

Preface

Boundary-value problems and initial-boundary-value problems for partial differential equations of continuum mechanics and mathematical physics that arise in applications in the physical sciences and engineering frequently contain ‘nonsmooth’ or ‘singular’ data, such as jumps in the coefficients in the equation, caused by discontinuities in material properties, or concentrated loads that are modelled as point sources, or indeed discontinuities in the solution at interfaces in transmission problems. There is a wealth of such practical examples. The present book, which arose from series of lectures given by the authors over a number of years at the University of Belgrade and the University of Oxford, respectively, is devoted to the construction and the mathematical analysis of numerical methods for the approximate solution of such problems. More specifically, we focus on the numerical solution of linear partial differential equations by variously generalized finite difference schemes in instances when the coefficients, source terms or initial or boundary data belong to spaces of weakly differentiable functions, e.g. Sobolev, Besov or Bessel-potential spaces of nonnegative order, or certain spaces of distributions, such as negative-order Sobolev, Besov or Bessel-potential spaces.

The fundamental mathematical result that underpins the convergence analysis of discretization methods for linear partial differential equations, and finite difference methods in particular, is the Lax equivalence theorem (cf. [156], Sect. 3.5), which, loosely speaking, states that a sequence of numerical solutions, generated on a family of meshes by means of a *consistent* finite difference approximation of a well-posed initial/boundary-value problem for a linear partial differential equation, *converges* to the analytical solution of the problem if, and only if, the finite difference method is *stable*.

Consistency of a finite difference scheme amounts to the requirement that the *truncation error*, defined by inserting the unknown analytical solution to the partial differential equation into the finite difference approximation of the equation, when measured in a suitable mesh-dependent norm, converges to zero, possibly at a certain rate, which is typically a positive power of the maximum mesh-size h , in the limit of h converging to zero.

The conventional mathematical tool for investigating the consistency of a finite difference approximation to a partial differential equation is multivariate Taylor series expansion. The truncation error is expanded to terms of order as high as is necessary so as to extract the highest possible power of h admitted by the finite difference scheme; the power of h in question is referred to as the *order of accuracy* or *order of consistency* of the finite difference method. The underlying assumption in such, frequently tedious, but completely elementary calculations based on Taylor series expansions is that the solution to the partial differential equation is sufficiently smooth, to the extent that it admits a Taylor series expansion up to derivatives whose order is as high as is needed in order to extract the highest possible power of h from the truncation error.

When confronted with partial differential equations whose solutions are known not to be differentiable or even continuous, and Taylor series expansion of the analytical solution, and thereby of the truncation error of the finite difference scheme, fails to make sense due to lack of regularity in the classical sense, a natural question is whether there are alternative mathematical tools one can resort to in a systematic fashion. A second, closely related and even more basic question is, of course, how, in the first place, should one construct finite difference approximations to partial differential equations whose coefficients, source terms or initial or boundary data are so ‘rough’ that sampling them at the points of the computational mesh is, quite evidently, a meaningless endeavour.

It is the mathematical analysis of these two questions that the present monograph is devoted to. The second question posed above, concerning the construction of finite difference schemes for partial differential equations with nonsmooth data, is addressed by mollifying the data through convolution (possibly in the sense of distributions) with suitable functions with compact support, which are typically (multivariate) B -splines whose support is commensurate with the mesh-size h . As for the first question, regarding the analysis of consistency in the absence of meaningful Taylor series expansions, we resort to a technique that is familiar in the realm of finite element methods but is seemingly alien to the world of finite difference schemes: interpreting the truncation error as a linear functional on a suitable function space (typically a certain Sobolev space of nonnegative order), scaling to a canonical ‘element’, which is chosen to be a scaled-up version of the support of the B -spline used in the definition of the mollification, followed by an application of a result known as the Bramble–Hilbert lemma and, finally, rescaling. The Bramble–Hilbert lemma plays the role of Taylor series expansion with remainder of the truncation error up to the highest possible derivative, with the lower-order terms in the Taylor polynomial cancelling: it simply states that a bounded linear functional on a Sobolev space with the property that the linear functional vanishes on polynomials of degree one less than the (positive) differentiability index of the Sobolev space, can be bounded by the highest-order Sobolev seminorm of the space. The subsequent rescaling from the canonical element then relies on the fact that the highest-order Sobolev seminorm is a homogeneous function of a certain degree in the mesh-size h (the homogeneity index of the Sobolev seminorm being dependent on the differentiability

ity and integrability indices of the Sobolev seminorm and the number of dimensions).

Our objective throughout the book is to systematically develop this methodology based on the combination of mollification of the nonsmooth data on the one hand and the application of variants of the Bramble–Hilbert lemma in conjunction with scaling arguments on the other, for a range of linear elliptic, parabolic and hyperbolic partial differential equations.

