $\frac{\partial^2 u}{\partial t^2} - \nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{x}}u = 0$. We will discuss simple hyperbolic equations in Chapter 2, and general hyperbolic equations in Chapter 4. If $\mathbf{D}$ has one zero diagonal entry, the equation may be **parabolic**. The canonical example of a parabolic equation is the heat equation $\frac{\partial u}{\partial t} + \nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{x}}u = 0$.

Example 1.0.1 Consider the differential equation

$$\frac{\partial^2 u}{\partial \mathbf{x}_1^2} + \frac{\partial^2 u}{\partial \mathbf{x}_2^2} - \frac{\partial^2 u}{\partial \mathbf{x}_3\partial \mathbf{x}_4} = 0$$

which arises in the Khokhlov–Zabolotskaya–Kuznetsov (KZK) equation for biomedical imaging. In this case, the coefficient matrix is

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1/2 \\ 0 & 0 & -1/2 & 0 \end{bmatrix}.$$

A coordinate transformation that diagonalizes $\mathbf{A}$ is given by

$$\mathbf{F} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

and the new coefficient matrix is

$$\mathbf{D} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & -1/2 \end{bmatrix}.$$

In this case, we see that the KZK equation is hyperbolic.

This book will discuss analytical and numerical methods for solving hyperbolic equations. Our emphasis will be on numerical methods and nonlinear problems, but a knowledge of some analytical approaches will be very useful for computation. Generally, our hyperbolic equations will arise from a physical law describing the conservation of some quantity, such as mass, momentum or energy. These will take a special form, which we will build into our numerical methods, so that our computations conserve these physical quantities as well.

Here is an outline of the analytical approaches in this book, whether they are applied to problems or numerical methods. In Chapter 2 we will study linear hyperbolic conservation laws in a single unknown. We will learn how the solution of such problems depends on initial and boundary data, so that we can construct numerical methods that respect this dependence. We will also develop some simple methods for analyzing the behavior of the numerical methods. First, we will use calculus to see how the approximations in the numerical method cause us to be solving a differential equation that is slightly different from the problem that was posed. This approach, called a modified equation analysis, gives us a qualititative feel for how the method should perform in practice. Second, we will use Fourier analysis to see how the methods propagate waves, and use this analysis to develop the very important Lax equivalence theorem.

In Chapter 3 we will begin our study of nonlinear hyperbolic conservation laws. We will learn about the development and propagation of discontinuities, and see that an understanding of infinitesimal diffusive effects is essential to understanding how nature selects certain solutions to these problems. We will also begin to learn how to build numerical diffusion into our computational methods, so that we can expect to compute the physically correct solutions as well. This numerical diffusion will arise in subtle ways, depending on how how numerical schemes use upwinding and averaging techniques. Some approaches will concentrate on building important analytical information about the wave propagation into the method, while other schemes will assiduously avoid such analytical work. We will apply these methods to problems in traffic flow and oil recovery/contaminant cleanup.

Chapter 4 will discuss hyperbolic systems of conservation laws. This is where the discussion becomes most practical, because the physical applications are so interesting. Once we understand the basic principles underlying the analytical solution of hyperbolic systems, we will perform case studies of shallow water, compressible gas dynamics, magnetohydrodynamics, solid mechanics and flow in porous media. The analytical solution of the equations of motion for these problems for special initial data (Riemann problems) can be very useful in building some of our numerical methods. Unfortunately, this analytical information is often expensive to compute and difficult to program, when it is available. As a result, we will find methods to approximate the solution of Riemann problems.

Amazingly enough, several of these approximate Riemann solvers produce better numerical results than the analytical methods, and at far less cost with far simpler programs.

In Chapter 5 we will try to analyze the numerical methods, and use the analysis to design better methods. We will run into an obstacle due to Godunov: linear schemes that preserve monotonicity are at best first-order accurate. In order to achieve higher-order accuracy, we will design nonlinear schemes, even for use on linear problems. These schemes will be very useful for solving problems with propagating discontinuities. They will not be the most effective schemes for solving linear problems with smooth solutions. We will extend these higher-order numerical schemes to solve hyperbolic systems in Chapter 6, and to solve problems in multiple dimensions in Chapter 7.

