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Stig Larsson Vidar Thomée

Partial Differential Equations with Numerical Methods

偏微分方程与数值方法

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《国外数学名著系列》(影印版)序

要使我国的数学事业更好地发展起来，需要数学家淡泊名利并付出更艰苦地努力。另一方面，我们也要从客观上为数学家创造更有利的发展数学事业的外部环境，这主要是加强对数学事业的支持与投资力度，使数学家有较好的工作与生活条件，其中也包括改善与加强数学的出版工作。

从出版方面来讲，除了较好较快地出版我们自己的成果外，引进国外的先进出版物无疑也是十分重要与必不可少的。从数学来说，施普林格（Springer）出版社至今仍然是世界上最具权威的出版社。科学出版社影印一批他们出版的好的新书，使我国广大数学家能以较低的价格购买，特别是在边远地区工作的数学家能普遍见到这些书，无疑是对推动我国数学的科研与教学十分有益的事。

这次科学出版社购买了版权，一次影印了 23 本施普林格出版社出版的数学书，就是一件好事，也是值得继续做下去的事情。大体上分一下，这 23 本书中，包括基础数学书 5 本，应用数学书 6 本与计算数学书 12 本，其中有些书也具有交叉性质。这些书都是很新的，2000 年以后出版的占绝大部分，共计 16 本，其余的也是 1990 年以后出版的。这些书可以使读者较快地了解数学某方面的前沿，例如基础数学中的数论、代数与拓扑三本，都是由该领域大数学家编著的“数学百科全书”的分册。对从事这方面研究的数学家了解该领域的前沿与全貌很有帮助。按照学科的特点，基础数学类的书以“经典”为主，应用和计算数学类的书以“前沿”为主。这些书的作者多数是国际知名的大数学家，例如《拓扑学》一书的作者诺维科夫是俄罗斯科学院的院士，曾获“菲尔兹奖”和“沃尔夫数学奖”。这些大数学家的著作无疑将会对我国的科研人员起到非常好的指导作用。

当然，23 本书只能涵盖数学的一部分，所以，这项工作还应该继续做下去。更进一步，有些读者面较广的好书还应该翻译成中文出版，使之有更大的读者群。

总之，我对科学出版社影印施普林格出版社的部分数学著作这一举措表示热烈的支持，并盼望这一工作取得更大的成绩。

王　元

2005 年 12 月 3 日

Preface

Our purpose in this book is to give an elementary, relatively short, and hopefully readable account of the basic types of linear partial differential equations and their properties, together with the most commonly used methods for their numerical solution. Our approach is to integrate the mathematical analysis of the differential equations with the corresponding numerical analysis. For the mathematician interested in partial differential equations or the person using such equations in the modelling of physical problems, it is important to realize that numerical methods are normally needed to find actual values of the solutions, and for the numerical analyst it is essential to be aware that numerical methods can only be designed, analyzed, and understood with sufficient knowledge of the theory of the differential equations, using discrete analogues of properties of these.

In our presentation we study the three major types of linear partial differential equations, namely elliptic, parabolic, and hyperbolic equations, and for each of these types of equations the text contains three chapters. In the first of these we introduce basic mathematical properties of the differential equation, and discuss existence, uniqueness, stability, and regularity of solutions of the various boundary value problems, and the remaining two chapters are devoted to the most important and widely used classes of numerical methods, namely finite difference methods and finite element methods.

Historically, finite difference methods were the first to be developed and applied. These are normally defined by looking for an approximate solution on a uniform mesh of points and by replacing the derivatives in the differential equation by difference quotients at the mesh-points. Finite element methods are based instead on variational formulations of the differential equations and determine approximate solutions that are piecewise polynomials on some partition of the domain under consideration. The former method is somewhat restricted by the difficulty of adapting the mesh to a general domain whereas the latter is more naturally suited for a general geometry. Finite element methods have become most popular for elliptic and also for parabolic problems, whereas for hyperbolic equations the finite difference method continues to dominate. In spite of the somewhat different philosophy underlying the two classes it is more reasonable in our view to consider the latter as further developments of the former rather than as competitors, and we feel that the practitioner of differential equations should be familiar with both.

