

**NUMERICAL SOLUTION OF
PARTIAL DIFFERENTIAL
EQUATIONS IN
SCIENCE AND ENGINEERING**

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A Wiley-Interscience Publication
JOHN WILEY & SONS

New York

Chichester

Brisbane

Toronto

Singapore

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ONE

Fundamental Concepts

This chapter serves as a detailed introduction to many of the concepts and characteristics of partial differential equations (hereafter abbreviated PDEs). Commonly encountered notation and the classification of PDE are discussed together with some features of analytical and numerical solutions.

1.0 NOTATION

Consider a partial differential equation (PDE) in which the independent variables are denoted by x, y, z, \dots and the dependent variables by u, v, w, \dots . Direct functionality is often written in the form

$$(1.0.1) \quad u = u(x, y, z),$$

which, in this particular case, designates u as a function of the independent variables x, y , and z . Partial derivatives are often denoted as follows:

$$(1.0.2) \quad u_x = \frac{\partial u}{\partial x}; \quad u_y = \frac{\partial u}{\partial y}; \quad u_{xx} = \frac{\partial^2 u}{\partial x^2}; \quad u_{xy} = \frac{\partial^2 u}{\partial x \partial y}; \quad \dots$$

Employing the definitions of (1.0.1) and (1.0.2), we can thus represent a PDE in the general form

$$(1.0.3) \quad F(x, y, u, u_x, u_y, u_{xx}, u_{yy}, u_{xy}, \dots) = 0,$$

where F is a function of the indicated quantities and at least one partial derivative exists.

As examples, consider the following PDEs:

$$u_{xx} + u_{yy} = 0$$

$$u_x = u + x^2 + y^2$$

$$u_{xxx} = u_{yy} + u^2$$

$$(u_x)^2 + (u_y)^2 = \exp(u).$$

The order of a PDE is defined by the highest-order derivative in the equation. Therefore,

$$u_x - bu_y = 0$$

is of first order,

$$u_{xx} + u_y = 0$$

is of second order, and

$$u_{xxxx} + u_{yyyy} = 0$$

is of fourth order. When several interdependent PDEs are encountered, the order is established by combining all the equations into a single equation. For example, the following system of equations is of second order although each contains only first-order derivatives; that is,

$$(1.0.4a) \quad u_x + v_y = u_z$$

$$(1.0.4b) \quad u = w_x$$

$$(1.0.4c) \quad v = w_y$$

can alternatively be written

$$(1.0.5) \quad w_{xx} + w_{yy} = w_{xz}.$$

When written in the form of (1.0.5), it is readily apparent that (1.0.4) is of second order.

In the solution of PDEs, the property of linearity plays a particularly important role. Consider, for example, the first-order equation

$$(1.0.6) \quad a(\cdot)u_x + b(\cdot)u_y = c(\cdot).$$

The linearity of this equation is established by the functionality of the coefficients $a(\cdot)$, $b(\cdot)$, and $c(\cdot)$. In the case of (1.0.6), if the coefficients are constant or functions of the independent variables only, $[(\cdot) \equiv (x, y)]$, the PDE is linear; if the coefficients are also functions of the dependent variable $[(\cdot) \equiv (x, y, u)]$, the PDE is quasilinear; if the coefficients are functions of the first derivatives, $[(\cdot) \equiv (x, y, u, u_x, u_y)]$, the PDE is nonlinear. Thus the following PDEs are classified as indicated:

$$u_x + bu_y = 0 \quad (\text{linear})$$

$$u_x + uu_y = x^2 \quad (\text{quasilinear})$$

$$u_x + (u_y)^2 = 0. \quad (\text{nonlinear})$$

In general, when the coefficients of an n th-order PDE depend upon n th-order derivatives, the equation is nonlinear; when they depend upon m th-order derivatives, $m < n$, the equation is quasilinear. These features are important because whereas many analytical properties of linear and even quasilinear PDEs are known, as a general rule, each nonlinear PDE must be considered individually.

The analytical solution of a PDE, which may be written

$$u = u(x, y),$$

denotes a function that, when substituted back into the PDE, generates an identity. Of course, when one discusses the solution of a PDE, it is necessary to consider appropriate auxiliary initial and boundary conditions. For example, the transient temperature distribution in a homogeneous rod of finite length with insulated sides is described by the system

$$u_x = u_{yy}, \quad x > 0, \quad 0 < y < 1 \quad (\text{PDE})$$

$$u(0, y) = f(y), \quad x = 0, \quad 0 < y < 1 \quad (\text{initial condition})$$

$$u(x, 0) = \phi(x), \quad y = 0, \quad x \geq 0$$

$$u(x, 1) = \theta(x), \quad y = 1, \quad x \geq 0. \quad (\text{boundary condition})$$

Such a specification usually leads to a well-posed problem. Almost all reasonable problems are well posed and yield a solution that is unique and depends continuously on the auxiliary conditions (Hadamard, 1923). Alternatively, a well-posed problem can be considered as one for which small perturbations in the auxiliary conditions lead to small changes in the solution.

It is instructive at this point to compare briefly the solution properties of ordinary differential equations, herein denoted as ODEs. The general form of a first-order ODE is

$$\frac{du}{dx} = f(x, u),$$

where f is a function of the indicated quantities. In the case of an ODE, a specification of (x, u) yields a unique value of du/dx ; by contrast, a specification of (x, y, u) in a first-order PDE only gives a connection between u_x and u_y but does not uniquely determine each. In the case of a second-order ODE, the solution specifies a point and a tangent line on the solution trajectory in a plane; by contrast, these concepts of a *point, plane, or tangent line* for the ODE are extended to a *curve, three-dimensional space, and tangent plane* for the PDE. In other words, for an ODE, there are solution curves in a two-dimensional space that are required to pass through a point, while for a PDE there are solution surfaces in three-dimensional space that are required to pass

$$u = u(x, y)$$

$$(1.1.2) \quad du = u_x dx + u_y dy$$

and thus $\{a, b, c\} \equiv \{dx, dy, du\}$.

The solution to (1.1.1) is readily obtained using the following theorem.

Theorem 1

The general solution of the quasilinear PDE

$$au_x + bu_y = c$$

is given by

$$G(v, w) = 0,$$

where G is an arbitrary function and where $v(x, y, u) = c_1$ and $w(x, y, u) = c_2$ form a solution of the equations

$$(1.1.3) \quad \frac{dx}{a} = \frac{dy}{b} = \frac{du}{c}.$$

Note that (1.1.3) comprises a set of two independent ODEs (a two-parameter family of curves in space). Further, one set of these can be written as

$$(1.1.4) \quad \frac{dy}{dx} = \frac{b(x, y, u)}{a(x, y, u)}$$

and is termed a *characteristic curve*. When $a = a(x, y)$ and $b = b(x, y)$ only, (1.1.4) is a function in (x, y) space. In this case we refer to the curve as a characteristic ground or base curve.

When a and b are constant, (1.1.4) defines a set of parallel lines in (x, y) space. In either of these last two cases (1.1.4) may be evaluated without knowing $u(x, y)$; in the quasilinear case (1.1.4) cannot be evaluated until $u(x, y)$ is also known. However, in any three-dimensional (x, y, u) plot, such as that in Figure 1.1, one can project down onto the x - y plane to obtain

$$\frac{dy}{dx} = \frac{b(x, y, u)}{a(x, y, u)}.$$

The characteristic equation (1.1.4) may be obtained directly through an examination of the PDE and (1.1.2). Restating these equations, we have two

through a curve or line. These differences are, of course, a direct result of the increase in number of independent variables in the PDE as compared to the ODE.

1.1 FIRST-ORDER PARTIAL DIFFERENTIAL EQUATIONS

In this section we consider some of the fundamental features of first-order PDEs. The principal objective is to present an overview of the basic concepts in this area; for a definitive analysis we recommend the books by Courant (1962) and Aris and Amundson (1973).

