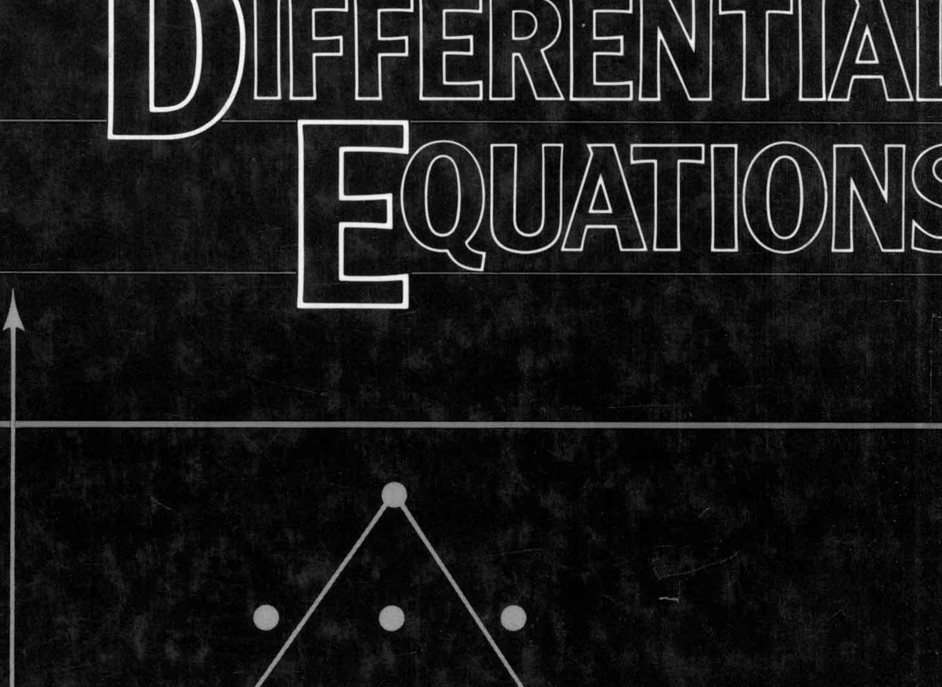
Numerical Analysis of Partial Differential Equations



CHARLES A. HALL
THOMAS A. PORSCHING

NUMERICAL ANALYSIS OF PARTIAL DIFFERENTIAL EQUATIONS

Charles A. Hall
Thomas A. Porsching
Institute for
Computational Mathematics and Applications
University of Pittsburgh

Prentice Hall, Englewood Cliffs, New Jersey 07632

Library of Congress Cataloging-in-Publication Data

HALL, CHARLES A., (date)
Numerical analysis of partial differential equations / Charles A. Hall, Thomas A. Porsching.
p. cm.
Includes bibliographical references.
ISBN 0-13-626557-X
1. Differential equations, Partial—Numerical solutions.
I. Porsching, Thomas A., (date). II. Title.
QA374.H29 1990
515'.353—dc20 89-16245
CIP

Editorial/production supervision
and interior design: *Kathleen M. Lafferty*
Cover design: *Lundgren Graphics, Ltd.*
Manufacturing buyer: *Paula Massenaro*

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

ISBN 0-13-626557-X

Prentice-Hall International (UK) Limited, *London*
Prentice-Hall of Australia Pty. Limited, *Sydney*
Prentice-Hall Canada Inc., *Toronto*
Prentice-Hall Hispanoamericana, S.A., *Mexico*
Prentice-Hall of India Private Limited, *New Delhi*
Prentice-Hall of Japan, Inc., *Tokyo*
Simon & Schuster Asia Pte. Ltd., *Singapore*
Editora Prentice-Hall do Brasil, Ltda., *Rio de Janeiro*

NUMERICAL ANALYSIS OF PARTIAL DIFFERENTIAL EQUATIONS

To our parents
George and Minnie Hall
and
August and Dorothy Porsching
for making it all possible

and to our wives
Mary and Eve
for sustaining it

Preface

In *Numerical Analysis of Partial Differential Equations* we present an account of the theory and methodology of the numerical solution of partial differential equations. This important subject forms much of the core of what is known more generally as "scientific computing," and it is one of the main areas that spawned the development of today's multimillion-dollar supercomputers.

