A First Course in the Numerical Analysis of Differential Equations

Numerical analysis presents different faces to the world. For mathematicians it is a *bona fide* mathematical theory with an applicable flavour. For scientists and engineers it is a practical, applied subject, part of the standard repertoire of modelling techniques. For computer scientists it is a theory on the interplay of computer architecture and algorithms for real-number calculations.

The tension between these standpoints is the driving force of this book, which presents a rigorous account of the fundamentals of numerical analysis both of ordinary and partial differential equations. The point of departure is mathematical, but the exposition strives to maintain a balance among theoretical, algorithmic and applied aspects of the subject.

This new edition has been extensively updated, and includes new chapters on developing subject areas: geometric numerical integration, an emerging paradigm for numerical computation that exhibits exact conservation of important geometric and structural features of the underlying differential equation; spectral methods, which have come to be seen in the last two decades as a serious competitor to finite differences and finite elements; and conjugate gradients, one of the most powerful contemporary tools in the solution of sparse linear algebraic systems.

Other topics covered include numerical solution of ordinary differential equations by multistep and Runge–Kutta methods; finite difference and finite elements techniques for the Poisson equation; a variety of algorithms to solve large, sparse algebraic systems; methods for parabolic and hyperbolic differential equations and techniques for their analysis. The book is accompanied by an appendix that presents brief back-up in a number of mathematical topics.

Professor ISERLES concentrates on fundamentals: deriving methods from first principles, analysing them with a variety of mathematical techniques and occasionally discussing questions of implementation and applications. By doing so, he is able to lead the reader to a theoretical understanding of the subject without neglecting its practical aspects. The outcome is a textbook that is mathematically honest and rigorous and provides its target audience with a wide range of skills in both ordinary and partial differential equations.

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A First Course in the Numerical Analysis of Differential Equations

Second Edition

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Contents

Preface to the second edition

In an ideal world this second edition should have been written at least three years ago but, needless to say, this is not an ideal world. Annoyingly, there are just 24 hours per day, rather less annoyingly I have joyously surrendered myself to the excitements of my own research and, being rather good at finding excuses, delayed the second edition again and again.

Yet, once I braced myself, banished my writer's block and started to compose in my head the new chapters, I was taken over by the sheer pleasure of writing. Repeatedly I have found myself, as I often do, thanking my good fortune for working in this particular corner of the mathematical garden, the numerical analysis of differential equations, and striving in a small way to communicate its oft-unappreciated beauty.

The last sentence is bound to startle anybody experienced enough in the fashions and prejudices of the mathematical world. Numerical analysis is often considered neither beautiful nor, indeed, profound. Pure mathematics is beautiful if your heart goes after the joy of abstraction, applied mathematics is beautiful if you are excited by mathematics as a means to explain the mystery of the world around us. But numerical analysis? Surely, we compute only when everything else fails, when mathematical theory cannot deliver an answer in a comprehensive, pristine form and thus we are compelled to throw a problem onto a number-crunching computer and produce boring numbers by boring calculations. This, I believe, is nonsense.

A mathematical problem does not cease being mathematical just because we have discretized it. The purpose of discretization is to render mathematical problems, often approximately, in a form accessible to efficient calculation by computers. This, in particular, means rephrasing and approximating analytic statements as a finite sequence of algebraic steps. Algorithms and numerical methods are, by their very design, suitable for *computation* but it makes them neither simple nor easy as *mathematical* constructs. Replacing derivatives by finite differences or an infinite-dimensional space by a hierarchy of finite-dimensional spaces does not necessarily lead to a more fuzzy form of reasoning. We can still ask proper mathematical questions with uncompromising rigour and seek answers with the full mathematical etiquette of precise definitions, statements and proofs. The rules of the game do not change at all.

Actually, it is almost inevitable that a discretized mathematical problem is, *as a mathematical problem,* more difficult and more demanding of our mathematical ingenuity. To give just one example, it is usual to approximate a partial differential equation of evolution, an infinite-dimensional animal, in a finite-dimensional space (using, for example, finite differences, finite elements or a spectral method). This finite-dimensional approximation makes the problem tractable on a computer, a machine that can execute a finite number of algebraic operations in finite time. However, once we wish to answer the big mathematical question underlying our discourse, how well does the finite-dimensional model approximate the original equation, we are compelled to consider not one finite-dimensional system but an infinite progression of such systems, of increasing (and unbounded) dimension. In effect, we are not just approximating a single equation but an entire infinite-dimensional function space. Of course, if all you want is numbers, you can get away with hand-waving arguments or use the expertise and experience of others. But once you wish to understand honestly the term 'analysis' in 'numerical analysis', prepare yourself for real mathematical experience.