But this book is not just about analysis of problems and methods. In each chapter, there are discussions of numerical results and comparisons of numerical methods. It is important that the student learn how to judge when a numerical method is working properly, sometimes by understanding its numerical stability, and often by performing mesh refinement studies to verify the correct order of convergence. Numerical methods can differ greatly in their achieved accuracy even when they have the same nominal order of accuracy. Methods can also differ greatly in their efficiency, meaning how much it costs us to achieve a given accuracy. Unfortunately, there is no best method in this book, that applies to all problems and is always most (or nearly most) efficient.

In order to assist the student in gaining knowledge about the design and performance of numerical methods, we have provided an interactive form of this book. Fortunately, you are currently reading that version. In this way, students can view computer programs to learn about code organization. Students can also run the programs from inside the book, and adjust parameters that control the numerical performance. Through the use of interactive graphics, the student can see the evolution of the numerical solution; this really helps in understanding instability and the spread of discontinuities due to numerical diffusion.

In order to execute programs from inside this book, it was necessary to use graphical user interfaces. These make the selection of program parameters easy once the code is written, but makes the example code somewhat larger than it needs to be just to solve the problem. In order to help the student here, we have provided a series of programs in Section 2.2.3 of Chapter 2. These programs start with short Fortran programs, proceed through more modular Fortran to mixed language programs, and end up with the more complicated program containing interactive graphics and graphical user interfaces. Students can write their own programs in any of these styles, as is appropriate for their experience or the expectations of their instructor.

If the student can learn about mixed language programming, then the discussion on adaptive mesh refinement in Chapter 8 should be interesting. This chapter describes the basic principles behind Marsha Berger's structured adaptive mesh refinement, and describes the basic ideas in the design of the author's adaptive mesh refinement program. The hope is that after study of the applications of adaptive mesh refinement to oil recovery, linear elasticity and gas dynamics, the student can apply adaptive mesh refinement to other research problems.

2

Scalar Hyperbolic Conservation Laws

In numerical analysis or scientific computing courses, it is common to examine ordinary differential equations and some basic numerical methods to solve these problems. In this chapter we will develop several basic numerical methods to solve initial value problems arising from a particular class of partial differential equations, namely scalar hyperbolic conservation laws. In some cases, we will be able to transform the solution of partial differential equations into ordinary differential equations. However, in many practical problems there are physical effects, such as diffusion, that prevent such analytical reductions. These ideas will be developed in Section 2.1.

The design of numerical methods for scalar conservation laws involves principles that are different from those commonly considered in the solution of ordinary differential equations. Some experimentation with obvious numerical discretizations in Section 2.2 will produce surprises, and illustrate the utility of interactive graphical displays in programming. Analysis of these basic numerical methods using Taylor series and Fourier transforms in Sections 2.3 and 2.5 will yield some basic numerical principles, and the limitations of the simple numerical methods.

2.1 Linear Advection

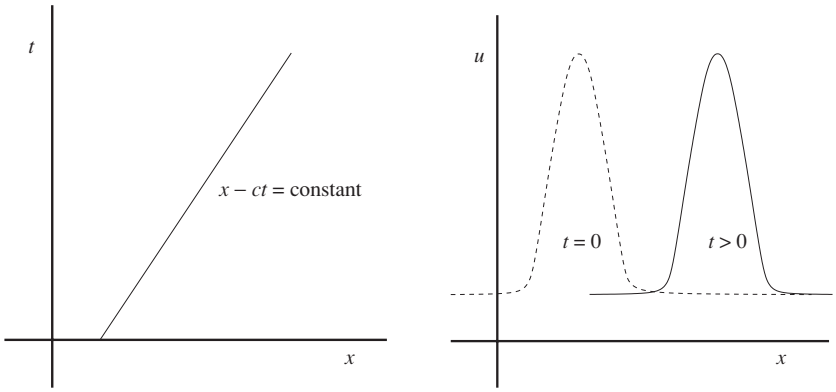
Linear advection describes the motion of some conserved quantity along a constant velocity field. This is the simplest conservation law, but it illustrates many of the important features we will see in more complicated conservation laws.