Scientific computing was defined by Garrett Birkhoff[1] in 1971 as "the art of utilizing physical intuition, mathematical theorems and algorithms, and modern computer technology to construct and explore realistic models of problems arising in the natural sciences and engineering." In this spirit, our goal is to present some problems from these disciplines that involve partial differential equations, discuss algorithms for their numerical solution, and provide sufficient theory for an intelligent analysis of such algorithms.

We have attempted to avoid the "recipe format" in which numerical algorithms are given with little or no theoretical justification. At the same time, it is not our intention to sacrifice practicality on the altar of abstract analysis. Thus, in this textbook we hope to strike a middle ground and provide a development of material that is a balance between finite difference and finite element methods, has both a practical

[1] G. Birkhoff, *The Numerical Solution of Elliptic Equations*, SIAM, Philadelphia, 1971.

and an analytic nature, and contains basic theoretical results at a level that is understandable to beginning graduate students in engineering and the sciences.

This book is divided into two parts. Part I, A Course in the Numerical Solution of Partial Differential Equations, is self-contained and is suitable for a one-term (40 to 45 one-hour lectures) introductory graduate course on the subject. This material treats stationary and evolutionary partial differential equations. Numerical algorithms for the evolution equations are based on finite difference approximations, whereas those for stationary equations are developed via the finite element method. In this way we cover the two most popular and successful methodologies in use today. Part II, Some Additional Topics, contains subject matter that may be used to supplement or replace material from Part I. The two-part structure is intended to give the text a modular format and allow additional or alternate chapters from Part II to be "snapped" into Part I. The price of this flexibility is a certain amount of redundancy, but we hope, this has been minimized. We have endeavored to keep Part II largely independent of Part I. However, the material on finite elements in Chapters 8 and 9 should be preceded by a reading of Section 1 of Chapter 5, and Chapter 6.

The chapters include explanatory examples in the main body of the text as well as sets of exercises. There are traditional pencil-and-paper problems that test the understanding of the material developed in the chapter. In addition, there are Computer Exercises that require the reader to develop computer programs and/or use software available from other sources such as mathematical software libraries. Notes and Remarks sections appear at the ends of chapters to provide historical comments and additional references.

We have followed a standard method of referencing key items such as theorems, tables, examples, and equations. They are ordered by chapter, section, and their order of occurrence. For numbering purposes no distinction is made among lemmas, theorems, and corollaries. Thus in Chapter 5, Section 2, the fourth equation is numbered (5.2.4). Similarly, Theorem 5.2.1 is the first theorem (lemma or corollary) in Section 2 of Chapter 5. Notes and remarks are numbered according to their relevancy to a specific section.

Any attempt to treat a subject as large as the numerical solution of partial differential equations in a single work necessarily entails the omission of many interesting and relevant subjects. In this respect, we have consciously decided not to include extensive material on the solution of the algebraic equation systems arising from finite difference and finite element algorithms. However, Section 3 of Chapter 10 does contain a brief survey of such methods, and numerical methods for the solution of *general* linear and nonlinear equation systems may be found, for instance, in Stewart [1973] and Ortega and Rheinboldt [1970], respectively. Other topics for which the diligent reader will search in vain include finite element methods for hyperbolic equations, collocation methods, eigenvalue problems, and boundary elements, among others.

This book is an outgrowth of lecture notes developed by the authors over the years for courses on the subject at the University of Pittsburgh. It is intended for first-year graduate students in the sciences and engineering. Some material has also been used with success at the senior undergraduate level. Prerequisites include courses in advanced calculus, linear algebra and matrix theory, and differential equations.

During the course of writing this book, we have benefited from the suggestions and advice of many people. In this respect, we wish to mention our colleagues Charles Cullen, Vincent Ervin, Donald French, William Layton, Walter Pilant, and Patrick Rabier. We also acknowledge the Math 307B students, especially Monica Brodzik, Yiping Huang, and Victoria Radel, who participated in the debugging of preliminary versions of the text. We appreciate the comments of the following reviewers: Richard Falk, Rutgers University; Bruce Kellogg, University of Maryland; Robert J. Krueger, Iowa State University; William Layton, University of Pittsburgh; J. Tinsley Oden, The University of Texas at Austin; Dennis Ryan, Wright State University; and Olof Widlund, New York University. Finally, the authors thank Catherine Morrow, administrative assistant, ICMA, for her skillful assistance in the preparation of the manuscript, and Monica Brodzik for painstakingly reviewing the galleys.

