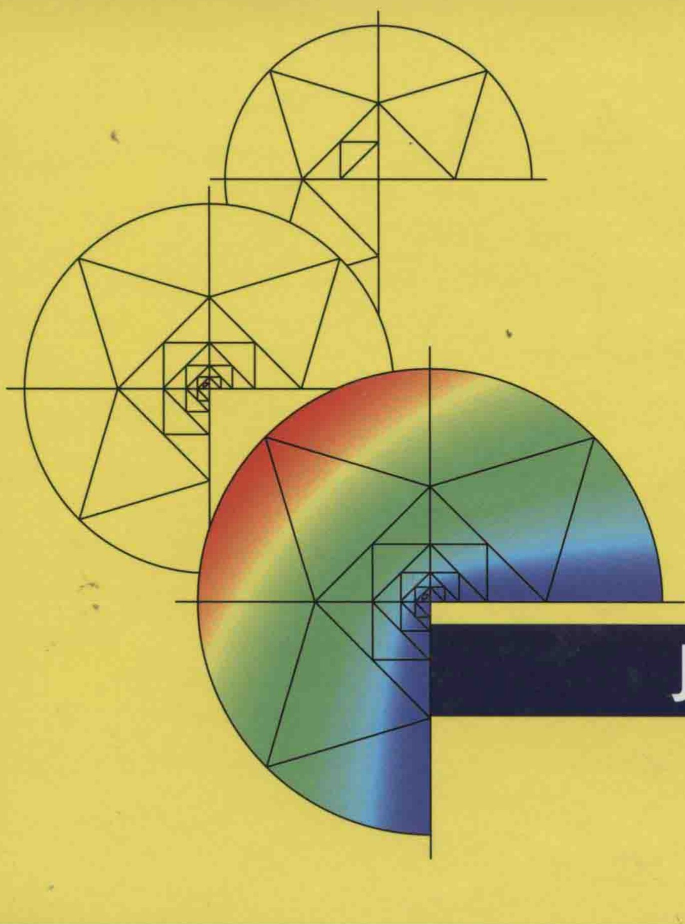
Numerical Solution of Elliptic and Parabolic Partial Differential Equations



John A. Trangenstein

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NUMERICAL SOLUTION OF ELLIPTIC AND PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

Numerical Solution of Elliptic and Parabolic Partial Differential Equations has been written for those who are interested in applying numerical methods to physical problems, but want solid mathematical justification for their numerical schemes. Throughout the book, numerical ideas are connected to finite difference or finite element software that accompanies this text. By seeing the complete description of the methods in both theory and implementation, students will more easily gain the knowledge needed to write their own application programs or develop new theory. This combination of theory and practice will make the book useful for classes that contain a mixture of mathematicians and engineers.

The book contains careful development of the mathematical tools needed for analysis of the numerical methods, including elliptic regularity theory and approximation theory. Variational crimes, due to quadrature, coordinate mappings, domain approximation and boundary conditions, are analyzed. The claims are stated with full statement of the assumptions and conclusions, and use subscripted constants which can be traced back to the origination (particularly in the electronic version). Mixed finite element methods are described in a manner that makes their numerical implementation more transparent, and the proof of their well-posedness and accuracy more understandable. The inf–sup condition for H^{div} approximations is handled in a direct fashion. Iterative methods for linear and nonlinear equations are described and analyzed before finite element methods are developed. The multigrid method has a purely algebraic proof. The former version contained too much detail for this purpose.

The accompanying software, also available from www.cambridge.org/trangenstein, implements the theory presented and solves some simple problems related to the applications in the book.

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To my wife, Rebecca, for her immense patience and infectious humor

Preface

Elliptic and parabolic partial differential equations arise in a number of important physical problems, such as solid mechanics, fluid dynamics, heat flow, oil recovery and electrocardiology. Engineering texts for these methods tend to emphasize a specific application while describing the methods. Such a presentation can make it difficult to understand the general principles, and prevent students in other application areas from fully understanding the ideas. On the other hand, mathematics books on these methods tend to emphasize analysis, rather than applications. Treatment of boundary conditions, systems of partial differential equations, iterative methods and other important implementation details are largely ignored. In some cases, practical applications are ignored in mathematical methods texts.

