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J.W. Thomas

Numerical Partial Differential Equations

Finite Difference Methods

偏微分方程的数值方法

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With 70 Illustrations

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Series Preface

Mathematics is playing an ever more important role in the physical and biological sciences, provoking a blurring of boundaries between scientific disciplines and a resurgence of interest in the modern as well as the classical techniques of applied mathematics. This renewal of interest, both in research and teaching, has led to the establishment of the series: *Texts in Applied Mathematics* (*TAM*).

The development of new courses is a natural consequence of a high level of excitement on the research frontier as newer techniques, such as numerical and symbolic computer systems, dynamical systems, and chaos, mix with and reinforce the traditional methods of applied mathematics. Thus, the purpose of this textbook series is to meet the current and future needs of these advances and encourage the teaching of new courses.

TAM will publish textbooks suitable for use in advanced undergraduate and beginning graduate courses and will complement the *Applied Mathematical Sciences* (*AMS*) series, which will focus on advanced textbooks and research level monographs.

Preface

This textbook is in two parts. The first part contains Chapters 1–7 and is subtitled *Finite Difference Methods*. The second part contains Chapters 8–11 and is subtitled *Conservation Laws and Elliptic Equations*. This text was developed from material presented in a year long, graduate course on using difference methods for the numerical solution of partial differential equations. Writing this text has been an iterative process, and much like the Jacobi iteration scheme presented in Chapter 10, it has been a *slow* iterative process. The course at Colorado State University is designed for graduate students in both applied mathematics and engineering. The students are required to have at least one semester of partial differential equations and some programming capability. Generally, the classes include a broad spectrum of types of students, ranging from first year mathematics graduate students with almost no physical intuition into the types of problems we might solve, to third year engineering graduate students who have a lot of physical intuition and know what types of problems they personally want to solve and why they want to solve them. Since the students definitely help shape the class that is taught, they probably have also helped to shape this text.

There are several distinct goals of the courses. One definite goal is to prepare the terminal mathematics masters degree students and the engineers to be competent practioners capable of solving a large range of problems, evaluating numerical results and understanding how and why results might be bad. Another goal is to prepare the applied mathematics Ph.D. students to take additional courses (the third course in our sequence is a course in computational fluid dynamics which requires both semesters taught out of this text) and to write theses in applied mathematics.

One of the premises on which this text is based is that in order to understand the numerical solution of partial differential equations the student must solve partial differential equations. The text includes homework problems that implement different aspects of most of the schemes discussed. As a part of the implementation phase of the text, discussions are included on how to implement the various schemes. In later parts of the text, we return to earlier problems to discuss the results obtained (or that should have been obtained) and to explain why the students got the results they did. Throughout the text, the problems sometimes lead to bad numerical results. As I explain to my students, since these types of results are very common in the area of numerical solutions of partial differential equations, they must learn how to recognize them and deal with them. A point of emphasis in my course, which I hope that I convey also in the text, is teaching the students to become experimentalists. I explain that before one runs an experiment, one should know as much as possible about the problem. In this book a complete problem usually includes the physical problem, the mathematical problem, the numerical scheme and the computer. I then try to show them how to run numerical experiments. As part of the training to be a numerical experimentalist, I include in the Prelude four nonlinear problems. I assume that the students do not generally know much about these problems initially. As we proceed in the text, I suggest that they try generalizations of some of our linear methods on these nonlinear problems. Of course, these methods are not always successful and in these cases I try to explain why we get the results that we get.

The implementation aspect of the text obviously includes a large amount of computing. Another aspect of computing included in the text is symbolic computing. When we introduce the concept of consistency, we show the calculations as being done on paper. However, after we have seen a few of these, we emphasize that a computer with a symbolic manipulator should be doing these computations. When we give algorithms for symbolic computations, we have tried to give it in a pseudo code that can be used by any of the symbolic manipulators. Another aspect of the new technologies that we use extensively is graphics. Of course, we ask the students to provide plots of their results. We also use graphics for analysis. For example, for the analyses of dissipation and dispersion, where much of this has traditionally been done analytically (where one obtains only asymptotic results), we have emphasized how easy it is to plot these results and interpret the dissipativity and dispersivity properties from the plots.