Charles A. Hall
Thomas A. Porsching

Contents

PART I

A COURSE IN THE NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS

1

Numerical Discretization: Finite Differences and Finite Elements

Although partial differential equations are used to describe many of the physical phenomena of science and engineering, few yield to closed-form solution. Numerical methods that have been developed to approximate solutions of partial differential equations can, for the most part, be grouped into two broad classes: *finite difference methods* and *finite element methods*. Our purpose in this book is to familiarize the reader with both classes of methods, to highlight their advantages and shortcomings, and above all, to present techniques that can be used for their analysis.

1.1 A MODEL PROBLEM

In this chapter we provide a description of both the finite difference and finite element methods applied to a simple transient convection–diffusion equation in one spatial dimension. This serves as an introduction to these methods and illustrates some of the computational pitfalls encountered in their implementation. Such pitfalls provide a partial justification for the need to analyze numerical methods.

Our model initial–boundary value problem is the following: Find $u(x, t)$ such that

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} - K\frac{\partial^2 u}{\partial x^2} = 0, \qquad 0 < x < 1, \quad t > 0 \tag{1.1.1}$$

subject to the *initial condition*

$$u(x, 0) = 0, \qquad 0 \le x \le 1, \tag{1.1.2}$$

and *boundary conditions*

$$u(0, t) = 0 \quad \text{and} \quad u(1, t) = 1, \qquad t > 0. \tag{1.1.3}$$

We assume that the constants $v > 0$ and $K > 0$ are specified. The variable u can be thought of as the temperature of a fluid moving at a velocity, v, through a thin tube occupying the interval $0 \le x \le 1$. The temperature is forced to be 0 at the inlet ($x = 0$) and 1 at the outlet ($x = 1$) (see also the Notes and Remarks for Section 2.3). The constant K is called the thermal diffusivity of the fluid. The fluid is initially ($t = 0$) at a temperature of 0. We seek the temperature $u(x, t)$ at each position x in the tube and for each subsequent time t.

1.2 FINITE DIFFERENCE METHODS

An elementary approach to finite difference methods is provided by Taylor's theorem, which we state as follows:

> Let $\phi \in C^{n+1}[a, b]$, where $C^{n+1}[a, b]$ denotes the class of functions that are $n + 1$ times continuously differentiable on the interval $[a, b]$. Then there exists a number ξ, $a < \xi < b$, such that
>
> $$\phi(b) = \sum_{i=0}^{n} \frac{\phi^{(i)}(a)}{i!}(b - a)^i + R_n,$$
>
> where
>
> $$R_n = \frac{\phi^{(n+1)}(\xi)(b - a)^{n+1}}{(n + 1)!}.$$

From this theorem it is easy to justify the following three approximations to $d\phi/dx(a)$:

1. *Forward difference:* $$\frac{\phi(a + h) - \phi(a)}{h},$$
2. *Backward difference:* $$\frac{\phi(a) - \phi(a - h)}{h},$$
3. *Centered difference:* $$\frac{\phi(a + h) - \phi(a - h)}{2h},$$

where h is a positive increment. Indeed, if ϕ is sufficiently smooth, then (1) and (2) approximate $d\phi/dx(a)$ with an error that is $O(h)$ as $h \to 0$, while (3) approximates $d\phi/dx(a)$ with an error that is $O(h^2)$ as $h \to 0$ (see Exercises 1.1 and 1.2). We say that (1) or (2) is a *first-order*, and (3) is a *second-order*, approximation to $d\phi/dx$.

The second derivative $d^2\phi/dx^2$ can be approximated similarly using the formula

4. *(Second) centered difference:* $$\frac{\phi(a+h) - 2\phi(a) + \phi(a-h)}{h^2},$$

which is also second order as $h \to 0$. These approximations are sufficient for our purposes, although it is worth mentioning that higher-order finite difference formulas can be derived as well as finite difference approximations of higher-ordered derivatives.

If L_h is a finite difference approximation to a differential operator L and

$$(L_h - L)[\phi](a) \to 0 \quad \text{as} \quad h \to 0,$$

then $L_h[\phi]$ is said to be a *consistent finite difference* approximation to $L[\phi]$ at a. For example,

$$L_h[\phi] \equiv \frac{\phi(a+h) - \phi(a)}{h}$$

is a consistent approximation to $L[\phi] \equiv d\phi/dx$ at a.

