1 Introduction

Partial differential equations (PDEs) form the basis of very many mathematical models of physical, chemical and biological phenomena, and more recently their use has spread into economics, financial forecasting, image processing and other fields. To investigate the predictions of PDE models of such phenomena it is often necessary to approximate their solution numerically, commonly in combination with the analysis of simple special cases; while in some of the recent instances the numerical models play an almost independent role.

Let us consider the design of an aircraft wing as shown in Fig. 1.1, though several other examples would have served our purpose equally well – such as the prediction of the weather, the effectiveness of pollutant dispersal, the design of a jet engine or an internal combustion engine,



Fig. 1.1. (a) A typical (inviscid) computational mesh around an aerofoil cross-section; (b) a corresponding mesh on a wing surface.

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the safety of a nuclear reactor, the exploration for and exploitation of oil, and so on.

In steady flight, two important design factors for a wing are the lift generated and the drag that is felt as a result of the flow of air past the wing. In calculating these quantities for a proposed design we know from boundary layer theory that, to a good approximation, there is a thin boundary layer near the wing surface where viscous forces are important and that outside this an inviscid flow can be assumed. Thus near the wing, which we will assume is locally flat, we can model the flow by

$$u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial y^2} = (1/\rho)\frac{\partial p}{\partial x},\tag{1.1}$$

where u is the flow velocity in the direction of the tangential co-ordinate x, y is the normal co-ordinate, ν is the viscosity, ρ is the density and p the pressure; we have here neglected the normal velocity. This is a typical *parabolic* equation for u with $(1/\rho)\partial p/\partial x$ treated as a forcing term.

Away from the wing, considered just as a two-dimensional crosssection, we can suppose the flow velocity to be inviscid and of the form $(u_{\infty} + u, v)$ where u and v are small compared with the flow speed at infinity, u_{∞} in the x-direction. One can often assume that the flow is irrotational so that we have

$$\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = 0; \tag{1.2a}$$

then combining the conservation laws for mass and the x-component of momentum, and retaining only first order quantities while assuming homentropic flow, we can deduce the simple model

$$(1 - M_{\infty}^2)\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$
 (1.2b)

where M_{∞} is the Mach number at infinity, $M_{\infty} = u_{\infty}/a_{\infty}$, and a_{∞} is the sound speed.

Clearly when the flow is subsonic so that $M_{\infty} < 1$, the pair of equations (1.2a, b) are equivalent to the Cauchy–Riemann equations and the system is *elliptic*. On the other hand for supersonic flow where $M_{\infty} > 1$, the system is equivalent to the one-dimensional wave equation and the system is *hyperbolic*. Alternatively, if we operate on (1.2b) by $\partial/\partial x$ and eliminate v by operating on (1.2a) by $\partial/\partial y$, we either obtain an equivalent to Laplace's equation or the second order wave equation.

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Thus from this one situation we have extracted the three basic types of partial differential equation: we could equally well have done so from the other problem examples mentioned at the beginning. We know from PDE theory that the analysis of these three types, what constitutes a well-posed problem, what boundary conditions should be imposed and the nature of possible solutions, all differ very markedly. This is also true of their numerical solution and analysis.

In this book we shall concentrate on model problems of these three types because their understanding is fundamental to that of many more complicated systems. We shall consider methods, mainly finite difference methods and closely related finite volume methods, which can be used for more practical, complicated problems, but can only be analysed as thoroughly as is necessary in simpler situations. In this way we will be able to develop a rigorous analytical theory of such phenomena as stability and convergence when finite difference meshes are refined. Similarly, we can study in detail the speed of convergence of iterative methods for solving the systems of algebraic equations generated by difference methods. And the results will be broadly applicable to practical situations where precise analysis is not possible.

Although our emphasis will be on these separate equation types, we must emphasise that in many practical situations they occur together, in a system of equations. An example, which arises in very many applications, is the Euler–Poisson system: in two space dimensions and time t, they involve the two components of velocity and the pressure already introduced; then, using the more compact notation ∂_t for $\partial/\partial t$ etc., they take the form

$$\partial_t u + u \partial_x u + v \partial_y u + \partial_x p = 0$$

$$\partial_t v + u \partial_x v + v \partial_y v + \partial_y p = 0$$

$$\partial_x^2 p + \partial_u^2 p = 0.$$
(1.3)

Solving this system requires the combination of two very different techniques: for the final elliptic equation for p one needs to use the techniques described in Chapters 6 and 7 to solve a large system of simultaneous algebraic equations; then its solution provides the driving force for the first two hyperbolic equations, which can generally be solved by marching forward in time using techniques described in Chapters 2 to 5. Such a model typically arises when flow speeds are much lower than in aero-dynamics, such as flow in a porous medium, like groundwater flow. The two procedures need to be closely integrated to be effective and efficient.