Chapter 1 provides a brief survey of some basic results from linear functional analysis, the theory of distributions and function spaces, Fourier multipliers and mollifiers in function spaces, and function space interpolation. Chapter 2 is concerned with the construction and the convergence analysis of finite difference schemes for elliptic boundary-value problems. One of the key contributions of the chapter is the derivation of optimal-order bounds on the error between the analytical solution and its finite difference approximation for elliptic equations with variable coefficients under minimal regularity hypotheses on the coefficients and the solution, the minimal regularity hypotheses on the coefficients being expressed in terms of spaces of multipliers in Sobolev spaces. In Chaps. 3 and 4 of the book we then pursue an analogous programme for some model linear parabolic and hyperbolic equations.

We shall consider finite difference methods on both uniform and nonuniform computational meshes. In order to avoid cluttering the presentation with the inclusion of technical details that are secondary to the central theme of the book, we shall confine ourselves throughout to boundary-value problems and initial-boundary-value problems on axiparallel domains. Curved boundaries give rise to additional complexities, which we do not address. Having said this, the starting point of a convergence analysis for any finite difference method is a stability result, which is typically a discrete counterpart of a stability or regularity result for the differential problem under consideration. For elliptic equations in arbitrary domains discrete versions of interior regularity results in L_2 and, more generally, L_p type norms were developed by Thomée and Westergren [179] and Shreve [166], respectively. Discrete versions of interior Schauder estimates were proved by Thomée [175]. For Lipschitz domains, discrete versions of elliptic regularity results, up to the boundary, were established by Hackbusch in [66] and [67]. For parabolic problems discrete interior regularity results in arbitrary spatial domains were proved by Brandt [22] and Bondesson [18, 19]. These, and related results, can be seen as a starting point for the development of a theoretical framework in arbitrary domains, analogous to the one considered here on axiparallel domains.

There are of course several excellent books concerned with the mathematical theory of finite difference schemes for partial differential equations. A classical source in the field is the influential monograph by R.D. Richtmyer and K.W. Morton: *Difference Methods for Initial-Value Problems* [156]; some other significant books include the following: A.A. Samarskiĭ: *The Theory of Difference Schemes* [159], J. Strikwerda: *Finite Difference Schemes and Partial Differential Equations* [170], B. Gustafsson, H.-O. Kreiss and J. Oliger: *Time Dependent Problems and Difference*

Methods [64], the short monograph by P. Brenner, V. Thomée and L.B. Wahlbin entitled *Besov Spaces and Applications to Difference Methods for Initial Value Problems* [24], the monograph by A.A. Samarskiĭ, R.D. Lazarov and L. Makarov: *Finite Difference Schemes for Differential Equations with Weak Solutions* (in Russian) [160], and Chap. 4 and Sects. 9.2, 10.2.2 and 11.3 of the book by W. Hackbusch entitled *Elliptic Differential Equations: Theory and Numerical Treatment* [68]. Instead of replicating the material contained in those and other books on the analysis of finite difference schemes for partial differential equations, our aim here has been to focus on ideas that have not been covered elsewhere in the literature previously, at least not in the form of a book. While we have made every effort to ensure that the text is reasonably accessible and self-contained, a disclaimer is in order: it is fair to say that this monograph has been written with a mathematical audience in mind. Some of the material we have included here has been successfully used in third- and fourth-year mathematics undergraduate courses on the numerical analysis of partial differential equations (e.g. Chap. 1, Sects. 1.1–1.4; Chap. 2, Sects. 2.1–2.4; Chap. 3, Sects. 3.1, 3.2; Chap. 4, Sects. 4.1, 4.2); however, the vast majority of the theoretical questions we discuss are firmly beyond the scope of the undergraduate numerical analysis syllabus, and will be of primary interest to graduate students, researchers and specialists working in the field of numerical analysis of partial differential equations. Readers will certainly find it helpful to possess prior knowledge of elements of linear functional analysis, the theory of linear partial differential equations, and basic concepts from the theory of distributions and function spaces. Although we chose to focus on linear problems throughout, it is nevertheless hoped that the methodology that is systematically developed here in the case of linear partial differential equations has some bearing on the mathematical analysis of finite difference approximations of nonlinear partial differential equations with nonsmooth solutions, particularly those that arise from continuum mechanics and the sciences in general. The recent upsurge of interest in numerical algorithms for atomistic models of crystalline materials, such as quasi-continuum methods, whose analysis relies on techniques from the theory of finite difference methods [14, 15, 29, 132, 133, 149, 150, 194], has provided added impetus to this book: we hope that some of the technical tools developed here will also prove useful to researchers working in that field.

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