I hope to have made the case that true numerical analysis operates according to standard mathematical rules of engagement (while, needless to say, fully engaging with the algorithmic and applied parts of its inner self). My stronger claim, illustrated in a small way by the material of this book, is that numerical analysis is perhaps the most eclectic and demanding client of the entire width and breadth of mathematics. Typically in mathematics, a discipline rests upon a fairly small number of neighbouring disciplines: once you visit a mathematical library, you find yourself time and again visiting a fairly modest number of shelves. Not so in the numerical analysis of differential equations. Once you want to understand the subject in its breadth, rather than specializing in a narrow and strictly delineated subset, prepare yourself to navigate across all library shelves! This volume, being a textbook, is purposefully steering well clear of deep and difficult mathematics. However, even at the sort of elementary level of mathematical sophistication suitable for advanced undergraduates, faithful to the principle that every unusual bit of mathematics should be introduced and explained I expect the reader to identify the many and varied mathematical sources of our discourse. This opportunity to revel and rejoice in the varied mathematical origins of the subject, of pulling occasional rabbits from all kinds of mathematical hats, is what makes me so happy to work in numerical analysis. I hope to have conveyed, in a small and inevitably flawed manner, how different strands of mathematical thinking join together to form this discipline.

Three chapters have been added to the first edition to reflect the changing face of the subject. The first is on geometric numerical integration, the emerging science of the numerical computation of differential equations in a way that renders exactly their qualitative features. The second is on spectral methods, an important competitor to the more established finite difference and finite element techniques for partial differential equations. The third new chapter reviews the method of conjugate gradients for the solution of the large linear algebraic systems that occur once partial differential equations are discretized.

Needless to say, the current contents cannot reflect all the many different ideas, algorithms, methods and insights that, in their totality, make the subject of computational differential equations. Writing a textbook, the main challenge is not what to include, but what to exclude! It would have been very easy to endure the publisher's unhappiness and expand this book to several volumes, reporting on numerous exciting themes such domain decomposition, meshless methods, wavelet-based methods, particle methods, homogenization – the list goes on and on. Easy, but perhaps not very illuminating, because this is not a cookbook, a dictionary or a compendium: it is a textbook that, ideally, should form the backdrop to a lecture course. It would not have been very helpful to bury the essential didactic message under a mountain of facts, exciting and useful as they might be. The main purpose of a lecture course – and hence of a textbook – is to provide enough material, insight and motivation to prepare students for further, often independent, study. My aim on these pages has been to provide this sort of preparation.

The flowchart on p. xix displays the connectivity and logical progression of the current 17 chapters. Although it is unlikely that the entire contents of the book can be encompased in less than a year-long intensive lecture course, the flowchart is suggestive of many different ways to pick and choose material while maintaining the inner integrity and coherence of the exposition.

This is the moment to thank all those who helped me selflessly in crafting an edition better than one I could have written singlehandedly. Firstly, all those users of the first edition who have provided me with feedback, communicated errors and misprints, queried the narrative, lavished praise or extended well-deserved criticism.[1] Secondly, those of my colleagues who read parts of the draft, offered remarks (mostly encouraging but sometimes critical: I appreciated both) and frequently saved me from embarrassing blunders: Ben Adcock, Alfredo Deaño, Euan Spence, Endre Süli and Antonella Zanna. Thirdly, my friends at Cambridge University Press, in particular David Tranah, who encouraged this second edition, pushed me when a push was needed, let me get along without undue harassment otherwise and was always willing to share his immense experience. Fourthly, my copy editor Susan Parkinson, as always pedantic in the best sense of the word. Fifthly, the terrific intellectual environment in the Department of Applied Mathematics and Theoretical Physics of the University of Cambridge, in particular among my colleagues and students in the Numerical Analysis Group. We have managed throughout the years to act not only as a testing bed, and sometimes a foil, to each other's ideas but also as a milieu where it is always delightful to abandon mathematics for a break of (relatively decent) coffee and uplifting conversation on just about anything. And last, but definitely not least, my wife and best friend, Dganit, who has encouraged and helped me always, in more ways than I can count or floating-number arithmetic can bear.

And so, over to you, the reader. I hope to have managed to convey to you, even if in a small and imperfect manner, not just the raw facts that, in their totality, make up the numerical analysis of differential equations, but the beauty and the excitement of the subject.

Arieh Iserles
August 2008

[1] I wish to thank less, though, those students who emailed me for solutions to the exercises before their class assignment was due.