1.1.1 First-Order Quasilinear Partial Differential Equations

Consider the quasilinear PDE

$$(1.1.1) \quad a(x, y, u)u_x + b(x, y, u)u_y = c(x, y, u)$$

in the two independent variables x and y . The extension to more independent variables is rather obvious and thus is not discussed here. Also, the linear PDE is considered as a special case of (1.1.1) and is mentioned specifically when appropriate.

Suppose that we are located at a point $P(x, y, u)$ on the solution surface $u = u(x, y)$ (Figure 1.1) and we move in a direction given by the vector $\{a, b, c\}$. But at any point on the surface, the direction of the normal is given by the vector $\{u_x, u_y, -1\}$. It is obvious from (1.1.1) that a scalar product of these two vectors vanishes (i.e., the two vectors are orthogonal). Thus $\{a, b, c\}$ is perpendicular to the normal and must lie in the tangent plane of the surface $u = u(x, y)$. Thus the PDE is a mathematical statement of the geometrical requirement that any solution surface through the point $P(x, y, u)$ must be tangent to a vector with components $\{a, b, c\}$. Further, since $\{a, b, c\}$ is always tangent to the surface, we never leave the surface. Note also that since

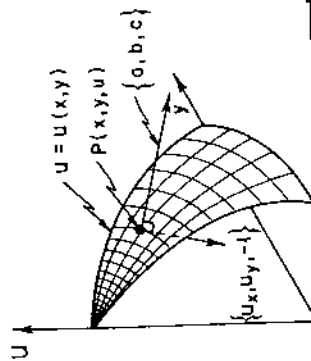


Figure 1.1. Solution surface $u = u(x, y)$ with vector $\{a, b, c\}$ tangent to u and vector $\{u_x, u_y, -1\}$ normal to u at point $P(x, y, u)$.

equations in the values u_x and u_y :

$$(1.1.5a) \quad au_x + bu_y = c$$

$$(1.1.5b) \quad (dx)u_x + (dy)u_y = du.$$

Obviously, both equations must hold on the solution surface and yet one can interpret each equation as a plane element; these plane elements intersect on a line along which different values of u_x and u_y may exist. In other words, u_x and u_y are themselves indeterminate along this line, but at the same time they are related or determinate to each other since the equations must hold.

To exploit this feature, we use a well-known principle of linear algebra. If a square coefficient matrix for a set of n linear simultaneous equations has a vanishing determinant, a necessary condition for finite solutions to exist is that when the right-hand side is substituted for any column of the coefficient matrix, the resulting determinants must also vanish. Thus, if we treat (1.1.5) as linear algebraic equations in u_x and u_y , we may write

$$(1.1.6) \quad \begin{bmatrix} a & b \\ dx & dy \end{bmatrix} \begin{bmatrix} u_x \\ u_y \end{bmatrix} = \begin{bmatrix} c \\ du \end{bmatrix}.$$

From the property above, it then follows that

$$(1.1.7) \quad \det \begin{bmatrix} a & b \\ dx & dy \end{bmatrix} = 0; \quad \det \begin{bmatrix} c & b \\ du & dy \end{bmatrix} = 0;$$

$$\det \begin{bmatrix} a & c \\ dx & du \end{bmatrix} = 0,$$

implying linear dependence of u_x and u_y . Evaluating the determinants leads directly to the statement of (1.1.3),

$$\frac{dx}{a} = \frac{dy}{b} = \frac{du}{c}.$$

1.1.2 Initial Value or Cauchy Problem

Now we raise the question of how initial data (initial or boundary conditions) specified on a prescribed curve or line Γ interact with the equations given by (1.1.3). Suppose that this space curve Γ prescribes the values of x, y , and u as a function of some parameter r . This means that

$$(1.1.8) \quad x = x(r), \quad y = y(r), \quad u = u(r).$$

The characteristic curves passing through Γ can be described using an independent variable, say s , along the characteristic. Thus (1.1.3) can be restated as the

set

$$(1.1.9a) \quad \frac{dx}{ds} = a$$

$$(1.1.9b) \quad \frac{dy}{ds} = b$$

and along this curve the PDE merely becomes

$$(1.1.9c) \quad \frac{du}{ds} = c.$$

Combination of (1.1.8) and (1.1.9) provides a solution to this problem which can be expressed in parametric terms as

$$(1.1.10) \quad x = x(r, s); \quad y = y(r, s); \quad u = u(r, s).$$

We have now involved the initial curve Γ and the characteristics to yield $u = u(r, s)$. The only problem that can occur is in the inversion of r, s , and u to functions of the independent variables x and y . This can be done (see Aris and Amundson, 1973, p. 9) provided that the Jacobian J , defined as

$$(1.1.11) \quad J = x_s y_r - y_s x_r = ay_r - bx_r,$$

is nonzero. When $J = 0$, the initial curve Γ is itself a characteristic curve and there are infinitely many solutions of the initial value or Cauchy problem.

1.1.3 Application of Characteristic Curves

Example 1

To illustrate some of the features of the abbreviated discussion above, we consider two examples. The first involves the solution to the following form of the transport equation:

$$(1.1.12) \quad u_x + v(\cdot)u_y = F(\cdot),$$

where $v(\cdot)$ is the velocity of propagation of an initial profile. When $v(\cdot) = v(x, y, u)$ the equation is quasilinear and the characteristics are curved and defined by substituting for a and b in (1.1.4):

$$(1.1.13) \quad \frac{dy}{dx} = v(x, y, u)$$

and, from (1.1.3),

$$(1.1.14) \quad \frac{du}{dx} = F(\cdot).$$

When $v(\cdot)$ is constant, the problem of solving (1.1.13) is simplified, because now the characteristic equation is

$$\frac{dy}{dx} = v = \text{constant}$$

and a given profile (see below) or initial condition at $x=0$ is propagated without change of shape in the direction of the x axis with velocity v .

When $v(\cdot) = \text{constant}$ and $F(\cdot) \equiv 0$, we have

$$(1.1.15) \quad u_x + vu_y = 0$$

and the equations of interest are

$$(1.1.16) \quad \frac{dx}{1} = \frac{dy}{v} = \frac{du}{0}.$$

The characteristics are now straight lines inclined to the x axis at an angle $\theta = \tan^{-1}v$ or with slope v . Along these characteristics $du=0$ or $u = \text{constant}$. This leads to a plot such as Figure 1.2, where the parallel straight lines are shown. Each straight line has the equation $y = vx + \text{constant}$ with the constant determined by the particular conditions at $x=0$ (initial conditions) or $y=0$ (boundary conditions). These are the conditions specified along the Γ data line. The solution $u(x, y)$ slides up a characteristic unchanged in its value.

Note that there is no approximation in this solution. The answer obtained is "correct" in the sense that only if $dx/ds = a$ needs to be integrated numerically along the characteristics will any error be involved.

