NUMERICAL DIFFERENTIAL EQUATIONS

Theory and Technique, ODE Methods, Finite Differences, Finite Elements and Collocation

John Loustau

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To all my students

Preface

This is a book in the mathematics of numerical differential equations. I present here the basic theoretical development supporting three common methods: finite difference method (FDM), finite element method (FEM), and collocation method (CM). I include description of the basic techniques and specific examples. The examples drive the interest in the topic while the technique supports the theoretical development. Our point of view on this topic is presented in more detail in the *Foreword*.

The intended purpose of the book is to help make the current literature accessible. This is not to say that the reader can jump into any current paper. Rather, the reader can take most papers, trace back into the supporting references and find an accessible starting point that will lead forward. By including both technique and theory, then the reader will find both the mathematical and the engineering literature accessible.

Our primary concern is with simulation. Mathematical modeling is a critical first step in the process. There are many current references that teach mathematical modeling of scientific observation. Two that are associated to biology are [Wodarz and Komarova (2015)] and [van der Berg (2011)]. Other references are cited throughout Part 1. In general, it is our point of view that developing a differential equation to represent observed data is only part of the story. The full treatment must also include numerical simulation. We present this point of view more completely in the Foreword.

We have chosen not to include discontinuous Galerkin FEM (GFEM). It is well known that discontinuous GFEM better conserves basic quantities associated to a particular setting, for instance, fluid incompressibility. Nevertheless, we contend that knowledge of FEM should begin with the continuous case. With a strong foundation in the continuous case, the discontinuous can be easily understood as a variant.

I imagine that the reader is a graduate student with background in basic real and complex analysis, functional analysis, and linear algebra. The level of the background is well within standard graduate level courses in these topics. Of course background in differential equations is important.

I use *Mathematica*. At this time they are at version 10. *Mathematica* related comments may be false as later versions improve the functionality of the programming product. The particular programming platform should not be a serious issue. Students at this level know how to program and have experience writing code for numerical applications. However, *Mathematica* does provide symbolic computation capability. There are times when I do suggest that a particular algebraic computation be carried out in *Mathematica*.

There are several pathways through this material. There is, of course, the intended or sequential path. I anticipate that any one presenting this material will pick and choose the examples that he finds most interesting. Alternatively, Chapters 1, 2, and 7 yield a basic FDM course. FEM could be presented using Chapters 1, 3, 8, and 9 along with parts of 6. CM is presented in Chapters 1, 5, parts of 6, and Chapter 10.

There is material on the important area of numerical solutions to PDE with stochastic coefficients. However, I only have space to introduce some of these ideas through a single example.

None of this work would have been possible without the input of many students over a period of years. In particular, I note that each of the following students contributed directly to the examples present here. As a matter of personal pride, I remark that most have completed their education and are currently contributing to the development of technology, many as professorial faculty. In no particular order, I acknowledge. Mimi Tsuruga, Hans Gilde, Joel Dodge, Alejandro Falchettore, Saumil Patel, Samuil Jubaed, Tony Markovina, Bolanle Bob-Egbe, Yevgeniy Milman, Henry Chong, Scott Irwin, Dymtro Kedyk, John Svadlenka, Lisa Ueda, Ariel Lindorf, Maurice Lepouttre, Daniel Keegan, Amy Wang, Evan Curcio, Jason Groob, Areum Cho, Nick Crispi, Patrick Brazil, Larry Fenn, Li Qian, Gregory Jarvens, Joseph Kaneko, and Pat Fay.

The cover honors John von Neumann. He understood the effect of computers on the direction of applied mathematics. It was this vision and his research in the years following WWII that lead to the mathematics included in this book.

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New York, NY
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Foreword

We begin with the role of numerical differential equations in science and the position the topic holds in Mathematics. First, we need to consider science and continuous mathematical models. Later, we see the role that numerical analysis plays.

Our knowledge of our environment is largely restricted to measuring change. We observe or measure changes and thereby infer knowledge to the entity that undergoes change. Mathematics first enters by providing quantifiable statements for scientific entities and their properties. The entity becomes a function, itself an idealized process, and properties such as mass, area or energy are integrals. It is by means of these mathematical constructs that we are able to quantize our abstractions. Next through observation, we identify conservation laws. Classically, these include conservation of mass or momentum. The 'no arbitrage' assumption in economics or finance is also a conservation law. No matter the source, when the conservation law is stated mathematically and then differentiated the result is zero. In other terms, conservation laws when given mathematical content give us differential equations, the equations of change. The object is a function, the change is represented as a derivative and the differential equation encapsulates our knowledge of the change. However, differential equations are largely intractable. In most cases, our knowledge of the solution is restricted to the data provided by numerical mathematics.

Writing in 1953, Braithwaite (1953) discussed this process in his book, Scientific Explanation. He used a paradigm to differentiate mathematics from science and to explain the role of mathematics in scientific development. The idea is to present science and math via a division of labor. The process is to first abstract observables as mathematical constructs and then to use conservation laws to provide the equations or relationships between the abstracted observables. In other terms, conservation laws are the means that yield mathematical models for observed reality. After the model is stated, the results of mathematical analysis are brought to bear on the problem. The expected outcome is that the differential equation is solved. With the solution at hand, the model generates data that can be used to predict observation. In the final step, if subsequent observation corresponds to prediction then the model is validated.

