SECOND EDITION

Numerical Methods for Partial Differential Equations

WILLIAM F. AMES

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Preface to second edition

Since the publication of the first edition, research in and applications of numerical analysis have expanded rapidly. The past few years have witnessed the maturation of numerical fluid mechanics and finite element techniques. Numerical fluid mechanics is addressed in substance in this second edition. I have also added material in several other areas of promise, including hopscotch and other explicit–implicit methods, Monte Carlo techniques, lines, the fast Fourier transform, and fractional steps methods. A new sixth chapter introduces the general concepts of weighted residuals, with emphasis on orthogonal collocation and the Bubnov–Galerkin method. In turn, the latter procedure is used to introduce the finite element concepts.

The spirit of the first edition was to be as self-contained as possible, to present many applications illustrating the theory, and to supply a substantial number of recent references to supplement the text material. This spirit has been retained—there are 38 more problems and 138 additional references. Also, a substantial number of additional applications have been included and references to others appended.

I wish to extend my special thanks to Ms. Mildred Buckalew for the preparation of an outstanding manuscript on the typewriter.

Georgia Institute of Technology

Preface to first edition

That part of numerical analysis which has been most changed by the ongoing revolution in numerical methods is probably the solution of partial differential equations. The equations from the technological world are often very complicated. Usually, they have variable coefficients, nonlinearities, irregular boundaries, and occur in coupled systems of differing types (say, parabolic and hyperbolic). The 'curse of dimensionality' is ever present – problems with two or three space variables, and time, are within our computational grasp.

Early development of calculational algorithms was based more upon the extension of methods for hand computation, empiricism, and intuition than on mathematical analyses. With increasing education and the subsequent development of the professional numerical analyst, the pattern is changing. New, useful methods are evolving which come closer to full utilization of the inherent powers of high-speed, large-memory computing machines. Many significant and powerful methods await discovery both for problems which are computable with existing techniques and those which are not.

Unfortunately, as in other portions of mathematics, the abstract and the applications have tended to diverge. A new field of pure mathematics has been generated and while it has produced some results of value to users, the complexities of real problems have yet to be significantly covered by the presently available theorems. Nevertheless, guidelines are now available for the person wishing to obtain the numerical solution to a practical problem.

The present volume constitutes an attempt to introduce to upper-level engineering and science undergraduate and graduate students the concepts of modern numerical analyses as they apply to partial differential equations. The book, while sprinkled liberally with practical problems and their solutions, also strives to point out the pitfalls – e.g., overstability, consistency requirements, and the danger of extrapolation to nonlinear problems methods which have proven useful on linear problems. The mathematics is by no means ignored, but its development to a keen-edge is not the major goal of this work.

The diligent student will find 248 problems of varying difficulty to test his mettle. Additionally, over 400 references provide a guide to the research and practical problems of today. With this text as a bridge, the applied student should find the professional numerical analysis journals more understandable.

I wish to extend special thanks to Mrs. Gary Strong and Mrs. Steven

Dukeshier for the typing of a difficult manuscript and Mr. Jasbir Arora for preparation of the ink drawings. Lastly, the excellent cooperation and patience of Dr. Alan Jeffrey and my publishers have made the efforts of the past two years bearable.

Contents

6 Weighted residuals and finite elements

1

Fundamentals

1-0 Introduction

Numerical calculation is commonplace today in fields where it was virtually unknown before 1950. The high-speed computing machine has made possible the solution of scientific and engineering problems of great complexity. This capability has, in turn, stimulated research in numerical analysis since effective utilization of such devices depends strongly upon the continual advance of research in relevant areas of mathematical analysis. One measure of the growth is the upsurge of books devoted to the subject in the years after 1953. A second measure is the development, during the same period, of at least six research journals whose primary concern is numerical analysis. The major research journals are *SIAM Journal of Numerical Analysis, Mathematics of Computation, Numerische Mathematik, Journal of Computational Physics, Computer Journal,* and *ACM Journal.*†