To make the presentation more easily accessible, the elliptic chapters are preceded by a chapter about the two-point boundary value problem for a second order ordinary differential equation, and those on parabolic and hyperbolic evolution equations by a short chapter about the initial value problem for a system of ordinary differential equations. We also include a chapter about eigenvalue problems and eigenfunction expansion, which is an important tool in the analysis of partial differential equations. There we also give some simple examples of numerical solution of eigenvalue problems.

The last chapter provides a short survey of other classes of numerical methods of importance, namely collocation methods, finite volume methods, spectral methods, and boundary element methods.

The presentation does not presume a deep knowledge of mathematical and functional analysis. In an appendix we collect some of the basic material that we need in these areas, mostly without proofs, such as elements of abstract linear spaces and function spaces, in particular Sobolev spaces, together with basic facts about Fourier transforms. In the implementation of numerical methods it will normally be necessary to solve large systems of linear algebraic equations, and these generally have to be solved by iterative methods. In a second appendix we therefore include an orientation about such methods.

Our purpose has thus been to cover a rather wide variety of topics, notions, and ideas, rather than to expound on the most general and far-reaching results or to go deeply into any one type of application. In the problem sections, which end the various chapters, we sometimes ask the reader to prove some results which are only stated in the text, and also to further develop some of the ideas presented. In some problems we propose testing some of the numerical methods on the computer, assuming that MATLAB or some similar software is available. At the end of the book we list a number of standard references where more material and more detail can be found, including issues concerned with implementation of the numerical methods.

This book has developed from courses that we have given over a rather long period of time at Chalmers University of Technology and Göteborg University originally for third year engineering students but later also in beginning graduate courses for applied mathematics students. We would like to thank the many students in these courses for the opportunities for us to test our ideas.

Göteborg,
January, 2003

Stig Larsson
Vidar Thomée

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1 Introduction

In this first chapter we begin in Sect. 1.1 by introducing the partial differential equations and associated initial and boundary value problems that we shall study in the following chapters. The equations are classified into elliptic, parabolic, and hyperbolic equations, and we indicate the corresponding type of problems in physics that they model. We discuss briefly the concept of a well posed boundary value problem, and the various techniques used in our subsequent presentation. In Sect. 1.2 we introduce some notation and concepts that will be used throughout the text, and in Sect. 1.3 we include a detailed derivation of the heat equation from physical principles explaining the meaning of all terms that occur in the equation and the boundary conditions. In the problem section, Sect. 1.4, we add some further illustrative material.

1.1 Background

In this text we study boundary value and initial-boundary value problems for partial differential equations, that are significant in applications, from both a theoretical and a numerical point of view. As a typical example of such a boundary value problem we consider first Dirichlet's problem for Poisson's equation,

$$-\Delta u = f(x) \quad \text{in } \Omega, \tag{1.1}$$

$$u = g(x) \quad \text{on } \Gamma, \tag{1.2}$$

where $x = (x_1, \dots, x_d)$, Δ is the Laplacian defined by $\Delta u = \sum_{j=1}^{d} \partial^2 u / \partial x_j^2$, and Ω is a bounded domain in d-dimensional Euclidean space $\mathbf{R}^d$ with boundary Γ. The given functions $f = f(x)$ and $g = g(x)$ are the *data* of the problem. Instead of Dirichlet's boundary condition (1.2) one can consider, for instance, Neumann's boundary condition

$$\frac{\partial u}{\partial n} = g(x) \quad \text{on } \Gamma, \tag{1.3}$$

where $\partial u / \partial n$ denotes the derivative in the direction of the exterior unit normal n to Γ. Another choice is Robin's boundary condition

$$\frac{\partial u}{\partial n} + \beta(x)u = g(x) \quad \text{on } \Gamma. \tag{1.4}$$