Though there is a strong emphasis in the text on implementing the schemes, there is also a strong emphasis on theory. Because of the audience, the theory is usually set in what might be called computational space (where the computations are or might be done) and the convergence is done in $\ell_{2,\Delta x}$ spaces in terms of the energy norm. Though at times these spaces might not be as nice mathematically, it seems that working in spaces that mimic the computational space is easier for the students to grasp. Throughout the text, we emphasize the meaning of consistency, stability and convergence. In my classes I emphasize that it is dangerous for a person who is using difference methods not to understand what it means for a scheme to converge. In my class and in the text, I emphasize that we sometimes get necessary and sufficient conditions for convergence and sometimes get only necessary conditions (then we must learn to accept that we have only necessary conditions and proceed with caution and numerical experimentation). In the text, not only do we prove the Lax Theorem, but we return to the proof to see how to choose an initialization scheme for multilevel schemes and how we can change the definition of stability when we consider higher order partial differential equations. For several topics (specifically for the stability of difference schemes for initial–boundary value problems by the GKSO theory presented in Chapter 8, the introduction to numerical schemes for the solution of problems involving conservation laws included in Chapter 9 and many of the results for elliptic equations presented in Chapter 10) we do not include all of the theory (specifically not all of the proofs) but discuss and present the material in a theoretically logical order. When theorems are used without proof, careful references are included for these results.

Lastly, it is hoped that the text will become a reference book for the students. In the preparation of the text, I have tried to include as many aspects of the numerical solution of partial differential equations as possible. Some of these topics, though I do not have time to include them in my course and might not want to include them even if I had time, must be available to the students so that they have a reference point when they are confronted with them. One such topic is the derivation of numerical schemes. I personally do not have a preference on whether a given numerical scheme is derived mathematically or based on some physical principles. I feel that it is important for the student to know that they can be derived both ways and that both ways can lead to good schemes and bad schemes. In Chapter 1, we begin by first deriving the basic difference mathematically, and then show how the same difference scheme can be derived by using the integral form of the conservation law. We emphasize in this section that the errors using the latter approach are errors in numerical integration. This is a topic that I discuss and that I want the students to know is there and that it is a possible approach. It is also a topic that I do not develop fully in my class. Throughout the text, we return to this approach to show how it differs when we have two dimensional problems, hyperbolic problems, etc. Also, throughout the text we derive difference schemes purely mathematically (heuristically, by the method of undetermined coefficients or by other methods). It is hoped the readers will understand that if they have to derive their own schemes for a partial differential equation not previously considered, they will know where to find some tools that they can use.

Because of the length of the text, as was stated earlier, the material is being given in two parts. The first part includes most of the basic material on time dependent equations including parabolic and hyperbolic problems, multi-dimensional problems, systems and dissipation and dispersion. The second part includes chapters on stability theory for initial–boundary value problems (the GKSO theory), numerical schemes for conservation laws, numerical solution of elliptic problems and an introduction to irregular regions and irregular grids. When I teach the course, I usually cover most of the first five chapters during the first semester. During the second semester I usually cover Chapters 6 and 7 (systems and dissipation and dispersion), Chapter 10 (elliptic equations) and selected topics from Chapters 8, 9 and 11. In other instances, I have covered Chapters 8 and 9 during the second semester. Other people who have used the notes have covered parts of Chapters 1–7 and Chapter 10 in one semester. In either case, there seems to be sufficient material for two semesters of course work.

At the end of most of the chapters of the text and in the middle of several, we include sections which we refer to as "Computatational Interludes." The original idea of these sections was to stop working on new methods, take a break from theory and compute for a while. These sections do include this aspect of the material, but as they developed, they also began to include more than just computational material. It is in these sections that we discuss results from previous homework problems. It is also in these sections that we suggest it is time for the students to try one of their new methods on one of the problems HW0.0.1–HW0.0.4 from the Prelude. There are also some topics included in these sections that did not find a home elsewhere. At times a more appropriate title for these sections might have been "etc.".