This book grew out of lecture notes that I have been modifying for 35 years. The notes began as a fusion of lecture notes from my finite element mentors in mathematics, namely Jim Douglas Jr., Todd Dupont and Jim Bramble. The notes grew as I gained contact with engineers, particularly Eric Reissner and Gerry Frazier at UCSD, and Gary Trudeau at LLNL. I also benefitted from collaborations with mathematicians working on applications, such as Phil Colella and John Bell.

I have written this book for others who are interested in applying numerical methods to physical problems, but want solid mathematical justification for their numerical schemes. Readers who are primarily interested in numerical methods for a particular application area, such as solid mechanics or fluid dynamics, will probably find other texts more suited to their needs. Nevertheless, I have included a number of applications in this book, in order to illustrate the mathematical ideas.

Throughout the book, I connect the numerical ideas to finite difference or finite element software that accompanies this text. By seeing the complete description of the methods in both theory and implementation, students should more easily gain the knowledge needed to write their own application programs or develop new theory.

Chapter 2 begins with finite difference methods for parabolic equations. This is an old topic, which is covered in more detail in classic texts by Richtmyer and Morton [213] or Forsythe and Wasow [121], and a more modern treatment by Strikwerda [239]. The analyses of finite difference methods tend to emphasize local truncation errors rather than global errors, and the methods prefer rectangular (or mappings of rectangular) problem domains. Finite difference methods can be modified to handle complicated immersed interfaces, as described by Li and Ito [177], although these techniques are not described in this book. Spatial operator splitting is included in this chapter because it is so simple to implement, and so effective on rectangular domains. The single most important analytical result in this chapter is the Lax equivalence theorem, which is based on Fourier analysis.

Students should understand that finite difference methods are relatively easy to understand and easy to implement. For all of us, it is important to remember that finite element methods can generally be implemented as finite differences, and that this approach can be important for numerical efficiency [137].

The book begins with parabolic equations so that I can discuss the competition between explicit and implicit solution methods for the resulting discretized equations. Linear systems of ordinary differential equations arising from the spatial discretization of parabolic equations are notoriously stiff, requiring explicit timesteps that are much smaller than the spatial grid width. This establishes a *minimal goal* for numerical linear algebra applied to implicit discretizations, namely to solve the linear systems more quickly than explicit time discretization. This is actually far harder than is popularly understood, especially as spatial and temporal meshes are refined for improved accuracy.

The iterative solution of linear and nonlinear equations is discussed in Chapter 3. This chapter includes many of the basic iterative techniques, such as iterative improvement, gradient methods, minimum residual methods and nonlinear iterations. The chapter concludes with a detailed algebraic discussion of multigrid methods, including an algebraic proof of the convergence of multigrid.

Iterative methods can be used in both unsteady- and steady-state computations, and unforced parabolic equations are known to approach steady states. This leads to a discussion of conforming finite element methods for elliptic problems in Chapters 4 through 6. I begin Chapter 4 with several examples of steady-state applications. However, the bulk of that chapter is devoted to an overview of finite element methods from an *implementation viewpoint*. I discuss reference shapes, polynomial shape functions, quadrature rules, mesh generation and linear system assembly. Unlike most mathematical texts on finite elements, I describe finite elements on both triangles and quadrilaterals in two dimensions, and tetrahedra, prisms and hexahedra in three dimensions. Each of these shape alternatives has its advantages and disadvantages, especially with regard to coordinate mappings and the treatment of essential or natural boundary conditions. In particular, high-order coordinate mappings for tessellations of tetrahedra are particularly difficult to handle, and are not discussed in competing books.

Chapter 5 contains a more traditional treatment of the mathematical theory of finite elements. Much of this material can be found in books by Brenner and Scott [56] or Braess [48]. My Ph.D. training with Jim Bramble led me to provide more background information on the well-posedness of elliptic boundary value problems, using material from Lions and Magenes [178] and Agmon [5].

There are common assumptions in the finite element theory, such as the approximation assumption, use of affine coordinate maps, exact integrals and exact satisfaction of essential boundary conditions. As Jim Douglas Jr. jokingly described the situation to me, the standard finite element theory assumes that the problem domain is a polygon with a smooth boundary. Following the careful treatment by Ciarlet and Raviart (see [76]), I discuss several finite element implementation details in Chapter 6.