More generally, a linear second order elliptic equation is of the form

$$\mathcal{A}u := -\sum_{i,j=1}^{d} \frac{\partial}{\partial x_i}\Big(a_{ij}(x)\frac{\partial u}{\partial x_j}\Big) + \sum_{j=1}^{d} b_j(x)\frac{\partial u}{\partial x_j} + c(x)u = f(x), \tag{1.5}$$

where $A(x) = (a_{ij}(x))$ is a sufficiently smooth positive definite matrix, and such an equation may also be considered in Ω together with various boundary conditions. In our treatment below we shall often restrict ourselves, for simplicity, to the isotropic case $A(x) = a(x)I$, where $a(x)$ is a smooth positive function and I the identity matrix.

Elliptic equations such as the above occur in a variety of applications, modeling, for instance, various potential fields (gravitational, electrostatic, magnetostatic, etc.), probability densities in random-walk problems, stationary heat flow, and biological phenomena. They are also related to important areas within pure mathematics, such as the theory of functions of a complex variable $z = x + iy$, conformal mapping, etc. In applications they often describe stationary, or time independent, physical states.

We also consider time dependent problems, and our two model equations are the heat equation,

$$\frac{\partial u}{\partial t} - \Delta u = f(x,t), \tag{1.6}$$

and the wave equation,

$$\frac{\partial^2 u}{\partial t^2} - \Delta u = f(x,t). \tag{1.7}$$

These will be considered for positive time t, and for x varying either throughout $\mathbf{R}^d$ or in some bounded domain $\Omega \subset \mathbf{R}^d$, on the boundary of which boundary conditions are prescribed as for Poisson's equation above. For these time dependent problems, the value of the solution u has to be given at the initial time $t = 0$, and in the case of the wave equation, also the value of $\partial u/\partial t$ at $t = 0$. In the case of the unrestricted space $\mathbf{R}^d$ the respective problems are referred to as the pure *initial value problem* or *Cauchy problem* and, in the case of a bounded domain Ω, a mixed *initial-boundary value problem.*

Again, these equations, and their generalizations permitting more general elliptic operators than the Laplacian Δ, appear in a variety of applied contexts, such as, in the case of the heat equation, in the conduction of heat in solids, in mass transport by diffusion, in diffusion of vortices in viscous fluid flow, in telegraphic transmission in cables, in the theory of electromagnetic waves, in hydromagnetics, in stochastic and biological processes; and, in the case of the wave equation, in vibration problems in solids, in sound waves in a tube, in the transmission of electricity along an insulated, low resistance cable, in long water waves in a straight canal, etc.

Some characteristics of equations of type (1.7) are shared with certain systems of first order partial differential equations. We shall therefore also have reason to study scalar linear partial differential equations of the form

$$\frac{\partial u}{\partial t} + \sum_{j=1}^{d} a_j(x,t)\frac{\partial u}{\partial x_j} + a_0(x,t)u = f(x,t),$$

and corresponding systems where the coefficients are matrices. Such systems appear, for instance, in fluid dynamics and electromagnetic field theory.

Applied problems often lead to partial differential equations which are nonlinear. The treatment of such equations is beyond the scope of this presentation. In many cases, however, it is useful to study linearized versions of these, and the theory of linear equations is therefore relevant also to nonlinear problems.

In applications, the equations used in the models normally contain physical parameters. For instance, in the case of the heat conduction problem, the temperature at a point of a homogeneous isotropic solid, extended over Ω, with the thermal conductivity k, density ρ, and specific heat capacity c, and with a heat source $f(x,t)$, satisfies

$$\rho c \frac{\partial u}{\partial t} = \nabla \cdot (k \nabla u) + f(x,t) \quad \text{in } \Omega.$$

If ρ, c, and k are constant, this equation may be written in the form (1.6) after a simple transformation, but if they vary with x, a more general elliptic operator is involved.