Finite difference methods for solving initial–boundary value problems such as (1.1.1)–(1.1.3) determine approximations at a finite number of points in the domain and involve four basic steps:

1. Subdivide the domain, for example by the uniform mesh $0 = x_0 < x_1 \cdots < x_N = 1$, where the *mesh points* are $x_j = j\,\Delta x$ and the *mesh gauge* is $\Delta x = 1/N$.
2. Approximate the differential equation at each mesh point x_j by replacing derivatives by appropriately chosen finite difference approximations.
3. Impose the boundary and initial conditions on the system generated in step 2.
4. Solve the finite difference equations generated in steps 2 and 3.

Hence we replace a differential equation and any auxiliary conditions by a system of (in this case) linear algebraic equations. The solution of the latter constitutes an approximation at mesh points to the solution of the former.

We now apply the finite difference method to the model convection–diffusion problem given above. There are choices to be made for the temporal and spatial discretizations, and we discuss each separately.

1.2.1 Spatial Discretization

Assume for the moment that u does not depend on time t (i.e., $\partial u/\partial t = 0$). The result is the steady-state boundary value problem[1]

$$\begin{cases} vu_x - Ku_{xx} = 0, & 0 < x < L = 1 \\ u(0) = 0, & u(1) = 1. \end{cases} \tag{1.2.1}$$

[1] Here we use subscript notation for partial differentiation. Thus $u_x = \partial u/\partial x$ and $u_{xx} = \partial^2 u/\partial x^2$. This is a practice we shall continue to employ whenever it is convenient.

One can verify that the solution of this boundary value problem is

$$u(x) = \frac{1 - e^{Rx}}{1 - e^{R}}, \tag{1.2.2}$$

where $R \equiv vL/K$ is called the *Péclet number.*

If the "standard" centered difference approximations are used, we obtain the second-order finite difference equations

$$v\frac{U_{j+1} - U_{j-1}}{2\Delta x} - K\frac{U_{j-1} - 2U_j + U_{j+1}}{\Delta x^2} = 0, \qquad 1 \le j \le N - 1, \tag{1.2.3}$$

where $U_j \approx u(x_j)$. This set of difference equations can be solved in closed form as follows. Let $P = R\,\Delta x/2$. Then (1.2.3) can be rewritten as

$$-(P + 1)U_{j-1} + 2U_j + (P - 1)U_{j+1} = 0, \qquad 1 \le j \le N - 1,$$

where $U_0 = 0$ and $U_N = 1$. Assume that $U_j = r^j$ for some nonzero number r. Substituting, we obtain the auxiliary equation

$$[(1 - P)r^2 - 2r + (P + 1)]r^{j-1} = 0,$$

from which it follows that $r = 1$ or $r = (1 + P)/(1 - P)$. If A and B are arbitrary constants, we see that

$$U_j = A + B\left(\frac{1 + P}{1 - P}\right)^j, \qquad 0 \le j \le N,$$

is also a solution. The boundary conditions then determine A and B and, for example, the closed-form solution of (1.2.3) is

$$U_j = \frac{1 - Z^j}{1 - Z^N}, \qquad 0 \le j \le N, \tag{1.2.4}$$

where $Z = (2 + R\,\Delta x)/(2 - R\,\Delta x)$. We note in passing that Z is the (1, 1)-Padé second-order rational approximation to $e^{R\,\Delta x}$ [cf. (1.2.2) and (1.2.4)]. The reader is referred to the Notes and Remarks section for a definition of Padé approximants.

Unfortunately, if $\Delta x > 2/R$, then Z is negative and U_j oscillates as j ranges from 1 to $N - 1$. For example, $R = 50$, $N = 10$, and $\Delta x = 0.1$ yields $Z = -7/3$ and $U_9 \approx -0.43$ (see Figure 1.2.1). However, the true solution $u(x)$ is positive, monotone, and ranges from 0 to 1. Of course, if Δx is chosen to be less than 0.04, then Z is positive and monotone, and we obtain much better agreement with the true solution. For more complicated problems in which v and R are position dependent, or for multidimensional problems, it is not easy to predict the size of mesh that will prevent oscillations. Also, this mesh size may be prohibitively small from a computational efficiency standpoint.

A popular means of avoiding this aphysical oscillatory behavior is through the use of *upwind differencing*, in which (1.2.1) is discretized as

$$v\frac{U_j^E - U_j^W}{\Delta x} - K\frac{U_{j-1} - 2U_j + U_{j+1}}{\Delta x^2} = 0, \qquad 1 \le j \le N - 1, \tag{1.2.5}$$