Finite difference approximations for derivatives were already in use by Euler [1]‡ in 1768. The simplest finite difference procedure for dealing with the problem $dx/dt = f(x, t)$, $x(0) = a$ is obtained by replacing $(dx/dt)_{n-1}$ with the crude approximation $(x_n - x_{n-1})/\Delta t$. This leads to the recurrence relation $x_0 = a$, $x_n = x_{n-1} + \Delta t f(x_{n-1}, t_{n-1})$ for $n > 0$. This procedure is known as Euler's method. Thus we see that for one-dimensional systems the finite difference approach has been deeply ingrained in computational algorithms for quite some time.

For two-dimensional systems the first computational application of finite difference methods was probably carried out by Runge [2] in 1908. He studied the numerical solution of the Poisson equation $u_{xx} + u_{yy} =$ constant. At approximately the same time Richardson [3], in England, was carrying on similar research. His 1910 paper was the earliest work on the application of iterative methods to the solution of continuous equilibrium problems by finite differences. In 1918 Liebmann [4], in considering the finite difference approximation to Laplace's equation, suggested an improved method of iteration. Today the name of Liebmann is associated with any method of iteration by single steps in which a fixed calculation sequence is followed.

The study of errors in finite difference calculations is still an area of prime research interest. Early mathematical convergence proofs were carried out by LeRoux [5], Phillips, and Wiener [6], and Courant, Friedrichs, and Lewy [7].

† SIAM is the common abbreviation for Society for Industrial and Applied Mathematics. ACM is the abbreviation for the Association for Computing Machinery.

‡ Numbers in brackets refer to the references at the end of each chapter.

Some consider the celebrated 1928 paper of Courant, Friedrichs, and Lewy as the birthdate of the modern theory of numerical methods for partial differential equations.

The algebraic solution of finite difference approximations is best accomplished by some iteration procedure. Various schemes have been proposed to accelerate the convergence of the iteration. A summary of those that were available in 1950, and which are adaptable to automatic programming, is given by Frankel [8]. Other methods require considerable judgment on the part of the computer and are therefore better suited to hand computation. Higgins [9] gives an extensive bibliography of such techniques. In the latter category the method of *relaxation* has received the most complete treatment. Relaxation was the most popular method in the decade of the thirties. Two books by Southwell [10, 11] describe the process and detail many examples. The *successive over-relaxation method*, extensively used on modern computers, is an outgrowth of this highly successful hand computation procedure.

Let us now consider some of the early technical applications. The pioneering paper of Richardson [3] discussed the approximate solution by finite differences of differential equations describing stresses in a masonry dam. Equilibrium and eigenvalue problems were successfully handled. Binder [12] and Schmidt [13] applied finite difference methods to obtain solutions of the diffusion equation. The classical explicit recurrence relation

$$u_{i,j+1} = ru_{i-1,j} + (1 - 2r)u_{i,j} + ru_{i+1,j}, \qquad r = \Delta t/(\Delta x)^2$$

for the diffusion equation $u_t = u_{xx}$ was given by Schmidt [13] in 1924.

For any given continuous system there are a multiplicity of discrete models which are usually comparable in terms of their relative truncation errors. Early approximations were second order—that is, $O(h^2)$†—and these still play an important role today. Higher order procedures were promoted by Collatz [14, 15] and Fox [16]. The relative economy of computation and accuracy of second-order processes utilizing a small interval size, compared with higher order procedures using larger interval sizes, has been discussed in the papers of Southwell [17] and Fox [18].

It is quite possible to formulate a discrete model in an apparently natural way which, upon computation, produces only garbage.‡ This is especially true in propagation problems—that is, problems described by parabolic and hyperbolic equations. An excellent historical example is provided by Richardson's pioneering paper [3], in which his suggested method for the conduction equation, describing the cooling of a rod, was found to be completely unstable by O'Brien, Hyman, and Kaplan [19]. Another example concerns the trans-

† The notation $O(h^2)$ is read '(term of) order h^2' and can be interpreted to mean 'when h is small enough the term behaves essentially like a constant times h^2'. Later we make this concept mathematically precise.