In Sect. 1.3 below we derive the heat equation from physical principles and explain, in the context given, the physical meaning of all terms in the elliptic operator (1.5) as well as the boundary conditions (1.2), (1.3), and (1.4). A corresponding derivation or the wave equation is given in Problem 1.2. Boundary value problems for elliptic equations, or stationary problems, may appear as limiting cases of the evolution problems as $\to \infty$.

One characteristic of mathematical modeling is that once the model is established, in our case as an initial or initial-boundary value problem for a partial differential equation, the analysis becomes purely mathematical and is independent of any specific application that the model describes. The results obtained are then valid for all the different examples of the model. We shall therefore not use much terminology from physics or other applied fields in our exposition, but invoke special applications in the exercises. It is often convenient to keep such examples in mind to enhance the intuitive understanding of a mathematical model.

The equations (1.1), (1.6), and (1.7) are said to be of elliptic, parabolic, and hyperbolic type, respectively. We shall return to the classification of partial differential equations into different types in Chapt. 11 below, and note here only that a differential equation in two variables x and t of the form

$$a\frac{\partial^2 u}{\partial t^2} + 2b\frac{\partial^2 u}{\partial x \partial t} + c\frac{\partial^2 u}{\partial x^2} + \ldots = f(x,t)$$

is said to be *elliptic, hyperbolic* or *parabolic* depending on whether $\delta = ac - b^2$ is positive, negative, or zero. Here $\ldots$ stands for a linear combination of derivatives of orders at most 1. In particular,

$$\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2 u}{\partial x^2} = f(x,t),$$

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = f(x,t),$$

and

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f(x,t),$$

are of these three types, respectively. Note that the conditions on the sign of δ are the same as those occurring in the classification of plane quadratic curves into ellipses, hyperbolas, and parabolas.

Together with the partial differential equations we also study numerical approximations by finite difference and finite element methods. For these problems, the continuous and the discretized equations, we prove results of the following types:

- *existence* of solutions,
- *uniqueness* of solutions,
- *stability*, or continuous dependence of solutions with respect to perturbations of data,
- *error estimates* (for numerical methods).

A boundary value problem that satisfies the three first of these conditions is said to be *well posed.* In order to prove such results we employ several techniques:

- *maximum principles*,
- *Fourier methods*; these are techniques that are based on the use of the Fourier transform, Fourier series expansion, or eigenfunction expansion,
- *energy estimates*,
- representation of solution operators by means of *Green's functions*.

1.2 Notation and Mathematical Preliminaries

In this section we briefly introduce some basic notation that will be used throughout the book. For more details on function spaces and norms we refer to App. A.

By $\mathbf{R}$ and $\mathbf{C}$ we denote the sets of real and complex numbers, respectively, and we write

$$\mathbf{R}^d = \{x = (x_1, \dots, x_d) : x_i \in \mathbf{R},\ i = 1, \dots, d\}, \quad \mathbf{R}_+ = \{t \in \mathbf{R} : t > 0\}.$$

A subset of $\mathbf{R}^d$ is called a domain if it is open and connected. By Ω we usually denote a bounded domain in $\mathbf{R}^d$, for $i = 1, 2$, or 3 (if $d = 1$, then Ω is a bounded open interval). Its boundary $\partial\Omega$ is usually denoted Γ. We assume throughout that Γ is either smooth or a polygon (if $d = 2$) or polyhedron (if $d = 3$). By $\bar{\Omega}$ we denote the closure of Ω, i.e., $\bar{\Omega} = \Omega \cup \Gamma$. The (length, area, or) volume of Ω is denoted by $|\Omega|$, the volume element in $\mathbf{R}^d$ is $\mathrm{d}x = \mathrm{d}x_1 \cdots \mathrm{d}x_d$, and $\mathrm{d}s$ denotes the element of arclength (if $d = 2$) or surface area (if $d = 3$) on Γ.