Example 2

As a second example, consider an isothermal plug flow reactor with a first-order reaction. The relevant PDE and boundary conditions are

$$(1.1.17a) \quad u_x + vu_y = -ku$$

$$(1.1.17b) \quad u=0, \quad x=0, \quad y \geq 0$$

$$(1.1.17c) \quad u=u_0, \quad x > 0, \quad y=0,$$

where u represents the concentration of material, v is the velocity of flow of material through the tube, and a first-order reaction (sink) is involved. The reactor contains no reactant initially and is then fed with a reactant with a fixed concentration u_0 . Defining the dimensionless groups

$$\eta = \frac{u}{u_0}, \quad \theta = kx, \quad \tau = \frac{y^2 k}{v}$$

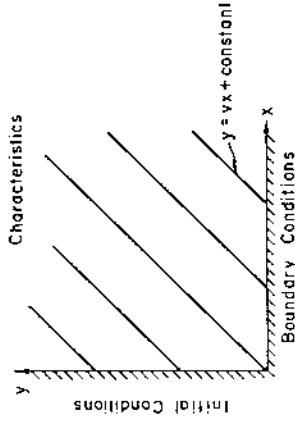


Figure 1.2. Characteristic curves $y = vx$ with boundary and initial conditions indicated.

we may rewrite (1.1.17) as

$$(1.1.18a) \quad \eta_\theta + \eta_\tau = -\eta$$

$$(1.1.18b) \quad \eta = 0, \quad \theta = 0, \quad \tau \geq 0$$

$$(1.1.18c) \quad \eta = 1, \quad \theta > 0, \quad \tau = 0.$$

The characteristic equations are

$$\frac{d\theta}{1} = \frac{d\tau}{1} = \frac{-d\eta}{\eta}$$

or

$$(1.1.19a) \quad \frac{d\tau}{d\theta} = 1; \quad \theta \geq 0, \quad \tau \geq 0$$

and

$$(1.1.19b) \quad \frac{d\eta}{d\tau} = -\eta; \quad \eta = 0, \quad \theta = 0, \quad \tau \geq 0 \\ \eta = 1, \quad \theta > 0, \quad \tau = 0.$$

Because (1.1.19) are linear they are easily integrated to yield

$$(1.1.20a) \quad \eta = 0, \quad \tau \geq \theta$$

$$(1.1.20b) \quad \eta = e^{-\tau}, \quad \tau < \theta.$$

Equations 1.1.20 represent the complete solution for the problem. Using the arbitrary numerical values of θ and τ of 2.5, Figures 1.3 and 1.4 can be developed. These are two- and three-dimensional representations of η as a function of τ and θ .

Although this is only a small sampling of applications of characteristic line to the solution of first-order PDE, it serves as an introduction to the scheme we use later in developing a classification for second-order PDEs. Before turning our attention to second-order PDEs, let us briefly extend the concept of characteristic lines to nonlinear first-order PDEs.

1.1.4 Nonlinear First-Order Partial Differential Equations

When the first-order PDE is nonlinear, it can be written (see Section 1.0)

$$(1.1.21) \quad F(x, y, u, u_x, u_y) = 0,$$

where

$$\left(\frac{\partial F}{\partial u_x} \right)^2 + \left(\frac{\partial F}{\partial u_y} \right)^2 \neq 0.$$

A well-known problem described by an equation of the form of (1.1.21) arises in geometric optics. The appropriate expression is

$$u_x^2 + u_y^2 = 1.$$

Much of what we introduced in the discussion of linear first-order PDE is still retained in the nonlinear case but in a more complex form. Now characteristic lines become characteristic strips; the so-called Monge cone in which the tangent to the solution surface must lie is a surface generated by a one-parameter family of straight lines through a fixed point of its vertex. In the quasilinear case, the cone becomes linear or a Monge axis.

Without attempting to present the details of the derivation of the characteristic equations, we indicate here that analogous to (1.1.9) (the initial value or Cauchy problem) there are now five ODEs:

$$(1.1.22a) \quad \frac{dx}{ds} = F_{u_x}$$

$$(1.1.22b) \quad \frac{dy}{ds} = F_{u_y}$$

$$(1.1.22c) \quad \frac{du}{ds} = u_x F_{u_x} + u_y F_{u_y}$$

$$(1.1.22d) \quad \frac{du_x}{ds} = -F_{u_x} - u_x F_{u_x}$$

$$(1.1.22e) \quad \frac{du_y}{ds} = -F_{u_y} - u_y F_{u_y}$$

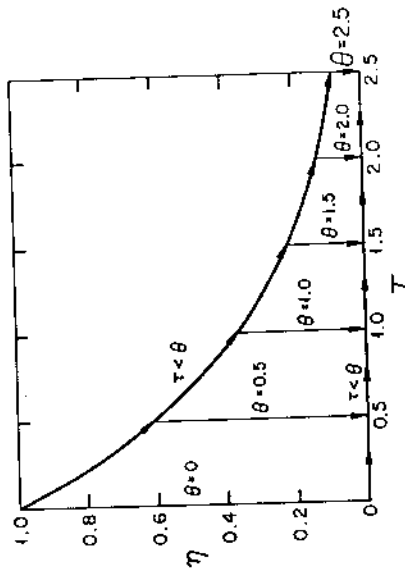


Figure 1.3. Two-dimensional representation of concentration (η) vs. distance (τ) with selected values of the second space variable θ also indicated (see Figure 1.4).

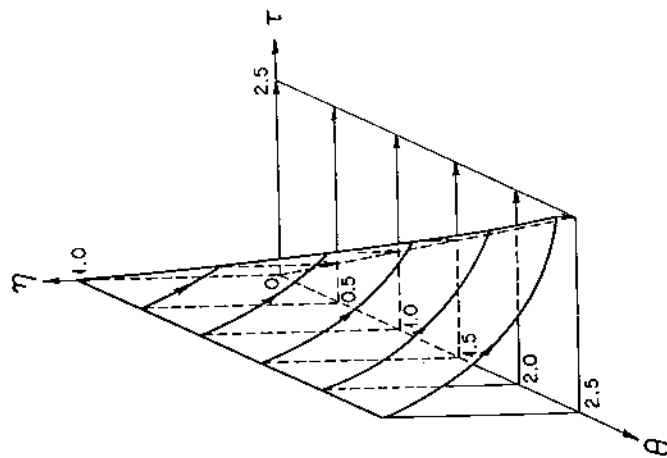


Figure 1.4. Three-dimensional representation of concentration (η) vs. the two space coordinates τ and θ .

When $F(x, y, u, u_x, u_y) = a(\cdot)u_x + b(\cdot)u_y - c = 0$, the quasilinear case, (1.1.22), becomes (1.1.9).

1.2 SECOND-ORDER PARTIAL DIFFERENTIAL EQUATIONS

Now let us consider some features of second-order PDE that will be useful in the ensuing chapters on numerical solutions. By comparison, the first-order PDE was relatively uncomplicated in the sense that the characteristic curves could be located and $u(x, y)$ determined along those curves. In the second-order case, the characteristics may or may not play a role.

Consider the following second-order PDE written in two independent variables:

$$(1.2.1) \quad a(\cdot)u_{xx} + 2b(\cdot)u_{xy} + c(\cdot)u_{yy} + d(\cdot)u_x + e(\cdot)u_y + f(\cdot)u + g(\cdot) = 0.$$

As in earlier sections, we denote (1.2.1) as linear if $a(\cdot)$, $b(\cdot)$, and $c(\cdot)$ are constant or functions only of x and y ; quasilinear if $a(\cdot)$, $b(\cdot)$, and $c(\cdot)$ are functions of x, y, u, u_x , and u_y ; and nonlinear in all other cases. Typical examples of second-order PDEs are the following well-known equations:

$$u_{xx} + u_{yy} = 0 \quad \text{Laplace's equation}$$

$$u_{xx} + u_{yy} = f(x, y) \quad \text{Poisson's equation}$$

$$u_x = u_{yy} \quad \text{heat flow or diffusion equation}$$

$$u_x = u_{yy} + u_{zz} \quad \text{heat flow or diffusion equation}$$

$$u_x + uu_y = ku_{yy} \quad \text{Burger's equation}$$

$$u_{xx} = u_{yy} \quad \text{wave equation}$$

1.2.1 Linear Second-Order Partial Differential Equations

There exists an extensive body of knowledge regarding linear PDEs. This information is generally cataloged according to the form of the PDE. Every linear second-order PDE in two independent variables can be converted into one of three standard or *canonical* forms which we identify as hyperbolic, parabolic, or elliptic. In this canonical form at least one of the second-order terms in (1.2.1) is not present.