‡ Misuse of computational algorithms has been described as GIGO—Garbage In and Garbage Out.

verse vibration of a beam. In 1936 Collatz [20] proposed a 'natural' finite difference procedure for the beam equation $u_{tt} + u_{xxxx} = 0$, but fifteen years later [21] the algorithm was found to be computationally unstable.

Nevertheless, the analyst usually strives to use methods dictated by the problem under consideration—these we call *natural methods*. Thus, a natural coordinate system may be toroidal (see Moon and Spencer [22]) instead of cartesian. Certain classes of equations have natural numerical methods which may be distinct from the finite difference methods. Typical of these are the *method of lines* for propagation problems and the *method of characteristics* for hyperbolic systems. Characteristics also provide a convenient way to classify partial differential equations.

1-1 Classification of physical problems

The majority of the problems of physics and engineering fall naturally into one of three *physical* categories: *equilibrium problems*, *eigenvalue problems*, and *propagation problems*.

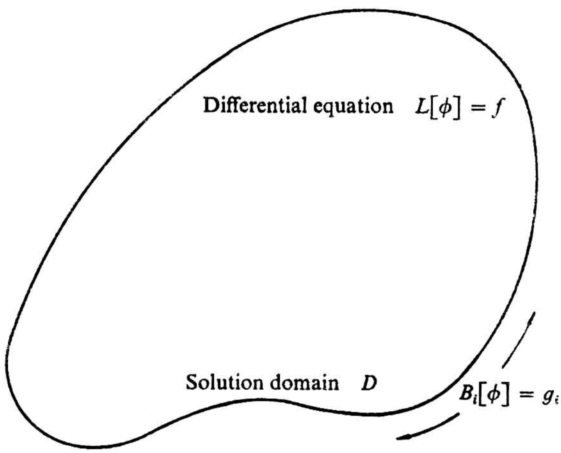

Fig. 1-1 Representation of the general equilibrium problem

Equilibrium problems are problems of steady state in which the equilibrium configuration ϕ in a domain D is to be determined by solving the differential equation

$$L[\phi] = f \tag{1-1}$$

within D, subject to certain boundary conditions

$$B_i[\phi] = g_i \tag{1-2}$$

on the boundary of D. Very often, but not always, the integration domain D is closed and bounded. In Fig. 1-1 we illustrate the general equilibrium problem. In mathematical terminology such problems are known as *boundary* *value problems*. Typical physical examples include steady viscous flow, steady temperature distributions, equilibrium stresses in elastic structures, and steady voltage distributions. Despite the apparent diversity of the physics we shall shortly see that the governing equations for equilibrium problems are *elliptic*.†

Eigenvalue problems may be thought of as extensions of equilibrium problems wherein critical values of certain parameters are to be determined in addition to the corresponding steady-state configurations. Mathematically the problem is to find one or more constants (λ), and the corresponding functions (ϕ), such that the differential equation

$$L[\phi] = \lambda M[\phi] \tag{1-3}$$

is satisfied within D and the boundary conditions

$$B_i[\phi] = \lambda E_i[\phi] \tag{1-4}$$

hold on the boundary of D. Typical physical examples include buckling and stability of structures, resonance in electric circuits and acoustics, natural frequency problems in vibrations, and so on. The operators L and M are of elliptic type.

Propagation problems are initial value problems that have an unsteady state or transient nature. One wishes to predict the subsequent behavior of a system given the initial state. This is to be done by solving the differential equation

$$L[\phi] = f \tag{1-5}$$

within the domain D when the initial state is prescribed as

$$I_i[\phi] = h_i \tag{1-6}$$

and subject to prescribed conditions

$$B_i[\phi] = g_i \tag{1-7}$$

on the (open) boundaries. The integration domain D is open. In Fig. 1-2 we illustrate the general propagation problem. In mathematical parlance such problems are known as *initial boundary value problems*.‡ Typical physical examples include the propagation of pressure waves in a fluid, propagation of stresses and displacements in elastic systems, propagation of heat, and the development of self-excited vibrations. The physical diversity obscures the fact that the governing equations for propagation problems are *parabolic or hyperbolic*.