Let u, v be scalar functions and $w = (w_1, \dots, w_d)$ a vector-valued function of $x \in \mathbf{R}^d$. We define the gradient, the divergence, and the Laplace operator (Laplacian) by

$$\nabla v = \operatorname{grad} v = \Big(\frac{\partial v}{\partial x_1}, \dots, \frac{\partial v}{\partial x_d}\Big),$$

$$\nabla \cdot w = \operatorname{div} w = \sum_{i=1}^{d} \frac{\partial w_i}{\partial x_i},$$

$$\Delta v = \nabla \cdot \nabla v = \sum_{i=1}^{d} \frac{\partial^2 v}{\partial x_i^2}.$$

We recall the *divergence theorem*

$$\int_\Omega \nabla \cdot w \, \mathrm{d}x = \int_\Gamma w \cdot n \, \mathrm{d}s,$$

where $n = (n_1, \dots, n_d)$ is the outward unit normal to Γ. Applying this to the product wv we obtain *Green's formula*:

$$\int_\Omega w \cdot \nabla v \, \mathrm{d}x = \int_\Gamma w \cdot n \, v \, \mathrm{d}s - \int_\Omega \nabla \cdot w \, v \, \mathrm{d}x.$$

When applied with $w = \nabla u$ the formula becomes

$$\int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}x = \int_\Gamma \frac{\partial u}{\partial n} v \, \mathrm{d}s - \int_\Omega \Delta u \, v \, \mathrm{d}x,$$

where $\partial u/\partial n = n \cdot \nabla u$ is the exterior normal derivative of u on Γ.

A *multi-index* $\alpha = (\alpha_1, \dots, \alpha_d)$ is a d-vector where the α_i are non-negative integers. The *length* $|\alpha|$ of a multi-index α is defined by $|\alpha| = \sum_{i=1}^{d} \alpha_i$. Given a function $v : \mathbf{R}^d \to \mathbf{R}$ we may write its partial derivatives of order $|\alpha|$ as

$$D^\alpha v = \frac{\partial^{|\alpha|} v}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}. \tag{1.8}$$

A linear partial differential equation of order k in Ω can therefore be written

$$\sum_{|\alpha|\le k} a_\alpha(x)D^\alpha u = f(x),$$

where the coefficients $a_\alpha(x)$ are functions of x in Ω. We also use subscripts to denote partial derivatives, e.g.,

$$v_t = D_t v = \frac{\partial v}{\partial t}, \quad v_{xx} = D_x^2 v = \frac{\partial^2 v}{\partial x^2}.$$

For $M \subset \mathbf{R}^d$ we denote by $\mathcal{C}(M)$ the linear space of continuous functions on M, and for bounded continuous functions we define the maximum-norm

$$\|v\|_{\mathcal{C}(M)} = \sup_{x\in M} |v(x)|. \tag{1.9}$$

For example, this defines $\|v\|_{\mathcal{C}(\mathbf{R}^d)}$. When M is a bounded and closed set, i.e., a compact set, the supremum in (1.9) is attained and we may write

$$\|v\|_{\mathcal{C}(M)} = \max_{x\in M} |v(x)|.$$

For a not necessarily bounded domain Ω and k a non-negative integer we denote by $\mathcal{C}^k(\Omega)$ the set of k times continuously differentiable functions in Ω. For a bounded domain Ω we write $\mathcal{C}^k(\bar\Omega)$ for the functions $v \in \mathcal{C}^k(\Omega)$ such that $D^\alpha v \in \mathcal{C}(\bar\Omega)$ for all $|\alpha| \le k$. For functions in $\mathcal{C}^k(\bar\Omega)$ we use the norm

$$\|v\|_{\mathcal{C}^k(\bar\Omega)} = \max_{|\alpha|\le k} \|D^\alpha v\|_{\mathcal{C}(\bar\Omega)},$$

and the seminorm, including only the derivatives of highest order,

$$|v|_{\mathcal{C}^k(\bar\Omega)} = \max_{|\alpha|=k} \|D^\alpha v\|_{\mathcal{C}(\bar\Omega)}.$$

When we are working on a fixed domain Ω we often omit the set in the notation and write simply $\|v\|_{\mathcal{C}}$, $|v|_{\mathcal{C}^k}$, etc.