2.1.1 Conservation Law on an Unbounded Domain

The unbounded linear advection problem takes the form

$$\frac{\partial u}{\partial t} + \frac{\partial cu}{\partial x} = 0 \quad \text{for all } x \in \mathbf{R} \quad \text{for all } t > 0, \tag{2.1a}$$

$$u(x, 0) = u_0(x) \quad \text{for all } x \in \mathbf{R}. \tag{2.1b}$$



(a) Characteristic line (b) Evolution

Fig. 2.1 Characteristics in linear advection

In this initial-value problem, we assume that the velocity c is constant. Then the differential equation (2.1a) can be rewritten in the form

$$0 = \begin{bmatrix} 1, & c \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial t} \\ \frac{\partial u}{\partial x} \end{bmatrix} \quad \text{for all } x \in \mathbf{R} \quad \text{for all } t > 0.$$

This equation says that the gradient of u is orthogonal to a constant vector. It follows that u is constant on lines parallel to that constant vector:

$$\text{for all } (x_0, t_0) \quad \text{for all } \tau \; u(x_0 + c\tau, t_0 + \tau) = \text{constant}.$$

Choosing $\tau = t - t_0$ gives us

$$u(x_0 + c(t - t_0), t) = u(x_0 - ct_0, 0) \equiv u_0(x_0 - ct_0).$$

Given x, choose $x_0 = x - ct + ct_0$ to get

$$u(x, t) = u_0(x - ct).$$

This is a formula for the solution of problem (2.1). It is clear from this formula that the **characteristic** lines

$$x - ct = \text{constant}$$

are especially important. Along a characteristic line, the solution of the conservation law at time $t > 0$ is equal to the initial value at time $t = 0$. These ideas are illustrated in Figure 2.1.

There is an easy way to verify this solution. Suppose that we define the new variables

$$\xi = x - ct, \quad \tau = t \tag{2.2}$$

and the function

$$\tilde{u}(\xi, \tau) \equiv u(x, t). \tag{2.3}$$

Then the chain rule implies that

$$\frac{\partial u}{\partial t} = \frac{\partial \tilde{u}}{\partial \tau} - \frac{\partial \tilde{u}}{\partial \xi} c \quad \text{and} \quad \frac{\partial u}{\partial x} = \frac{\partial \tilde{u}}{\partial \xi}.$$

It follows that $\tilde{u}$ solves the initial value problem

$$0 = \frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = \frac{\partial \tilde{u}}{\partial \tau},$$
$$\tilde{u}(\xi, 0) = u_0(\xi).$$

The differential equation for $\tilde{u}$ shows that $\tilde{u}$ is a function of ξ alone. In summary, after we change to characteristic coordinates the original partial differential equation becomes a system of ordinary differential equations, parameterized by ξ. Further, these ordinary differential equations have the trivial solution

$$\tilde{u}(\xi) = u_0(\xi).$$

2.1.2 Integral Form of the Conservation Law

In general, a **conservation law** in one dimension takes the form

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0. \tag{2.4}$$

Here u is the conserved quantity, and f is the flux. For example, the linear advection flux is $f = cu$.

There is a physical reason for calling Equation (2.4) a conservation law. By integrating over the space-time rectangle $(a, b) \times (0, t)$ and applying the divergence theorem, we obtain

$$\int_a^b u(x, t)\, dx = \int_a^b u(x, 0)\, dx + \int_0^t f(a, \tau)\, d\tau - \int_0^t f(b, \tau)\, d\tau. \tag{2.5}$$

We can interpret the conservation law (2.5) as follows. The quantity u represents a density, *i.e.*, the conserved quantity per length. Thus the spatial integrals represent the total conserved quantity in the interval (a, b) at some advanced time t and the initial time 0. The temporal integrals represent the total amount of the conserved quantity flowing through ends of the interval in space during the given interval in time. Thus equation (2.5) says that the total conserved quantity in the interval (a, b) at time t is equal to the total conserved quantity in the same interval initially, plus what flows into the interval on the left and minus what flows out on the right.

2.1.3 Advection–Diffusion Equation

Many physically realistic problems actually involve some amount of diffusion. For example, the miscible displacement problem described in Section 3.2.2 is a linear advection problem involving a physical diffusion. In general, one-dimensional linear advection with constant diffusion takes the form

$$\frac{\partial u}{\partial t} + \frac{\partial cu}{\partial x} = \frac{\partial}{\partial x}\left(\epsilon \frac{\partial u}{\partial x}\right) \quad \text{for all } x \in \mathbf{R} \quad \text{for all } t > 0, \tag{2.6a}$$

$$u(x, 0) = u_0(x) \quad \text{for all } x \in \mathbf{R}. \tag{2.6b}$$

Here, we assume that the diffusion coefficient satisfies $\epsilon > 0$, so that the conservation law is well-posed. The need for this restriction on ϵ will become obvious in Equation (2.8) below.