The distinction between equilibrium and propagation problems was well

† The original mathematical formulation of an equilibrium problem will generate an elliptic equation or system. Later mathematical approximations may change the type. A typical example is the boundary layer approximation of the equations of fluid mechanics. Those elliptic equations are approximated by the parabolic equations of the boundary layer. Yet the problem is still one of equilibrium.

‡ Sometimes only the terminology initial value problem is utilized.

stated by Richardson [23] when he described the first as *jury* problems and the second as *marching* problems. In equilibrium problems the entire solution is passed on by a jury requiring satisfaction of all the boundary conditions and all the internal requirements. In propagation problems the solution marches out from the initial state guided and modified in transit by the side boundary conditions.

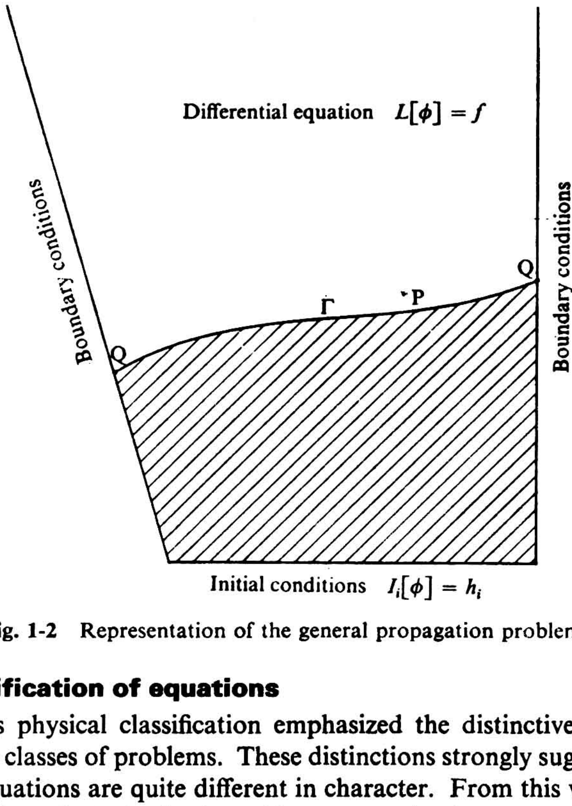

Fig. 1-2 Representation of the general propagation problem

1-2 Classification of equations

The previous physical classification emphasized the distinctive features of basically two classes of problems. These distinctions strongly suggest that the governing equations are quite different in character. From this we infer that the numerical methods for both problems must also have some basic differences. Classification of the equations is best accomplished by developing the concept of *characteristics*.

Let the coefficients $a_1, a_2, \ldots, f_1, f_2$ be functions of x, y, u, and v and consider the simultaneous first-order quasilinear system†

$$\begin{aligned} a_1 u_x + b_1 u_y + c_1 v_x + d_1 v_y &= f_1 \\ a_2 u_x + b_2 u_y + c_2 v_x + d_2 v_y &= f_2 \ddagger \end{aligned} \tag{1-8}$$

† A quasilinear system of equations is one in which the highest order derivatives occur linearly.

‡ We shall often use the notation u_x to represent $\partial u/\partial x$.

This set of equations is sufficiently general to represent many of the problems encountered in engineering where the mathematical model is second order.

Suppose that the solution for u and v is known from the initial state to some curve Γ.† At any boundary point P of this curve, we know the continuously differentiable values of u and v and the directional derivatives of u and v in directions *below* the curve (see Fig. 1-2).