There is a practical reason for identifying the type of PDE in which one is interested. When coupled with initial and boundary conditions, the method and form of solution will be dependent on the type of PDE.

The classification can take many forms. We assume (for now) that if

$$(1.2.2a) \quad b^2 - ac > 0 \quad \text{the PDE is hyperbolic}$$

$$(1.2.2b) \quad b^2 - ac = 0 \quad \text{the PDE is parabolic}$$

$$(1.2.2c) \quad b^2 - ac < 0 \quad \text{the PDE is elliptic.}$$

Let us now examine the canonical forms and their associated transformations. The three canonical forms are written in terms of the new variables ξ and η as:

$$(1.2.3a) \quad u_{\xi\xi} - u_{\eta\eta} + \dots = 0 \quad \checkmark$$

or $u_{\xi\xi} + \dots = 0$ *hyperbolic*

$$(1.2.3b) \quad u_{\xi\xi} + \dots = 0 \quad \text{parabolic}$$

$$(1.2.3c) \quad u_{\xi\xi} + u_{\eta\eta} + \dots = 0. \quad \text{elliptic}$$

We shall see that the hyperbolic PDE has two real characteristic curves, the parabolic PDE has one real characteristic curve, and the elliptic PDE has no real characteristic curves.

From (1.2.2) or (1.2.3) we can see that the heat flow equation $u_x = u_{yy}$ is parabolic and already in canonical form, and the Laplace equation $u_{xx} + u_{yy} = 0$ is elliptic and already in canonical form. There are other cases, however, in which (1.2.2) must be used and the equations and their classifications may change because of coefficients. Thus

$$yu_{xx} + u_{yy} = 0$$

Tricomi's equation, elliptic for $y > 0$, hyperbolic for $y < 0$

$$(1 + y^2)u_{xx} + (1 + y^2)u_{yy} - u_x = 0$$

elliptic

$$u_{xx} + uu_{yy} = 0$$

elliptic for $u > 0$
hyperbolic for $u < 0$

$$u_{xx} + (1 - x^2 - y^2)u_{yy} = 0$$

elliptic inside unit circle
hyperbolic outside

$$yu_{xx} + xu_{xy} + yu_{yy} = 0.$$

hyperbolic, $x > 2y$
parabolic, $x = 2y$
elliptic, $x < 2y$

With these preliminaries in hand, let us now consider the canonical transformations. We ignore all terms in (1.2.1) except the second derivatives because the lower-order terms do not influence the results. We introduce the change of variables (implicit here) of

$$(1.2.4) \quad \xi = \phi(x, y), \quad \eta = \psi(x, y)$$

and develop, using the chain rule,

$$(1.2.5a) \quad u_x = u_\xi \phi_x + u_\eta \psi_x$$

$$(1.2.5b) \quad u_y = u_\xi \phi_y + u_\eta \psi_y$$

$$(1.2.6) \quad u_{xx} = u_{\xi\xi} \phi_x^2 + 2u_{\xi\eta} \phi_x \psi_x + u_{\eta\eta} \psi_x^2 + \dots$$

$$(1.2.7) \quad u_{xy} = u_{\xi\xi} \phi_x \phi_y + u_{\xi\eta} (\phi_x \psi_y + \phi_y \psi_x) + u_{\eta\eta} \psi_x \psi_y + \dots$$

$$(1.2.8) \quad u_{yy} = u_{\xi\xi} \phi_y^2 + 2u_{\xi\eta} \phi_y \psi_y + u_{\eta\eta} \psi_y^2 + \dots$$

Substitution into (1.2.1) yields

$$(1.2.9) \quad au_{xx} + 2bu_{xy} + cu_{yy} = Au_{\xi\xi} + 2Bu_{\xi\eta} + Cu_{\eta\eta} + \dots,$$

where

$$(1.2.10) \quad A = a\phi_x^2 + 2b\phi_x\phi_y + c\phi_y^2$$

$$(1.2.11) \quad B = a\phi_x\psi_x + b(\phi_x\psi_y + \phi_y\psi_x) + c\phi_y\psi_y$$

$$(1.2.12) \quad C = a\psi_x^2 + 2b\psi_x\psi_y + c\psi_y^2.$$

From (1.2.10), (1.2.11), and (1.2.12) one can obtain the following relationship between a, b, c and A, B, C :

$$(1.2.13) \quad B^2 - AC = (b^2 - ac)(\phi_x\psi_y - \phi_y\psi_x)^2.$$

It is apparent that, under this change of variables, the sign of $b^2 - ac$ remains invariant with respect to $B^2 - AC$; moreover, $\phi_x\psi_y - \phi_y\psi_x$, which is the Jacobian of the transformation, must always be kept nonzero. If an explicit change of variables had been used,

$$\xi = \alpha_1 x + \beta_1 y + \gamma_1$$

$$\eta = \alpha_2 x + \beta_2 y + \gamma_2,$$

the Jacobian requirement would mean that $\alpha_1\beta_2 - \alpha_2\beta_1 \neq 0$.

Now let us consider the case where the discriminant $b^2 - ac$ is everywhere greater than zero, equal to zero, or less than zero. For illustration, take $b^2 - ac > 0$, which is the hyperbolic PDE case. We wish to show that (1.2.9) can be converted into either of the two canonical forms in (1.2.3a). To simplify the problem, let us consider the case wherein $u_{\xi\eta} + \dots = 0$. To do this we need to make A and C of (1.2.10) and (1.2.12) vanish. These equations are of the form (with $A = 0, B = 0$)

$$(1.2.14a) \quad a\phi_x^2 + 2b\phi_x\phi_y + c\phi_y^2 = 0$$

and

$$(1.2.14b) \quad a\psi_x^2 + 2b\psi_x\psi_y + c\psi_y^2 = 0.$$

If we choose

$$(1.2.15) \quad \phi_x = \lambda_1 \phi_y \quad \text{and} \quad \psi_x = \lambda_2 \psi_y,$$

where λ_1 and λ_2 are the roots of (1.2.14), then $A = 0$ and $B = 0$.

But these equations are both first-order linear PDEs in ϕ and ψ and thus, from Theorem 1 in Section 1.1, it follows that

$$(1.2.16a) \quad \frac{dx}{1} = \frac{-dy}{\lambda_1} = \frac{d\phi}{0}$$

and

$$(1.2.16b) \quad \frac{dx}{1} = \frac{-dy}{\lambda_2} = \frac{d\psi}{0}.$$

From (1.2.16) we obtain directly

$$(1.2.17a) \quad \frac{dy}{dx} + \lambda_1 = 0$$

$$(1.2.17b) \quad \frac{dy}{dx} + \lambda_2 = 0$$

$$(1.2.18a) \quad \xi = \phi(x, y) = c_1 = \text{constant}$$

$$(1.2.18b) \quad \eta = \psi(x, y) = c_2 = \text{constant}.$$

Thus we now get two characteristic curves in (x, y) space [i.e., (1.2.17)] arising out of the linear second-order PDE. In (ξ, η) space these curves are no longer curved but rather correspond to horizontal and vertical lines since (1.2.18) holds.

In summary, we see that we can convert the original hyperbolic PDE into its canonical form by defining two sets of one-parameter families of curves, the characteristic curves in (x, y) space.

In addition, if we substitute (1.2.17) into (1.2.15), we obtain

$$\frac{dy}{dx} = \frac{-\phi_x}{\phi_y} \quad \text{and} \quad \frac{dy}{dx} = \frac{-\psi_x}{\psi_y}$$

and combination of this expression with (1.2.14) yields

$$(1.2.19) \quad a(dy)^2 - 2b dx dy + c(dx)^2 = 0.$$

Because this is a quadratic in dy/dx , we obtain

$$(1.2.20) \quad \frac{dy}{dx} = \frac{b(\cdot) \pm \sqrt{b^2(\cdot) - a(\cdot)c(\cdot)}}{a(\cdot)}.$$

Since $b^2 - ac > 0$, the right-hand side has two real values, which are λ_1 and λ_2 . Because they are real, they are both positive if a, b , and c are all of the same sign, both negative if b has a sign opposite to a and c , and contrary signs if the signs of a and c are different. Note that

$$\lambda_1 - \lambda_2 = \frac{2\sqrt{b^2 - ac}}{a} \neq 0$$

and thus the two characteristic curves cannot be tangent at any point.