Let us transform again to characteristic coordinate $\xi = x - ct$ and time $\tau = t$ as in Equation (2.2) and define the solution $\tilde{u}$ in terms of these coordinates as in (2.3). Then substitution into the advection–diffusion equation (2.6) leads to

$$\frac{\partial \tilde{u}}{\partial \tau} = \epsilon \frac{\partial^2 \tilde{u}}{\partial \xi^2} \quad \text{for all } \xi \in \mathbf{R} \quad \text{for all } \tau > 0,$$

$$\tilde{u}(\xi, 0) = u_0(\xi) \quad \text{for all } \xi \in \mathbf{R}. \tag{2.7}$$

This is the one-dimensional **heat equation** on an unbounded interval. If the initial data u_0 grow sufficiently slowly for large values of its argument, then it is well known that the analytical solution of this equation is

$$\tilde{u}(\xi, \tau) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi\epsilon\tau}} e^{-(\xi - y)^2/(4\epsilon\tau)} u_0(y) dy \equiv \int_{-\infty}^{\infty} G(\xi - y, \tau) u_0(y) dy. \tag{2.8}$$

Here

$$G(\xi, \tau) = \frac{1}{\sqrt{4\pi\epsilon\tau}} e^{-\xi^2/(4\epsilon\tau)}$$

is called the **Green's function**. Because the diffusion constant ϵ is positive, the Green's function is real-valued. Here $\tilde{u}$ is smooth for $t > 0$ because derivatives of $\tilde{u}$ involve derivatives of the smooth Green's function G, and not derivatives of the initial data u_0.

It follows that the solution of the linear advection–diffusion problem (2.6) is

$$u(x, t) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi\epsilon t}} e^{-(x - ct - y)^2/(4\epsilon t)} u_0(y) dy.$$

The lines $x - ct =$ constant are still important, in that they carry the bulk of the initial information for small diffusion, but they are no longer lines along which the solution u is constant.

Note that the Green's function G approaches a delta-function as the diffusion coefficient $\epsilon \to 0$. On the other hand, after sufficiently large time even a small diffusion will spread the effect of disturbances in the initial data over significant intervals in space. If the initial data is zero outside some bounded interval, then at very large times the solution $\tilde{u}$ will decay to zero. These observations are important, because in many practical situations we are interested in the solution of conservation laws obtained in the limit as the diffusion tends to zero. The study of the interplay between small diffusion and large times is an appropriate matter for asymptotics, and would take the current discussion too far astray.

It is sometimes useful to note that the linear advection–diffusion equation (2.6a) is a conservation law. In fact, we can rewrite it in the form

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(cu - \epsilon \frac{\partial u}{\partial x} \right) = 0 \quad \text{for all } x \in \mathbf{R} \quad \text{for all } t > 0.$$

Here the flux $f(x,t) \equiv cu - \epsilon \frac{\partial u}{\partial x}$ is the difference of the advective flux cu and the diffusive flux $\epsilon \frac{\partial u}{\partial x}$. We can develop an integral form of this conservation law by using (2.5).

2.1.4 Advection Equation on a Half-Line

Here is another important modification to the problem (2.1). For both practical and computational purposes, we might be interested in solving a semi-infinite problem with boundary data:

$$\frac{\partial u}{\partial t} + \frac{\partial (cu)}{\partial x} = 0 \quad \text{for all } x > 0 \quad \text{for all } t > 0, \tag{2.9a}$$

$$u(0,t) = v(t) \quad \text{for all } t > 0, \tag{2.9b}$$

$$u(x,0) = u_0(x) \quad \text{for all } x > 0. \tag{2.9c}$$

If we transform to characteristic coordinates as in Equation (2.2), we see that the solution of (2.9) depends on the data $v(t)$ at the left-hand boundary only for $x - ct < 0$. If $c < 0$, this inequality cannot be satisfied for any (x,t) in the problem domain; in other words, no points in the problem domain will depend on the data at the left-hand boundary. Thus in this case we assume that the velocity c is positive: $c > 0$. Since the solution of (2.9) is constant along characteristics, we can easily solve to get

$$u(x,t) = \begin{cases} u_0(x - ct), & x - ct > 0 \\ v(t - x/c), & x - ct < 0. \end{cases}$$