At this time I would like to acknowledge some people who have helped me with various aspects of this text. I thank Drs. Michael Kirby, Steve McKay and K. McArthur for teaching parts of the text and providing me with feedback. I also thank Drs. Kirby, McArthur, Jay Bourland, Paul DuChateau and David Zachmann for many discussions about various aspects of the text. Finally, I thank the many students who over the years put up with the dreadfully slow convergence of this material from notes to text. Whatever the result, without their input the result would not be as good. And, finally, though all of the people mentioned above tried, there are surely still some typos and errors of thought. Though I do so sadly, I take the blame for all of these mistakes. I would appreciate it if you would send any mistakes that you find to thomasvon-neumann.math.colostate.edu. Thank you.

J.W. Thomas

Contents of Part 2: Conservation Laws and Elliptic Equations

Chapter 8 will be devoted to applying the GKSO theory to prove stability of initial–boundary–value problem schemes. The emphasis of this chapter will be on understanding and applying the results rather than on proofs of the results. We will also discuss the relationship between the GKSO stability theory and convergence.

Chapter 9 Conservation Laws

1. Theory of Conservation Laws
   (a) Shock Formation
   (b) Weak Solutions
   (c) The Entropy Condition
   (d) Solution of Scalar Conservation Laws
   (e) Systems of Conservation Laws
   (f) Solutions to Riemann Problems
2. Numerical Methods for Conservation Laws
   (a) Conservative Difference Schemes
   (b) Monotone Schemes
   (c) Total Variation Decreasing Schemes
   (d) High Resolution Methods
   (e) Flux Splitting Schemes

Chapter 9 will include some of the most current work on conservation law schemes. We begin by giving a background on conservation laws. Then, using results from Volume 1, we motivate the need for better schemes for conservation laws. We then proceed to discuss the various properties and implementations of numerical schemes for solving conservation laws.

Chapter 10 Elliptic Equations

1. Solvability of Elliptic Difference Equations
2. Convergence of Elliptic Difference Schemes
3. Approximate Solution of Ellitpic Equations
4. Residual Correction Methods
   (a) Analysis of Residual Correction Schemes
   (b) Jacobi Relaxation Scheme
   (c) Analysis of the Jacobi Relaxation Scheme
   (d) Stopping Criteria
   (e) Implementation of the Jacobi Scheme
   (f) Gauss-Seidel Scheme

In Chapter 10 we give a complete survey of results and methods for the numerical solution of elliptic problems. Though we have not included many of the proofs, the material is presented in an order that is consistent with a rigorous approach and complete references are included.

Chapter 11 Irregular Grids and Regions.

Chapter 11 is our confession that all physical problems are not uniform and rectangular. We discuss various approaches to including irregular grids into finite difference schemes and methods for treating irregular regions. Some of these techniques are reviewed (and referenced) and some of these techniques are included.

Contents

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Prelude

Numerical partial differential equations is a large area of study. The subject includes components in the areas of applications, mathematics and computers. These three aspects of a problem are so strongly tied together that it is virtually impossible to consider one in isolation from the other two. It is impossible (or at least fool-hardy) to consider the applied aspect of a problem without considering at least some of the mathematical and computing aspects of that problem. Often, the mathematical aspects of numerical partial differential equations can be developed without considering applications or computing, but experience shows that this approach does not generally yield useful results.

Of the many different approaches to solving partial differential equations numerically (finite differences, finite elements, spectral methods, collocation methods, etc.), we shall study **difference methods**. We will provide a review of a large range of methods. A certain amount of theory and rigor will be included, but at all times implementation of the methods will be stressed. The goal is to come out of this course with a large number of methods about which you have **theoretical knowledge** and with which you have **numerical experience**.

Often, when numerical techniques are going to be used to solve a physical problem, it is not possible to thoroughly analyze the methods that are used. Any time we use methods that have not been thoroughly analyzed, we must resort to methods that become a part of **numerical experimentation**. As we shall see, often such experimentation will also become necessary for linear problems. In fact, we often do not even know what to try to prove analytically until we have run a well-designed series of experiments.