Finally, it is worth pointing out that we could have performed this transformation by an explicit approach rather than the implicit one used. In the explicit formulation, we would define

$$\xi = c_1 = \frac{-b + \sqrt{b^2 - ac}}{a}x + y$$

and

$$\eta = c_2 = \frac{-b - \sqrt{b^2 - ac}}{a}x + y$$

to convert to the characteristic coordinate system directly.

An analysis, analogous to the one conducted above for the hyperbolic case, can be performed on parabolic and elliptic PDEs. In the parabolic case $b^2 - ac = 0$ and when c is eliminated, there is one root and one family of characteristic curves. These correspond to $\lambda_1 = \lambda_2 = -b/a$ and to $\psi(x, y) = c_2 = \text{constant}$. Thus we can define ξ as before and η as any function of x and y that is independent of ξ . In the elliptic case, $b^2 - ac < 0$ and no real roots exist.

1.2.2 Classification and Canonical Form of Selected Partial Differential Equations

To illustrate certain features of the discussion above let us now consider several examples. The first case is presented in detail and others are summarized with it in Table 1.1. Consider the hyperbolic equation

$$u_{xx} = \alpha^2 u_{yy}, \quad a = 1, \quad b = 0, \quad c = -\alpha^2$$

$$\alpha^2 > 0, \quad b^2 - ac = \alpha^2 > 0.$$

The two roots of the quadratic equation become

$$\frac{dy}{dx} = \alpha; \quad \frac{dy}{dx} = -\alpha,$$

which yields

$$y - \alpha x = \text{constant}; \quad y + \alpha x = \text{constant}.$$

Thus

$$\xi = \phi(x, y) = y - \alpha x \quad \text{and} \quad \eta = \psi(x, y) = y + \alpha x.$$

Substitution of ξ and η into the PDE reduces it to the canonical form

$$u_{\xi\eta} + \dots = 0.$$

1.2.3 Quasilinear Partial Differential Equations and Other Ideas

It is apparent that the hyperbolic, linear, second-order PDE is much like the linear first-order PDE. Instead of one characteristic curve, there are now two but, because these are only functions of x and y , they are ground or base curves. When we go to a quasilinear second-order PDE, these curves are no longer simply given because the coefficients are functions of x, y, u, u_x , and u_y . One can show that such a quasilinear hyperbolic second-order PDE is reducible to a canonical form of five first-order PDEs in the five unknowns x, y, u, u_x , and u_y . As before, the initial curve cannot be a characteristic, and discontinuities in the initial data are propagated, in the hyperbolic case, into the solution domain along the characteristics. Thus, if u_x and u_y are known along the initial data curve, the discontinuities in the second derivative may occur along the characteristic lines. To show this and a few other items, we invoke the concepts of linear algebraic equations mentioned in Section 1.1. Thus we write

$$au_{xx} + 2bu_{xy} + cu_{yy} = H$$

together with

$$(dx)u_{xx} + (dy)u_{xy} = du_x$$

$$(dx)u_{xy} + (dy)u_{yy} = du_y.$$

In matrix form, these three equations become

$$\begin{bmatrix} a & 2b & c \\ dx & dy & 0 \\ 0 & dx & dy \end{bmatrix} \begin{bmatrix} u_{xx} \\ u_{xy} \\ u_{yy} \end{bmatrix} = \begin{bmatrix} H \\ du_x \\ du_y \end{bmatrix}.$$

For linear dependence of the type already mentioned, the right-hand side of the matrix equation is substituted for a column of the coefficient matrix, and the determinant of the resulting matrix set to zero.

$$\det \begin{bmatrix} a & 2b & c \\ dx & dy & 0 \\ 0 & dx & dy \end{bmatrix} = 0; \quad \det \begin{bmatrix} a & H & c \\ dx & du_x & 0 \\ 0 & du_y & dy \end{bmatrix} = 0; \quad \text{etc.}$$

The first determinant merely gives us our characteristic curves

$$(1.2.21) \quad \frac{dy}{dx} = \frac{b \pm \sqrt{b^2 - ac}}{a},$$

as before. However, the second determinant yields some new information that we have not previously obtained, namely that

$$\frac{du_y}{du_x} = -\frac{a}{c} \frac{dy}{dx} + \frac{H}{c} \frac{dy}{du_x}.$$

When the characteristic equation is substituted for dy/dx we arrive at

$$(1.2.22) \quad \frac{du_y}{du_x} = -\frac{b \pm \sqrt{b^2 - ac}}{c} + \frac{H}{c} \frac{dy}{du_x},$$

which shows how u_x and u_y vary along a characteristic. Actually, (1.2.22) is exactly the type of information we picked up in the first-order PDE case to confirm our stated theorem on the behavior of du [see (1.1.6) and (1.1.7)].

We may concisely summarize these results using the terminology that the two characteristic slopes are λ_1 and λ_2 and noting that

$$(1.2.23) \quad du = u_x dx + u_y dy.$$

TABLE 1.1. Summary of Information Required to Obtain Canonical Form and Characteristic Curves for Selected PDEs.*

PDE	Type	a	b	c	Root (dy/dx)	$\phi(x, y)$	$\psi(x, y)$
$u_{xx}^2 - a_2^2 u_{yy}^2 = 0$	Hyperbolic	1	0	$-a^2$	a^2	$\pm ax$	$y + ax$
$u_{xx} - x^2 u_{yy} = 0$	Hyperbolic	1	0	$-x^2$	x^2	$\pm x$	$y + \frac{1}{2}x^2$
$u_{xx} + 2u_{xy} + u_{yy} = 0$	Parabolic	1	1	1	0	1	$y - x$
$u_{xx} + 4u_{xy} + 5u_{yy} = 0$	Elliptic	1	2	5	-1	$\pm \sqrt{-y}$	$y - x$
$u_{xx} + y u_{yy} = 0$	Hyperbolic	1	0	y	$-y$	$\pm \sqrt{-y}$	$y + x$ (arbitrary)
$u_{xx} + y u_{yy} = 0$	Hyperbolic	1	0	y	$-y$	$\pm \sqrt{-y}$	No real roots
$u_{xx} + y u_{yy} = 0$	Hyperbolic	1	0	y	$-y$	$\pm \sqrt{-y}$	$x + 2\sqrt{-y}$
$u_{xx} + y u_{yy} = 0$	Hyperbolic	1	0	y	$-y$	$\pm \sqrt{-y}$	$x - 2\sqrt{-y}$
$u_{xx} - LL'u_{xy} + \dots = 0$	Hyperbolic	$HL - HL'$	$HL - HL'$	$-LL'$	$(HL - HL')^2$	$\frac{H}{L}$ and $-\frac{H}{L'}$	Requires additional information on L, H, L', H'

*The first example is presented in detail in the text.