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Fig. 1.2. A typical multi-aerofoil: (a) a general view; (b) a detail of the mesh that might be needed for a Navier–Stokes calculation. (Courtesy of DRA, Farnborough.)

Returning to our wing design example, however, it will be as well to mention some of the practical complications that may arise. For a civil aircraft most consideration can be given to its behaviour in steady flight at its design speed; but, especially for a military aircraft, manoeuvrability is important, which means that the flow will be unsteady and the equations time-dependent. Then, even for subsonic flow, the equations corresponding to (1.2a, b) will be hyperbolic (in one time and two space variables), similar to but more complicated than the Euler–Poisson system (1.3). Greater geometric complexity must also be taken into account: the three-dimensional form of the wing must be taken into consideration particularly for the flow near the tip and the junction with the aircraft body; and at landing and take-off, the flaps are extended to give greater lift at the slower speeds, so in cross-section it may appear as in Fig. 1.2.

In addition, rather than the smooth flow regimes which we have so far implicitly assumed, one needs in practice to study such phenomena as shocks, vortex sheets, turbulent wakes and their interactions. Developments of the methods we shall study are used to model all these situations but such topics are well beyond the scope of this book. Present capabilities within the industry include the solution of approximations to the Reynolds-averaged Navier–Stokes equations for unsteady viscous flow around a complete aircraft, such as that shown in Fig. 1.3.

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(Courtesy of British Aerospace.)

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Moreover, the ultimate objective is to integrate these flow prediction capabilities into the complete design cycle – rather than calculating the flow around a given aircraft shape, one would like to design the shape to obtain a given flow.

Finally, to end this introductory chapter there are a few points of notation to draw to the reader's attention. We use the notation \approx to mean 'approximately equal to', usually in a numerical sense. On the other hand, the notation \sim has the precise meaning 'is asymptotic to' in the sense that $f(t) \sim t^2$ as $t \to 0$ means that $t^{-2}[f(t) - t^2] \to 0$ as $t \to 0$. The notation $f(t) = t^2 + o(t^2)$ has the same meaning; and the notation $f(t) = O(t^2)$ means that $t^{-2}f(t)$ is bounded as $t \to 0$. We have often used the notation := to mean that the quantity on the left is *defined* by that on the right. We shall usually use bold face to denote vectors.

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Parabolic equations in one space variable

2.1 Introduction

In this chapter we shall be concerned with the numerical solution of parabolic equations in one space variable and the time variable t. We begin with the simplest model problem, for heat conduction in a uniform medium. For this model problem an explicit difference method is very straightforward in use, and the analysis of its error is easily accomplished by the use of a maximum principle, or by Fourier analysis. As we shall show, however, the numerical solution becomes unstable unless the time step is severely restricted, so we shall go on to consider other, more elaborate, numerical methods which can avoid such a restriction. The additional complication in the numerical calculation is more than offset by the smaller number of time steps needed. We then extend the methods to problems with more general boundary conditions, then to more general linear parabolic equations. Finally we shall discuss the more difficult problem of the solution of nonlinear equations.

2.2 A model problem

Many problems in science and engineering are modelled by special cases of the linear parabolic equation for the unknown u(x, t)

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(b(x,t) \frac{\partial u}{\partial x} \right) + c(x,t)u + d(x,t)$$
(2.1)

where b is strictly positive. An *initial condition* will be needed; if this is given at t = 0 it will take the form

$$u(x,0) = u^0(x)$$
 (2.2)

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Parabolic equations in one space variable

where $u^0(x)$ is a given function. The solution of the problem will be required to satisfy (2.1) for t > 0 and x in an open region R which will be typically either the whole real line, the half-line x > 0, or an interval such as (0,1). In the two latter cases we require the solution to be defined on the closure of R and to satisfy certain *boundary conditions*; we shall assume that these also are linear, and may involve u or its first space derivative $\partial u/\partial x$, or both. If x = 0 is a left-hand boundary, the boundary condition will be of the form

$$\alpha_0(t)u + \alpha_1(t)\frac{\partial u}{\partial x} = \alpha_2(t) \tag{2.3}$$

where

$$\alpha_0 \ge 0, \ \alpha_1 \le 0 \quad \text{and} \quad \alpha_0 - \alpha_1 > 0. \tag{2.4}$$

If x = 1 is a right-hand boundary we shall need a condition of the form

$$\beta_0(t)u + \beta_1(t)\frac{\partial u}{\partial x} = \beta_2(t) \tag{2.5}$$

where

$$\beta_0 \ge 0, \ \beta_1 \ge 0 \quad \text{and} \quad \beta_0 + \beta_1 > 0.$$
 (2.6)

The reason for the conditions on the coefficients α and β will become apparent later. Note the change of sign between α_1 and β_1 , reflecting the fact that at the right-hand boundary $\partial/\partial x$ is an outward normal derivative, while in (2.3) it was an inward derivative.