Other issues, such as mesh regularity and connectivity, affect the conditioning of finite element methods. I end Chapter 6 with a discussion of condition numbers and maximum attainable accuracy. Using the proved error estimates, I show that high-order discretizations have much greater maximum attainable accuracy and much lower memory requirements than the lowest-order methods, provided that the problems are smooth enough to produce smooth solutions. This may surprise some engineers who habitually use only the lowest-order methods.

I have devoted Chapter 7 to mixed and hybrid finite elements. These are very useful in problems with rough coefficients, such as flow in random porous media. Other authors see advantage in these schemes because they provide direct approximations to quantities that could be computed in standard finite element methods only by differentiation. Typically, these schemes involve greater computational cost, and larger linear systems with poorer conditioning, when compared to standard finite element methods. I have worked hard to provide this chapter with a better discussion of implementation details, especially the Piola transformations. In particular, each of the mixed polynomial families is described together with its corresponding Lagrange multiplier family, and all mixed polynomial families are described for all tessellation shapes. As a result, students should find it possible to implement these mixed methods for tessellations involving a mixture of tetrahedra, prisms and hexahedra in three dimensions. I have also strived to offer a cleaner presentation of the proofs.

I return to parabolic equations in Chapter 8, in this case via finite element methods. This discussion is adapted from college lecture notes by Douglas and Dupont, and from the book by Thomée [244]. I begin with a discussion of the well-posedness of parabolic boundary value problems, using material from Friedman

[123, 124] and Ladyženskaja *et al.* [171]. Then I discuss some of the standard error estimates for parabolic problems, including the choice of approximation of the initial values. These problems can be solved by the method of lines, using any of a variety of time integration techniques.

The book finishes with discussions of multigrid methods via finite elements, and *a posteriori* error estimation. The purpose of the multigrid discussion is to prove the one assumption needed in the earlier multigrid convergence theorem, but not easily proved by purely algebraic techniques. The final chapter on error estimation leads to techniques for automatic local mesh refinement, and a discussion of mortar methods.

This book is offered in two forms: a printed version and an electronic version, which is available on the accompanying CD-ROM. The printed form of this book is limited by the publisher. In order to cover the range of topics and remain within the publication limits, almost all of the proofs are available only in the electronic form of the book. I think that this makes the printed form of the book easier to read, especially given the limitations of the printed page. The results are easier to find, without having to thumb through pages of proofs.

The electronic form of the book allows the reader to click on links to references for definitions, assumptions and results, as well as computer source code and web resources. This form is roughly 250 pages longer than the printed form because the proofs are included.

In both forms of the book, I have taken great effort to state the claims carefully. There are lengthy statements of assumptions, sometimes segregated into separate lists of assumptions that would otherwise have been made repeatedly. Quantifiers and qualifiers are listed cautiously. Perhaps the biggest change from the standard finite element literature is that I avoided the use of the generic constant C. To the best of my ability, all constants have a subscript given by the inequality in which they first appear. This allows the reader to trace back to that point of use to examine the quantifiers and qualifiers that apply to the use of that constant. In the electronic form of the text, clicking on that subscript takes the user to the equation or inequality where the constant first appears. This means that the electronic form of this text is particularly effective in following the full development of a proof.

The CD-ROM contains accompanying software to perform many of the numerical methods. For the finite difference methods in Chapters 2 and 3, these programs are written in a combination of Fortran and C^{++}. Fortran is very effective for array operations, and C^{++} is very useful for graphics and graphical user interfaces, as well as dynamic memory allocation.

Several chapters of the book, especially Chapter 4, contain references to a finite element programming environment written in C^{++}. This finite element code was adapted from the **DEAL.II** code, due to Wolfgang Bangerth *et al.* [34]. The organization of this code corresponds well to the discussion in this book, but may not use the most computationally effective programming strategies, particularly for rectangular grids or adaptive mesh refinement. I have made substantial changes to the DEAL.II code, in order to incorporate shapes other than parallelepipeds, and to include interactive graphics and graphical user interfaces.

The DEAL.II license allows for free distribution and modification for non-commercial use under the Q Public License. We have extended this agreement to our modifications and extensions of the DEAL.II code.

Finally, emotional support throughout a project of this sort is essential. I want to thank my wife, Becky, for all her love and understanding throughout our years together. I could not have written this book without her.

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