Thus (1.2.21)-(1.2.23) yield

$$(1.2.24a) \quad \frac{dy}{dx} = \lambda_i$$

$$(1.2.24b) \quad \left. \frac{du_y}{du_x} = \frac{-a}{c} \lambda_i + \frac{H}{c} \frac{dy}{du_x} \right\} \text{ along characteristics with slope } \lambda_i$$

$$(1.2.24c) \quad \frac{du}{dx} = u_x + \lambda_i u_y$$

Finally, we wish to briefly mention what happens when n independent variables x_1, x_2, \dots, x_n are involved rather than only the two, x and y . There are still canonical reductions that can be carried out, the forms being

$$\sum_{k=1}^{n-1} u_{x_k x_k} - u_{x_n x_n} + \dots = 0 \quad \text{hyperbolic}$$

$$\sum_{k=2}^n u_{x_k x_k} + a_1 u_{x_1} + \dots = 0 \quad \text{parabolic, } a_1 \neq 0$$

$$\sum_{k=1}^n u_{x_k x_k} + \dots = 0. \quad \text{elliptic}$$

In this context, the following PDEs can be classified as

$$u_{x_1 x_1} + u_{x_2 x_2} - u_{x_3 x_3} = 0 \quad \text{hyperbolic}$$

$$u_{x_1 x_1} + u_{x_2 x_2} + u_{x_3 x_3} - u_{x_4 x_4} = 0 \quad \text{hyperbolic}$$

$$u_{x_2 x_2} + u_{x_3 x_3} + u_{x_4 x_4} - u_{x_1} = 0. \quad \text{parabolic}$$

On the other hand, the equation

$$u_{x_1} = u_{x_2 x_2}$$

does not fit into any category. In addition, an equation of the form

$$u_{4x} + 2u_{2x2y} + u_{4y} + \dots = 0$$

is called elliptic because it has no real characteristics.

1.3 SYSTEMS OF FIRST-ORDER PDES

In this section we consider sets of coupled first-order PDEs. For ease in presentation, we usually use only two equations and later generalize the development. Let us consider the two dependent variables $u(x, y)$ and $v(x, y)$ coupled via the equations

$$(1.3.1a) \quad a_1(\cdot)u_x + b_1(\cdot)u_y + c_1(\cdot)v_x + d_1(\cdot)v_y = h_1(\cdot)$$

$$(1.3.1b) \quad a_2(\cdot)u_x + b_2(\cdot)u_y + c_2(\cdot)v_x + d_2(\cdot)v_y = h_2(\cdot),$$

where, as before, the functionality in $a_1(\cdot), b_1(\cdot), \dots, b_2(\cdot)$ defines the terminology of linear, quasilinear, and nonlinear PDEs. Equation (1.3.1) may also be written in matrix form as

$$(1.3.2) \quad [A]\{u_x\} + [B]\{u_y\} = \{h\},$$

where

$$\{u_x\} = \begin{bmatrix} u_x \\ v_x \end{bmatrix}; \quad \{u_y\} = \begin{bmatrix} u_y \\ v_y \end{bmatrix}; \quad [A] = \begin{bmatrix} a_1 & c_1 \\ a_2 & c_2 \end{bmatrix};$$

$$(1.3.3) \quad [B] = \begin{bmatrix} b_1 & d_1 \\ b_2 & d_2 \end{bmatrix}; \quad \{h\} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}.$$

Equations of the form defined by (1.3.1) and (1.3.2) may result from a change of variables in a second-order (or higher) PDE or, and this is usually the case, as a direct result of the description of a physical system. Because of the connection to second-order PDEs one might anticipate that (1.3.1) would be classified in the usual three forms of hyperbolic, parabolic, and elliptic and that the number of real characteristic curves would determine the particular form.

1.3.1 First-Order and Second-Order PDEs

One can usually obtain a set of first-order equations such as (1.3.1) from a second-order PDE; conversely, (1.3.1) can be converted to a second-order equation. To demonstrate this, we show that the wave equation, heat flow equation, and Poisson's equation are all convertible to a form such as (1.3.2).

Wave equation: $f_{xx} - f_{yy} = H(x, y)$

define $u = f_x, \quad v = f_y.$

The PDE and the requirement that u_x, v_x can be written in matrix form as the set of two first-order PDEs:

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} u_x \\ v_x \end{bmatrix} + \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} u_y \\ v_y \end{bmatrix} = \begin{bmatrix} H \\ 0 \end{bmatrix}.$$

Note that for $H \equiv 0$, this is equivalent to the set

$$\begin{aligned} u_x - v_y &= 0 \\ v_x - u_y &= 0. \end{aligned}$$

Heat flow equation: $f_x - f_{yy} = H(x, y)$

define $u = f, v = f_y$.

Once again the PDE and the requirement that $u_y = v$ results in a set of two first-order PDEs:

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} u_x \\ v_x \end{bmatrix} + \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} u_y \\ v_y \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} H \\ 0 \end{bmatrix}.$$

Poisson's equation: $f_{xx} + f_{yy} = H(x, y)$

define $u = f, v = f_x, w = f_y$.

In this case, we obtain three first-order PDEs, which can be written

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_x \\ v_x \\ w_x \end{bmatrix} + \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_y \\ v_y \\ w_y \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} + \begin{bmatrix} H \\ 0 \\ 0 \end{bmatrix}.$$

Now let us go in the opposite direction and generate a second-order PDE from two first-order PDEs. Consider

$$\begin{aligned} u_x + gv_y &= 0 \\ v_x + ku_y &= 0. \end{aligned}$$

Differentiation of the first with respect to y and the second with respect to x , multiplication of the second by g , and subtraction yields (g and k are independent of x and y)

$$u_{xx} - gku_{yy} = 0.$$

Next consider the equations describing a counter-current heat exchange item. The temperature balances can be written as

$$\begin{aligned} Hcu_x &= -Lcu_y - k(u - v) \\ H'c'v_x &= L'c'v_y + k(u - v), \end{aligned}$$

where u, v = temperatures of the two phases

H = holdup
 c = heat capacity
 L = flow rate
 k = heat transfer coefficient
 x = time variable
 y = position variable
 the prime designates parameters identified with the second phase.

If the second equation is solved for v and then differentiated with respect to x and y , the resulting expression can be substituted into the first to give

$$\begin{aligned} HH'u_{xx} + (H'L - HL')u_{xy} - LL'u_{yy} &= -k\left[\frac{H}{c'} + \frac{H'}{c}\right]u_x \\ &\quad - k\left[\frac{L}{c'} - \frac{L'}{c}\right]u_y. \end{aligned}$$

Finally, let us transform the general form of the second-order PDE

$$af_{xx} + 2bf_{xy} + cf_{yy} = H.$$

Substitution of the variables

$$u = f_x \quad \text{and} \quad v = f_y$$

yields the following set of first-order PDEs:

$$\begin{aligned} au_x + 2bv_y + cv_y &= H \\ u_y - v_x &= 0. \end{aligned}$$

This example possibly shows most clearly the connection between the standard second-order PDE and (1.3.1).

1.3.2 Characteristic Curves

To develop the characteristic curves for the first-order equations described by (1.3.1), we rewrite them together with two auxiliary conditions:

$$(1.3.1a) \quad a_1(\cdot)u_x + b_1(\cdot)u_y + c_1(\cdot)v_x + d_1(\cdot)v_y = u_1(\cdot)$$

$$(1.3.1b) \quad a_2(\cdot)u_x + b_2(\cdot)u_y + c_2(\cdot)v_x + d_2(\cdot)v_y = u_2(\cdot)$$

$$u_x dx + u_y dy = du$$

$$v_x dx + v_y dy = dv$$

These equations may be expressed in matrix form as

$$(1.3.4) \quad \begin{bmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{bmatrix} \begin{bmatrix} u_x \\ u_y \\ v_x \\ v_y \end{bmatrix} = \begin{bmatrix} u_1 \\ u_2 \\ du \\ dv \end{bmatrix}$$

Setting the determinant of the coefficient matrix in (1.3.4) to zero, we obtain

$$(1.3.5) \quad a(dy)^2 - 2b(dx)(dy) + c(dx)^2 = 0,$$

where

$$(1.3.6a) \quad a = a_1c_2 - a_2c_1$$

$$(1.3.6b) \quad 2b = a_1d_2 - a_2d_1 + b_1c_2 - b_2c_1$$

$$(1.3.6c) \quad c = b_1d_2 - b_2d_1.$$

As before, this is a quadratic equation for dy/dx . Depending upon whether $b^2 - ac$ has two real values, one real value or zero real values, we call (1.3.1) hyperbolic, parabolic, or elliptic.