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Arieh Iserles
Frontmatter
More information

Preface to the first edition

Books – so we are often told – should be born out of a sense of mission, a wish to share knowledge, experience and ideas, a penchant for beauty. This book has been born out of a sense of frustration.

For the last decade or so I have been teaching the numerical analysis of differential equations to mathematicians, in Cambridge and elsewhere. Examining this extensive period of trial and (frequent) error, two main conclusions come to mind and both have guided my choice of material and presentation in this volume.

Firstly, mathematicians are different from other varieties of *homo sapiens.* It may be observed that people study numerical analysis for various reasons. **Scientists** and **engineers** require it as a means to an end, a tool to investigate the subject matter that *really* interests them. Entirely justifiably, they wish to spend neither time nor intellectual effort on the finer points of mathematical analysis, typically preferring a style that combines a cook-book presentation of numerical methods with a leavening of intuitive and hand-waving explanations. **Computer scientists** adopt a different, more algorithmic, attitude. Their heart goes after the clever algorithm and its interaction with computer architecture. Differential equations and their likes are abandoned as soon as decency allows (or sooner). They are replaced by discrete models, which in turn are analysed by combinatorial techniques. **Mathematicians,** though, follow a different mode of reasoning. Typically, mathematics students are likely to participate in an advanced numerical analysis course in their final year of undergraduate studies, or perhaps in the first postgraduate year. Their studies until that point in time would have consisted, to a large extent, of a progression of formal reasoning, the familiar sequence of axiom $\Rightarrow$ theorem $\Rightarrow$ proof $\Rightarrow$ corollary $\Rightarrow \ldots$. Numerical analysis does not fit easily into this straitjacket, and this goes a long way toward explaining why many students of mathematics find it so unattractive.

Trying to teach numerical analysis to mathematicians, one is thus in a dilemma: should the subject be presented purely as a mathematical theory, intellectually pleasing but arid insofar as applications are concerned or, alternatively, should the audience be administered an application-oriented culture shock that might well cause it to vote with its feet?! The resolution is not very difficult, namely to present the material in a *bona fide* mathematical manner, occasionally veering toward issues of applications and algorithmics but never abandoning honesty and rigour. It is perfectly allowable to omit an occasional proof (which might well require material outside the scope of the presentation) and even to justify a numerical method on the grounds of plausibility and a good track record in applications. But plausibility, a good track record, intuition and old-fashioned hand-waving do not constitute an honest mathematical argument and should never be presented as such.

Secondly, students should be exposed in numerical analysis to both ordinary and partial differential equations, as well as to means of dealing with large sparse algebraic systems. The pressure of many mathematical subjects and sub-disciplines is such that only a modest proportion of undergraduates are likely to take part in more than a single advanced numerical analysis course. Many more will, in all likelihood, be faced with the need to solve differential equations numerically in the future course of their professional life. Therefore, the option of restricting the exposition to ordinary differential equations, say, or to finite elements, while having the obvious merit of cohesion and sharpness of focus is counterproductive in the long term.

To recapitulate, the ideal course in the numerical analysis of differential equations, directed toward mathematics students, should be mathematically honest and rigorous and provide its target audience with a wide range of skills in both ordinary and partial differential equations. For the last decade I have been desperately trying to find a textbook that can be used to my satisfaction in such a course – in vain. There are many fine textbooks on particular aspects of the subject: numerical methods for ordinary differential equations, finite elements, computation of sparse algebraic systems. There are several books that span the whole subject but, unfortunately, at a relatively low level of mathematical sophistication and rigour. But, to the best of my knowledge, no text addresses itself to the right mathematical agenda at the right level of maturity. Hence my frustration and hence the motivation behind this volume.

This is perhaps the place to review briefly the main features of this book.

★ We cover a broad range of material: the numerical solution of ordinary differential equations by multistep and Runge–Kutta methods; finite difference and finite element techniques for the Poisson equation; a variety of algorithms for solving the large systems of sparse algebraic equations that occur in the course of computing the solution of the Poisson equation; and, finally, methods for parabolic and hyperbolic differential equations and techniques for their analysis. There is probably enough material in this book for a one-year fast-paced course and probably many lecturers will wish to cover only part of the material.

★ This is a textbook for mathematics students. By implication, it is not a textbook for computer scientists, engineers or natural scientists. As I have already argued, each group of students has different concerns and thought modes. Each assimilates knowledge differently. Hence, a textbook that attempts to be different things to different audiences is likely to disappoint them all. Nevertheless, non-mathematicians in need of numerical knowledge can benefit from this volume, but it is fair to observe that they should perhaps peruse it somewhat later in their careers, when in possession of the appropriate degree of motivation and background knowledge.