By $\mathcal{C}_0^k(\Omega)$ we denote the set of functions $v \in \mathcal{C}^k(\Omega)$ that vanish outside some compact subset of Ω, in particular, such functions satisfy $D^\alpha v = 0$ on the boundary of Ω for $|\alpha| \le k$. Similarly, $\mathcal{C}_0^\infty(\mathbf{R}^d)$ is the set of functions that have continuous derivatives of all orders and vanish outside some bounded set.

We say that a function is *smooth* if, depending on the situation, it has sufficiently many continuous derivatives.

We also frequently employ the space $L_2(\Omega)$ of square integrable functions with scalar product and norm

$$(v,w) = (v,w)_{L_2(\Omega)} = \Big(\int_\Omega vw\,\mathrm{d}x\Big)^{1/2}, \quad \|v\| = \|v\|_{L_2(\Omega)} = \Big(\int_\Omega v^2\,\mathrm{d}x\Big)^{1/2}.$$

For Ω a domain we also employ the Sobolev space $H^k(\Omega)$, $k \geq 1$, of functions v such that $D^\alpha v \in L_2(\Omega)$ for all $|\alpha| \leq k$, equipped with the norm and seminorm

$$\|v\|_k = \|v\|_{H^k(\Omega)} = \Big(\sum_{|\alpha| \leq k} \|D^\alpha v\|^2 \Big)^{1/2},$$

$$|v|_k = |v|_{H^k(\Omega)} = \Big(\sum_{|\alpha| = k} \|D^\alpha v\|^2 \Big)^{1/2}.$$

Additional norms are defined and used locally when the need arises.

We use the letters c, C to denote various positive constants that need not be the same at each occurrence.

1.3 Physical Derivation of the Heat Equation

Many equations in physics are derived by combining a conservation law with constitutive relations. A conservation law states that a physical quantity, such as energy, mass, or momentum, is conserved as the physical process develops in time. Constitutive relations express our assumptions about how the material behaves when the state variables change.

In this section we we consider the conduction of heat in a body $\Omega \subset \mathbf{R}^3$ with boundary Γ and derive the heat equation using conservation of energy together with linear constitutive relations.

Conservation of Energy

Consider the balance of heat in an arbitrary subset $\Omega_0 \subset \Omega$ with boundary Γ_0. The energy principle says that the rate of change of the total energy in Ω_0 equals the inflow of heat through Γ_0 plus the heat power produced by heat sources inside Ω_0. To express this in mathematical terms we introduce some physical quantities, each of which is followed, within brackets, by the associated standard unit of measurement.

With $e = e(x,t)$ [J/m^3] the *density of internal energy* at the point x [m] and time t [s], the total amount of heat in Ω_0 is $\int_{\Omega_0} e\,\mathrm{d}x$ [J]. Further with the vector field $j = j(x,t)$ [J/(m^{2}s)] denoting the *heat flux* and n the exterior unit normal to Γ_0, the net outflow of heat through Γ_0 is $\int_{\Gamma_0} j \cdot n\,\mathrm{d}s$ [J/s]. Introducing also the power density of heat sources $p = p(x,t)$ [J/(m^{3}s)], the energy principle then states that

$$\frac{d}{dt}\int_{\Omega_0} e\,\mathrm{d}x = -\int_{\Gamma_0} j \cdot n\,\mathrm{d}s + \int_{\Omega_0} p\,\mathrm{d}x.$$

Applying the divergence theorem we obtain