If, in addition, we replace the fourth column in the coefficient matrix with the right-hand side of (1.3.4) and set the determinant equal to zero, there results

$$(1.3.7) \quad e(du) + \left[a \frac{dy}{dx} - f \right] dv = \left(g - h \frac{dy}{dx} \right) dx.$$

where

$$(1.3.8a) \quad e = a_1b_2 - a_2b_1$$

$$(1.3.8b) \quad f = b_1c_2 - b_2c_1$$

$$(1.3.8c) \quad g = u_1b_2 - u_2b_1$$

$$(1.3.8d) \quad h = u_1a_2 - u_2a_1.$$

Equation (1.3.7) tells us how du and dv change along a characteristic curve dy/dx . If the PDE is hyperbolic, then there are two roots $\lambda_i, i = 1, 2$, both real, and we may now write

$$(1.3.9a) \quad \frac{dy}{dx} = \lambda_i$$

$$(1.3.9b) \quad e(du) + [a\lambda_i - f] dv = (g - h\lambda_i) dx.$$

Thus, just as we have done previously, we now have the necessary equations to solve for the hyperbolic case.

Two words of caution are required in the use of (1.3.5) and (1.3.9). These equations relate to specific cases which occur frequently in physical systems. We often find, however, that the two first-order PDEs are written as

$$(1.3.10a) \quad a_1u_x + b_1u_y = h_1(\cdot)$$

$$(1.3.10b) \quad c_2v_x + d_2v_y = h_2(\cdot),$$

wherein the only coupling terms are $h_1(\cdot)$ and $h_2(\cdot)$. In such a case, e in (1.3.9b) will be equal to zero ($e = 0$), and only dv/dx can be calculated; no information is obtainable on how both u and v vary along a characteristic. The characteristic curves themselves are still available, however. In other cases, even one or more of the a_i, b_i, c_i, d_i in (1.3.10) may be zero and now a in (1.3.6) may also be zero ($a = 0$). In this situation the characteristic curves themselves cannot be calculated. Fortunately, all is not lost since (1.3.10) behave as quasilinear first-order PDEs and therefore we can invoke Theorem 1 in Section 1.1. Thus

$$(1.3.11a) \quad \frac{dx}{a_1} = \frac{dy}{b_1} = \frac{du}{h_1}$$

$$(1.3.11b) \quad \frac{dx}{c_2} = \frac{dy}{d_2} = \frac{dv}{h_2},$$

leading to

$$(1.3.12) \quad \frac{dy}{dx} = \frac{b_1}{a_1} \quad \text{and} \quad \frac{dy}{dx} = \frac{d_2}{c_2}$$

as the two characteristic curves and

$$(1.3.13) \quad \frac{du}{dx} = \frac{h_1}{a_1} \quad \text{and} \quad \frac{dv}{dy} = \frac{h_2}{a_2}$$

as equations for the dependent variables along the characteristic curves.

Alternatively, we could begin by writing the matrix equation (1.3.2),

$$(1.3.2) \quad [A]\{u_x\} + [B]\{u_y\} = \{h\}.$$

It is possible to show that when $\det[B] \neq 0$ and the equation

$$(1.3.14) \quad \det([A] - \lambda[B]) = 0$$

has real distinct roots or eigenvalues, (1.3.2) is hyperbolic. In the same fashion if $\det[B] \neq 0$, we may write (1.3.2) as

$$(1.3.15) \quad \{u_x\} = [A']\{u_y\} + \{h'\}$$

and now the requirement for hyperbolic form is that the equation $\det[A'] = 0$ has all real roots or eigenvalues. Finally, we also point out that if the PDE is written as

$$(1.3.16) \quad \{u_x\} = [A']\{u_y\} + [B']\{u_z\},$$

the hyperbolic character is retained if $[A']$ and $[B']$ are symmetric.

1.3.3 Applications of Characteristic Curves

To demonstrate the use of the foregoing theory we now outline a series of examples.

Example 1

Consider the wave equation written in the form

$$(1.3.17a) \quad u_{xx} - u_{yy} = 0.$$

This second-order PDE may be transformed to the pair of first-order PD.

$$(1.3.17b) \quad u_x - v_y = 0$$

$$(1.3.17c) \quad u_y - v_x = 0,$$

where $u \equiv u_x$ and $v \equiv u_y$ are the new dependent variables. In the notation of (1.3.1), we have

$$a_1(\cdot) = b_2(\cdot) = 1$$

$$c_2(\cdot) = d_1(\cdot) = -1$$

$$b_1 = c_1 = h_1 = a_2 = d_2 = h_2 = 0$$

and thus, from (1.3.5),

$$a = -1$$

$$b = 0$$

$$c = 1,$$

which yields the following roots:

$$(1.3.18) \quad \frac{dy}{dx} = \frac{b \pm \sqrt{b^2 - ac}}{a} = \pm 1.$$

To determine how du and dv change along the characteristic lines, we utilize (1.3.8) and (1.3.9):

$$a = -1$$

$$e = 1$$

$$f = g = h = 0$$

and

$$du - \frac{dy}{dx} dv = 0.$$

The last equation shows that along the characteristics of (1.3.18),

$$du \pm dv = 0$$

or

$$u + v = \text{constant}$$

$$u - v = \text{constant}.$$

Example 2

Consider the following set of equations, which describe a model of single-component chromatography wherein the solution contains concentrated solute:

$$(1.3.19a) \quad v^* u_x + u_y = -R_1(u, v, v^*)$$

$$(1.3.19b) \quad v_x^* = -R_2(u, v, v^*)$$

$$(1.3.19c) \quad v_y = R(u, v, v^*),$$

where $R(u, v^*) =$ rate of transfer between liquid and solid

$u =$ liquid solute concentration

$v =$ solid solute concentration

$v^* =$ velocity of flow [$v^* = v^*(x, y)$].

Equation (1.3.19) leads to the following sets of characteristic equations and associated ODEs:

$$\frac{dy}{dx} = \frac{1}{v^*}; \quad \frac{du}{dx} = -\frac{R_1}{v^*}$$

$$\frac{dy}{dx} = 0, \quad y = \text{constant}; \quad \frac{dv^*}{dx} = -R_2$$

$$\frac{dx}{dy} = 0, \quad x = \text{constant}; \quad \frac{dv^*}{dy} = R.$$

1.4 INITIAL AND BOUNDARY CONDITIONS

To this point we have only briefly mentioned the initial and boundary conditions associated with a PDE. The term "initial" refers to the fact that in many physical problems one of the independent variables x, y, z, \dots may be time x . Thus a specification of $u(x, y)$ at $x = 0$ is referred to as an initial condition.

In general terms, initial and boundary conditions have the form

$$(1.4.1) \quad \alpha(x, y)u(x, y) + \beta(x, y)u_n(x, y) = \gamma(x, y),$$

where $u_n = \partial u / \partial n =$ a derivative normal to a boundary. Frequently, $\partial u / \partial n =$

u_x or u_y . We can categorize (1.4.1) as being homogeneous ($\gamma = 0$) or nonhomogeneous ($\gamma \neq 0$). Moreover, specific forms of (1.4.1) are denoted as follows:

Name	Form	Comment
Dirichlet (first kind)	$\beta = 0$	Value specified
Neumann (second kind)	$\alpha = 0$	Slope specified
Cauchy	Two equations: $\alpha = 0$ in one and $\beta = 0$ in other	Both slope and value specified
Robbins (third kind)	α and $\beta \neq 0$	At least homogeneous form of (1.4.1) is specified

The combination of PDE and initial and boundary conditions must lead to a well-posed problem. Depending on the form of the x, y region of interest, this usually means that

1. Hyperbolic equations are associated with Cauchy conditions in an open region.
2. Parabolic equations are associated with Dirichlet or Neumann conditions in an open region.
3. Elliptic equations are associated with Dirichlet or Neumann conditions in a closed region.