We now seek the answer to the question: 'Is the behavior of the solution just above P uniquely determined by the information below and on the curve?' Stated alternatively: 'Are these data sufficient to determine the directional derivatives at P in directions that lie above the curve Γ?' By way of reducing this question, suppose that θ (an angle with the horizontal) specifies a direction along which σ measures distance. If u_x and u_y are known at P, then the directional derivative

$$u_\sigma|_\theta = u_x \cos\theta + u_y \sin\theta = u_x \frac{dx}{d\sigma} + u_y \frac{dy}{d\sigma} \tag{1-9}$$

is also known, so we restate the question in the simpler form: 'Under what conditions are the derivatives u_x, u_y, v_x, and v_y uniquely determined at P by values of u and v on Γ?' At P we have four relations, Eqns (1-8) and

$$\begin{aligned} du &= u_\sigma\, d\sigma = u_x\, dx + u_y\, dy \\ dv &= v_\sigma\, d\sigma = v_x\, dx + v_y\, dy \end{aligned} \tag{1-10}$$

whose matrix form is

$$\begin{bmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{bmatrix} \begin{bmatrix} u_x \\ u_y \\ v_x \\ v_y \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ du \\ dv \end{bmatrix} \tag{1-11}$$

With u and v known at P the coefficient functions $a_1, a_2, \ldots, f_1, f_2$ are known. With the direction of Γ known, dx and dy are known; and if u and v are known along Γ, du and dv are also known. Thus, the four equations [Eqns (1-11)] for the four partial derivatives have known coefficients. A unique solution for u_x, u_y, v_x, and v_y exists if the determinant of the 4×4 matrix in Eqns (1-11) is *not zero*. If the determinant is not zero, then the directional derivatives have the same value above and below Γ.

The exceptional case, when the determinant is zero, implies that a multiplicity of solutions are possible. Thus, the system of Eqns (1-11) does not determine the partial derivatives uniquely. Consequently, discontinuities in

† We restrict this discussion to a finite domain in which discontinuities do not occur. Later developments consider the degeneration of smooth solutions into discontinuous ones. Additional information is available in Jeffrey and Taniuti [24] and Ames [25].

the partial derivatives may occur as we cross Γ. Upon equating to zero the determinant of the matrix in Eqns (1-11) we find the *characteristic equation*

$$(a_1c_2 - a_2c_1)(dy)^2 - (a_1d_2 - a_2d_1 + b_1c_2 - b_2c_1)\, dxdy + (b_1d_2 - b_2d_1)(dx)^2 = 0 \qquad (1\text{-}12)$$

which is a quadratic equation in dy/dx. If the curve Γ (Fig. 1-2) at P has a slope such that Eqn (1-12) is satisfied, then the derivatives u_x, u_y, v_x, and v_y are not uniquely determined by the values of u and v on Γ. The directions specified by Eqn (1-12) are called *characteristic directions*; they may be real and distinct, real and identical, or not real according to whether the discriminant

$$(a_1d_2 - a_2d_1 + b_1c_2 - b_2c_1)^2 - 4(a_1c_2 - a_2c_1)(b_1d_2 - b_2d_1) \qquad (1\text{-}13)$$

is positive, zero, or negative. This is also the criterion for classifying Eqns (1-8) as hyperbolic, parabolic, or elliptic. They are *hyperbolic* if Eqn (1-13) is positive—that is, has two *real* characteristic directions; *parabolic* if Eqn (1-13) is zero; and *elliptic* if there are no real characteristic directions.

Next consider the quasilinear second-order equation

$$au_{xx} + bu_{xy} + cu_{yy} = f \qquad (1\text{-}14)$$

where a, b, c, and f are functions of x, y, u, u_x, and u_y. The classification of Eqn (1-14) can be examined by reduction to a system of first-order equations† or by independent treatment. Taking the latter course we ask the conditions under which a knowledge of u, u_x, and u_y on Γ (see Fig. 1-2) serve to determine u_{xx}, u_{xy},‡ and u_{yy} uniquely so that Eqn (1-14) is satisfied. If these derivatives exist we must have

$$\begin{aligned} d(u_x) &= u_{xx}\, dx + u_{xy}\, dy \\ d(u_y) &= u_{xy}\, dx + u_{yy}\, dy \end{aligned} \qquad (1\text{-}15)$$

† Transformation of Eqn (1-14) into a system of first-order equations is *not unique*. This 'nonuniqueness' is easily demonstrated. Substitutions (i) $w = u_x$, $v = u_y$, and (ii) $w = u_x$, $v = u_x + u_y$ both reduce Eqn (1-14) to two first-order equations.