On an even more basic level of restriction, this is a textbook, not a monograph or a collection of recipes. Emphatically, our mission is *not* to bring the exposition to the state of the art or to highlight the most advanced developments. Likewise, it is not our intention to provide techniques that cater for all possible problems and eventualities.

★ An annoying feature of many numerical analysis texts is that they display inordinately long lists of methods and algorithms to solve any one problem. Thus, not just one Runge–Kutta method but twenty! The hapless reader is left with an arsenal of weapons but, all too often, without a clue which one to use and why. In this volume we adopt an alternative approach: methods are derived from underlying principles and these principles, rather than the algorithms themselves, are at the centre of our argument. As soon as the underlying principles are sorted out, algorithmic fireworks become the least challenging part of numerical analysis – the real intellectual effort goes into the mathematical analysis.

This is not to say that issues of software are not important or that they are somehow of a lesser scholarly pedigree. They receive our attention in Chapter 6 and I hasten to emphasize that good software design is just as challenging as theorem-proving. Indeed, the proper appreciation of difficulties in software and applications is enhanced by the understanding of the analytic aspects of numerical mathematics.

★ A truly exciting aspect of numerical analysis is the extensive use it makes of different mathematical disciplines. If you believe that numerics are a mathematical cop-out, a device for abandoning mathematics in favour of something 'softer', you are in for a shock. Numerical analysis is perhaps the most extensive and varied user of a very wide range of mathematical theories, from basic linear algebra and calculus all the way to functional analysis, differential topology, graph theory, analytic function theory, nonlinear dynamical systems, number theory, convexity theory – and the list goes on and on. Hardly any theme in modern mathematics fails to inspire and help numerical analysis. Hence, numerical analysts must be open-minded and ready to borrow from a wide range of mathematical skills – this is not a good bolt-hole for narrow specialists!

In this volume we emphasize the variety of mathematical themes that inspire and inform numerical analysis. This is not as easy as it might sound, since it is impossible to take for granted that students in different universities have a similar knowledge of pure mathematics. In other words, it is often necessary to devote a few pages to a topic which, in principle, has nothing to do with numerical analysis *per se* but which, nonetheless, is required in our exposition. I ask for the indulgence of those readers who are more knowledgeable in arcane mathematical matters – all they need is simply to skip few pages . . .

★ There is a major difference between recalling and understanding a mathematical concept. Reading mathematical texts I often come across concepts that are familiar and which I have certainly encountered in the past. Ask me, however, to recite their precise definition and I will probably flunk the test. The proper and virtuous course of action in such an instance is to pause, walk to the nearest mathematical library and consult the right source. To be frank, although sometimes I pursue this course of action, more often than not I simply go on reading. I have every reason to believe that I am not alone in this dubious practice.

In this volume I have attempted a partial remedy to the aforementioned phenomenon, by adding an appendix named 'Bluffer's guide to useful mathematics'. This appendix lists in a perfunctory manner definitions and major theorems in a range of topics – linear algebra, elementary functional analysis and approximation theory – to which students should have been exposed previously but which might have been forgotten. Its purpose is neither to substitute elementary mathematical courses nor to offer remedial teaching. If you flick too often to the end of the book in search of a definition then, my friend, perhaps you had better stop for a while and get to grips with the underlying subject, using a proper textbook. Likewise, if you always pursue a virtuous course of action, consulting a proper source in each and every case of doubt, please do not allow me to tempt you off the straight and narrow.

★ Part of the etiquette of writing mathematics is to attribute material and to refer to primary sources. This is important not just to quench the vanity of one's colleagues but also to set the record straight, as well as allowing an interested reader access to more advanced material. Having said this, I entertain serious doubts with regard to the practice of sprinkling each and every paragraph in a *textbook* with copious references. The scenario is presumably that, having read the sentence '...suppose that $\boldsymbol{x} \in \mathbb{U}$, where $\mathbb{U}$ is a foliated widget [37]', the reader will look up the references, identify '[37]' with a paper of J. Bloggs in *Proc. SDW,* recognize the latter as *Proceedings of the Society of Differentiable Widgets,* walk to the library, locate the journal (which will be actually on the shelf, rather than on loan, misplaced or stolen)... All this might not be far-fetched as far as advanced mathematics monographs are concerned but makes very little sense in an undergraduate context. Therefore I have adopted a practice whereby there are no references in the text proper. Instead, each chapter is followed by a section of 'Comments and bibliography', where we survey briefly further literature that might be beneficial to students (and lecturers).

Such sections serve a further important purpose. Some students – am I too optimistic? – might be interested and inspired by the material of the chapter. For their benefit I have given in each 'Comments and bibliography' section a brief discussion of further developments, algorithms, methods of analysis and connections with other mathematical disciplines.