We shall begin by considering a simple model problem, the equation for which models the flow of heat in a homogeneous unchanging medium, of finite extent, with no heat source. We suppose that we are given homogeneous *Dirichlet boundary conditions*, i.e., the solution is given to be zero at each end of the range, for all values of t. After changing to dimensionless variables this problem becomes: find u(x, t) defined for $x \in [0, 1]$ and $t \ge 0$ such that

$$u_t = u_{xx}$$
 for $t > 0, \ 0 < x < 1$, (2.7)

$$u(0,t) = u(1,t) = 0$$
 for $t > 0$, (2.8)

$$u(x,0) = u^0(x), \text{ for } 0 \le x \le 1.$$
 (2.9)

Here we have introduced the common subscript notation to denote partial derivatives.

2.3 Series approximation

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2.3 Series approximation

This differential equation has special solutions which can be found by the method of *separation of variables*. The method is rather restricted in its application, unlike the finite difference methods which will be our main concern. However, it gives useful solutions for comparison purposes, and leads to a natural analysis of the stability of finite difference methods by the use of Fourier analysis.

We look for a solution of the special form u(x,t) = f(x)g(t); substituting into the differential equation we obtain

i.e.,
$$fg' = f''g,$$

 $g'/g = f''/f.$ (2.10)

In this last equation the left-hand side is independent of x, and the right-hand side is independent of t, so that both sides must be constant. Writing this constant as $-k^2$, we immediately solve two simple equations for the functions f and g, leading to the solution

$$u(x,t) = \mathrm{e}^{-k^2 t} \, \sin kx.$$

This shows the reason for the choice of $-k^2$ for the constant; if we had chosen a positive value here, the solution would have involved an exponentially increasing function of t, whereas the solution of our model problem is known to be bounded for all positive values of t. For all values of the number k this is a solution of the differential equation; if we now restrict k to take the values $k = m\pi$, where m is a positive integer, the solution vanishes at x = 1 as well as at x = 0. Hence any linear combination of such solutions will satisfy the differential equation and the two boundary conditions. This linear combination can be written

$$u(x,t) = \sum_{m=1}^{\infty} a_m e^{-(m\pi)^2 t} \sin m\pi x.$$
 (2.11)

We must now choose the coefficients a_m in this linear combination in order to satisfy the given initial condition. Writing t = 0 we obtain

$$\sum_{m=1}^{\infty} a_m \sin m\pi x = u^0(x).$$
 (2.12)

This shows at once that the a_m are just the coefficients in the Fourier sine series expansion of the given function $u^0(x)$, and are therefore given by

$$a_m = 2 \int_0^1 u^0(x) \sin m\pi x \, \mathrm{d}x.$$
 (2.13)

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Parabolic equations in one space variable

This final result may be regarded as an exact analytic solution of the problem, but it is much more like a numerical approximation, for two reasons. If we require the value of u(x,t) for specific values of x and t, we must first determine the Fourier coefficients a_m ; these can be found exactly only for specially simple functions $u^0(x)$, and more generally would require some form of numerical integration. And secondly we can only sum a finite number of terms of the infinite series. For the model problem, however, it is a very efficient method; for even quite small values of t a few terms of the series will be quite sufficient, as the series converges extremely rapidly. The real limitation of the method in this form is that it does not easily generalise to even slightly more complicated differential equations.

2.4 An explicit scheme for the model problem

To approximate the model equation (2.7) by finite differences we divide the closed domain $\overline{R} \times [0, t_F]$ by a set of lines parallel to the *x*- and *t*-axes to form a grid or mesh. We shall assume, for simplicity only, that the sets of lines are equally spaced, and from now on we shall assume that \overline{R} is the interval [0, 1]. Note that in practice we have to work in a finite time interval $[0, t_F]$, but t_F can be as large as we like.

We shall write Δx and Δt for the line spacings. The crossing points

$$(x_j = j\Delta x, t_n = n\Delta t), j = 0, 1, \dots, J, n = 0, 1, \dots,$$
 (2.14)

where

$$\Delta x = 1/J,\tag{2.15}$$

are called the *grid points* or *mesh points*. We seek approximations of the solution at these mesh points; these approximate values will be denoted by

$$U_j^n \approx u(x_j, t_n). \tag{2.16}$$

We shall approximate the derivatives in (2.7) by finite differences and then solve the resulting difference equations in an evolutionary manner starting from n = 0.

We shall often use notation like U_j^n ; there should be no confusion with other expressions which may look similar, such as λ^n which, of course, denotes the *n*th power of λ . If there is likely to be any ambiguity we shall sometimes write such a power in the form $(\lambda_j)^n$.