For (i) we find the system

$$\begin{aligned} aw_x + bw_y + cv_y &= f \\ w_y - v_x &= 0 \end{aligned}$$

and for (ii) we have

$$\begin{aligned} aw_x + (b - c)w_y + cv_y &= f \\ w_y - v_x - w_x &= 0 \end{aligned}$$

Some forms may be more convenient than others during computation. An example of this, from a paper by Swope and Ames [26], will be discussed in Chapter 4.

‡ Throughout, unless otherwise specified, we shall assume that the continuity condition, under which $u_{xy} = u_{yx}$, is satisfied.

Eqns (1-15), together with Eqn (1-14), has the matrix form

$$\begin{bmatrix} a & b & c \\ dx & dy & 0 \\ 0 & dx & dy \end{bmatrix} \begin{bmatrix} u_{xx} \\ u_{xy} \\ u_{yy} \end{bmatrix} = \begin{bmatrix} f \\ d(u_x) \\ d(u_y) \end{bmatrix} \tag{1-16}$$

Thus the solution for u_{xx}, u_{xy}, and u_{yy} exists, and it is unique unless the determinant of the coefficient matrix vanishes, that is

$$a(dy)^2 - b\,dydx + c(dx)^2 = 0. \tag{1-17}$$

Accordingly, the characteristic equation for the second-order quasilinear equation is (1-17). Equation (1-14) is hyperbolic if $b^2 - 4ac > 0$, parabolic if $b^2 - 4ac = 0$, and elliptic if $b^2 - 4ac < 0$. Since a, b, and c are functions of x, y, u, u_x, and u_y, an equation may change its type from region to region.

In the hyperbolic case there are two real characteristic curves. Since the higher order derivatives are indeterminate along these curves they provide paths for the propagation of discontinuities. Indeed, shock waves and other disturbances do propagate into media along characteristics.

The characteristic directions for the linear wave equation

$$u_{xx} - \alpha^2 u_{yy} = 0 \quad (\alpha \text{ constant}) \tag{1-18}$$

are

$$(dy)^2 - \alpha^2(dx)^2 = 0$$

or

$$y \pm \alpha x = \beta. \tag{1-19}$$

These are obviously straight lines.

A more complicated example is furnished by the nozzle problem. The governing equations of steady two-dimensional irrotational isentropic flow of a gas are (see, for example, Shapiro [27]):

$$\begin{aligned} uu_x + vu_y + \rho^{-1}p_x &= 0 \\ uv_x + vv_y + \rho^{-1}p_y &= 0 \\ (\rho u)_x + (\rho v)_y &= 0 \\ v_x - u_y &= 0 \end{aligned} \tag{1-20}$$

$$p\rho^{-\gamma} = \text{constant}, \qquad \frac{dp}{d\rho} = c^2$$

where u and v are velocity components, p is pressure, ρ is density, c is the velocity of sound, and γ is the ratio of specific heats (for air $\gamma = 1.4$).

By multiplying the first of Eqns (1-20) by ρu, the second by ρv, using $dp = c^2\,d\rho$, and adding the two resulting equations we find that Eqns (1-20) are equivalent to the following pair of first-order equations for u and v,

$$\begin{aligned} (u^2 - c^2)u_x + (uv)u_y + (uv)v_x + (v^2 - c^2)v_y &= 0 \\ -u_y + v_x &= 0 \end{aligned} \tag{1-21}$$