★ Clarity of exposition often hinges on transparency of notation. Thus, throughout this book we use the following convention:

- lower-case lightface sloping letters $(a, b, c, \alpha, \beta, \gamma, \ldots)$ represent scalars;
- lower-case boldface sloping letters $(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}, \ldots)$ represent vectors;
- upper-case lightface letters $(A, B, C, \Theta, \Phi, \ldots)$ represent matrices;
- letters in calligraphic font $(\mathcal{A}, \mathcal{B}, \mathcal{C}, \ldots)$ represent operators;
- shell capitals $(\mathbb{A}, \mathbb{B}, \mathbb{C}, \ldots)$ represent sets.

> Mathematical constants like $\mathrm{i} = \sqrt{-1}$ and e, the base of natural logarithms, are denoted by roman, rather than italic letters. This follows British typesetting convention and helps to identify the different components of a mathematical formula.
>
> As with any principle, our notational convention has its exceptions. For example, in Section 3.1 we refer to Legendre and Chebyshev polynomials by the conventional notation, P_n and T_n: any other course of action would have caused utter confusion. And, again as with any principle, grey areas and ambiguities abound. I have tried to eliminate them by applying common sense but this, needless to say, is a highly subjective criterion.

This book started out life as two sets of condensed lecture notes – one for students of Part II (the last year of undergraduate mathematics in Cambridge) and the other for students of Part III (the Cambridge advanced degree course in mathematics). The task of expanding lecture notes to a full-scale book is, unfortunately, more complicated than producing a cup of hot soup from concentrate by adding boiling water, stirring and simmering for a short while. Ultimately, it has taken the better part of a year, shared with the usual commitments of academic life. The main portion of the manuscript was written in Autumn 1994, during a sabbatical leave at the California Institute of Technology (Caltech). It is my pleasant duty to acknowledge the hospitality of my many good friends there and the perfect working environment in Pasadena.

A familiar computer proverb states that, while the first 90% of a programming job takes 90% of the time, the remaining 10% also takes 90% of the time . . . Writing a textbook follows similar rules and, back home in Cambridge, I have spent several months reading and rereading the manuscript. This is the place to thank a long list of friends and colleagues whose help has been truly crucial: Brad Baxter (Imperial College, London), Martin Buhmann (Swiss Institute of Technology, Zürich), Yu-Chung Chang (Caltech), Stephen Cowley (Cambridge), George Goodsell (Cambridge), Mike Holst (Caltech), Herb Keller (Caltech), Yorke Liu (Cambridge), Michelle Schatzman (Lyon), Andrew Stuart (Stanford), Stefan Vandewalle (Louven) and Antonella Zanna (Cambridge). Some have read the manuscript and offered their comments. Some provided software well beyond my own meagre programming skills and helped with the figures and with computational examples. Some have experimented with the manuscript upon their students and listened to their complaints. Some contributed insight and occasionally saved me from embarrassing blunders. All have been helpful, encouraging and patient to a fault with my foibles and idiosyncrasies. None is responsible for blunders, errors, mistakes, misprints and infelicities that, in spite of my sincerest efforts, are bound to persist in this volume.

This is perhaps the place to extend thanks to two 'friends' that have made the process of writing this book considerably easier: the TEX typesetting system and the `MATLAB` package. These days we take mathematical typesetting for granted but it is often forgotten that just a decade ago a mathematical manuscript would have been hand-written, then typed and retyped and, finally, typeset by publishers – each stage requiring laborious proofreading. In turn, `MATLAB` allows us a unique opportunity to turn our office into a computational-cum-graphic laboratory, to bounce ideas off the computer screen and produce informative figures and graphic displays. Not since the discovery of coffee have any inanimate objects caused so much pleasure to so many mathematicians!

The editorial staff of Cambridge University Press, in particular Alan Harvey, David Tranah and Roger Astley, went well beyond the call of duty in being helpful, friendly and cooperative. Susan Parkinson, the copy editor, has worked to the highest standards. Her professionalism, diligence and good taste have done wonders in sparing the readers numerous blunders and the more questionable examples of my hopeless wit. This is a pleasant opportunity to thank them all.

Last but never the least, my wife and best friend, Dganit. Her encouragement, advice and support cannot be quantified in conventional mathematical terms. Thank you!

I wish to dedicate this book to my parents, Gisella and Israel. They are not mathematicians, yet I have learnt from them all the really important things that have motivated me as a mathematician: love of scholarship and admiration for beauty and art.

Arieh Iserles
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Frontmatter
More information

Flowchart of contents