The meaning of the terms "open" or "closed" region will be apparent shortly. Figure 1.5 illustrates an (x, y) diagram for the hyperbolic, parabolic, and elliptic problems. The dashed lines are characteristic curves. The case $x = 0$ corresponds to an initial condition, and the cases $y = 0$ and $y = 1$ might correspond to boundary conditions, assuming that y is always finite. The extension to more dependent variables (x, y, z) is difficult to present diagrammatically but is usually conceptually apparent when discussed.

Let us first consider the hyperbolic equation $u_{xx} = u_{yy}$ as a convenient PDE. We see that we require two initial conditions and two boundary conditions (x is chosen to represent time). These conditions are shown in Figure 1.5 as

$$(1.4.2a) \quad u(0, y) = \text{given}, \quad x = 0$$

and

$$(1.4.2b) \quad u_x(0, y) = \text{given}, \quad x = 0$$

and

$$(1.4.2c) \quad u(x, 0) = \text{given} \quad u(x, 1) = \text{given}$$

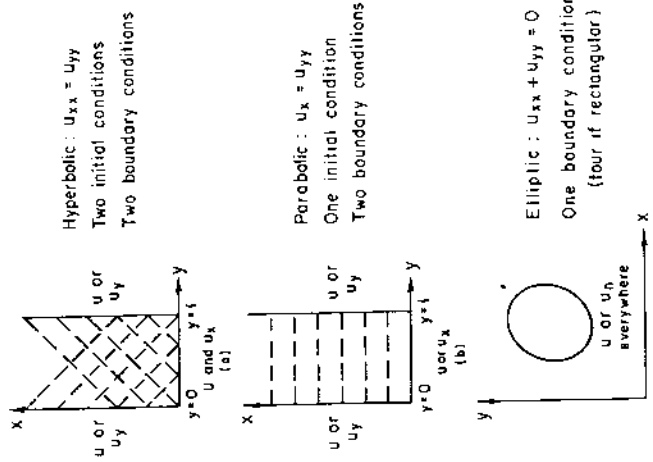


Figure 1.5. Diagrammatic representation of conditions imposed on hyperbolic, parabolic, and elliptic equations. Dashed lines are characteristic curves.

or

$$(1.4.2d) \quad u_y(x, 0) = \text{given} \quad u_y(x, 1) = \text{given}.$$

The term "given" in (1.4.2) refers to a specified numerical value for the function or the appropriate derivative. Alternatively, we might write

$$\begin{aligned} u(0, y) &= f(y), & x &= 0 \\ u_y(0, y) &= g(y), & x &= 0 \\ u(x, 0) &= h(x), & y &= 0 \\ & & & \vdots \end{aligned}$$

indicating that the function or its slope is given but not as a constant. Obviously, these are all special forms of (1.4.1) with a proper selection of $\alpha, \beta,$ and γ .

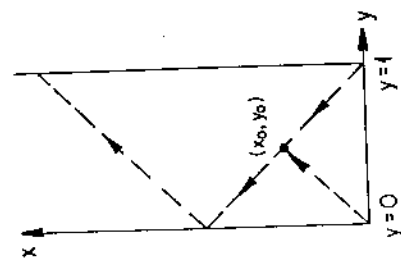


Figure 1.6. Simplified representation of characteristics arising in the hyperbolic equation $u_{xx} = u_{yy}$.

The characteristics shown in Figure 1.5 for this case correspond to

$$\frac{dx}{dy} = \pm 1,$$

which are crossing lines propagating up from $x=0$. Figure 1.6 shows a simplified version of the lower portion of Figure 1.5. The value of $u(x_0, y_0)$ depends only on the initial data between the characteristics shown; in other words, the solution at x_0, y_0 is affected only by the data on the baseline. If a discontinuity in the initial data occurs on the baseline, this discontinuity is propagated along the characteristic through that point. Moreover, this characteristic is continued, as shown, due to the reflection condition along the boundary $y=0$. Of course, now the data at $y=0$ influence the reflected values of $u(x, y)$. The region below the point x_0, y_0 and the appropriate characteristics is referred to as the domain of dependence of the point x_0, y_0 . When one considers a physical system, such as a countercurrent heat exchanger, then a discontinuity of one phase temperature is propagated along with its derivative. When this information reaches the end of the exchanger, a new discontinuity in the other phase temperature derivative propagates back along with its second derivative. In effect, a reflection in temperature derivatives (a reflection of waves) occurs along the characteristics.

Next consider the case of a parabolic PDE, using $u_x = u_{yy}$ as an illustration, in the finite domain of $0 \leq y \leq 1$. Here one initial condition and two boundary conditions are required. For boundary conditions we have chosen

$$u(x, 0) = \text{given} \quad u(x, 1) = \text{given}$$

or

$$u_y(x, 0) = \text{given} \quad u_y(x, 1) = \text{given},$$

with the "given" value having the same meaning as before. It should be apparent from (1.4.1) that these boundary conditions could be written

$$\alpha_1 u + \beta_1 u_y = \gamma_1 \quad \text{at} \quad y = 0$$

and

$$\alpha_2 u + \beta_2 u_y = \gamma_2 \quad \text{and} \quad y = 1,$$

with $\alpha_1, \alpha_2 \geq 0, \beta_1, \beta_2 \leq 0$ and $\alpha_1 - \beta_1 > 0, \alpha_2 - \beta_2 > 0$ in any combination desired. The initial condition could be given as

$$u(0, y) = f(y) \quad \text{at} \quad x = 0.$$

Further, the domain y need not be restricted to $y = 1$ but could be semi-infinite, $y \rightarrow +\infty$, and even infinite in both directions, $-\infty < y < +\infty$. Now we must specify continuity at infinity rather than the specific conditions stated below.

There is only one set of characteristics in the parabolic case; these are shown as horizontal lines in Figure 1.5. The function $u(x, y)$ is now determined by all the initial data plus the data on the sides which are on or below a horizontal characteristic. The domain of determination is now the complete rectangle.

Finally, we consider the elliptic case, $u_{xx} + u_{yy} = 0$. Now there are four boundary conditions (for a rectangular-shaped domain). These could be any combination of the following:

$$u(x, y) = \text{given}$$

$$u_n(x, y) = \text{given}$$

or

$$\alpha u + \beta u_n = \gamma.$$

It is important to point out that when only the normal derivative is given completely around the domain, the solution can only be obtained to an arbitrary constant. Since the elliptic PDE has no real characteristics, none are shown in Figure 1.5.

This is only a small sampling of possible PDEs and associated initial and boundary conditions; others are specified later when we consider specific physical problems.

Finally, we wish to mention a discontinuity that can occur at a corner of a finite domain. Consider, for example, the temperature distribution defining the boundary conditions for a parabolic PDE as illustrated in Figure 1.7. The temperature is 500° on the $x = 0$ line and 100° on the $y = 0$ line. Thus there is a discontinuity in temperature at the corner, $x = 0$ and $y = 0$, because the

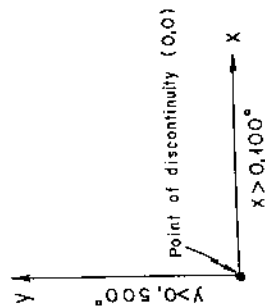


Figure 1.7. Diagrammatic representation of discontinuity at (0,0) arising from different Dirichlet conditions specified along each space coordinate.

temperature will be different as we approach this point from above or from the right. A common practice for handling this discontinuity is to use an average of the two limiting values.

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