In 1947, John von Neumann (Grcar, 2011) knew that mathematical analysis alone could not produce the results necessary to support scientific and technological progress. The resolution of differential equations would also use numerical analysis. When the actual solution was not available then necessary information would be produced by discrete simulation. This observation must have been accepted fact for some time prior to 1947. However, the difference in the post WWII era was that computers provided the means for effective simulation.

Already at this time many of the fundamental techniques for approximating the solutions to differential equations were in place. The Runge–Kutta method for ordinary differential equations dates back to the 19th century. The mathematical foundation for this technique rested firmly on the Taylor series. For partial differential equations, finite difference method or FDM, Galerkin finite element method or GFEM, and spectral collocation were commonly applied by engineers. Indeed, this was the case as far back as the 1930s. However, little or nothing was known about the convergence and stability of these procedures. Hence, there was no means to validate much of the data that was being generated. Indeed, von Neumann recognized that convergence and stability questions were critical to the useful application of numerical analysis. In his 1947 paper with Herman

Goldstine, von Neumann set out on the path of reshaping numerical analysis as the mathematics necessary to support science and technology in the forthcoming computer age.

In terms of R. B. Braithwaite, in order to generate the data necessary to apply a mathematical model, there would need to be a second layer of theory, the stability and convergence theory. In the original setting, the conservation laws were the enabling results that interfaced between science and the continuous mathematical model. Now, there would need to be a second level of theory, the convergence and stability results, and these would be purely mathematical in nature. These results would bridge from the continuous model to the discrete model. They would validate the numerically generated data as trusted representations of the continuous mathematical model.

Early in this book, we will see an example of exactly the process just outlined. In this case, we begin with a conservation law related to conservation of energy. When this statement is rendered mathematically and differentiated, the result is the heat equation. We next apply Fourier transforms to the 1D case to arrive at a closed form solution for a specific set of boundary conditions. But beyond those specific cases, we are left with no alternative to numerical processes. In this case, the numerical technique that we choose is finite differences. As the example unfolds, the reader sees the entire process. Later in the book, we prove the Lax equivalence theorem. This result resolves the stability and convergence issue.

The purpose of this book is to present the reader with the basic techniques necessary to numerically resolve ODE and PDE and to present the underlying mathematics that supports these methods.

Historically, the stability and convergence theory has always lagged behind the technique. Even today research papers that propose to fill gaps in the convergence theory appear regularly. These gaps arise as engineers need to simulate specific cases that are beyond the current state of the theory. Often engineers introduce methods that are subsequently abstracted by mathematicians or engineers so that they may derive the convergence theorems. The theory is the offspring of the technique. As such, the theory is only fully understood when one also understands the corresponding application.

This last statement is nicely illustrated by an example. The FEM theory is written for Sobolev spaces. The idea is that you have a PDE defined for a function on a domain. Mathematical analysis has proved the existence of a solution u for certain cases but without providing a specific representation. FEM provides a family of approximate solutions u_h for partitions of the domain. In this case, h is a parameter associated to the partition size. The convergence theorem should state that $u_h \to u$ as $h \to 0$. But then there must be a metric space that contains both u and the family u_h. Since u is the solution to a PDE, then it must be differentiable. However, the u_h are usually piecewise polynomial functions and often not differentiable. They are however weakly differentiable and Sobolev spaces are metric spaces of weakly differentiable functions. Hence, this structure is the natural space to support convergence. However, this is only natural for people who have experienced doing FEM.

But we do not begin with the numerical technique. We begin with the application. The applications are the source. They give rise to the continuous mathematical model. The numerical technique is the means to resolving the mathematical model while the theory validates the connection between method and model. Therefore, we begin with applications. Some of these applications are historical while others are current. We use them as a vehicle to methods. Later, we turn our attention to the validating theory.

It is not our intention to be encyclopedic. This is a basic introduction to the topic for a graduate student with mathematical background in linear algebra and mathematical analysis including the elements of measure theory, functional analysis and Fourier transforms. In an introduction, the writer can be narrow in scope and complete in treatment or broad in scope but somewhat superficial in treatment. We are broad in scope in that we look at several techniques. However, we are not superficial in what we do and the questions we pose. Rather, we have restricted our treatment to the standard cases. It is our contention that this introduction will provide the reader or student with sufficient background to be able to access the numerical analysis literature and thereby develop the deep understanding of those settings of particular interest. We present here the background necessary to do advanced work.

We have tried to include most of what is necessary based on a standard background in measure theory and some basic results of functional analysis. Beyond this, we have included most proofs. However, theory based on special constructs is omitted. In these cases, we point the reader to a currently available reference. We do not want the reader to get bogged down in details whose inclusion has more to do with completeness than with understanding. Our singular purpose is to introduce numerical analysis both as applied technique and as theoretical mathematics. We remain focused on this goal.

This book proceeds as follows. In Part 1, we focus on applications and techniques or methods. In Part 2, we present the theory. We begin Part 1 with techniques as seen from a list of interesting and important application areas. These include finance, mechanical engineering, civil engineering and biology. More specifically, we include fluids, traffic, environmental protection, population studies, chemotaxis and options pricing. We have chosen the list to illustrate the breadth of the topic.

We have matched techniques to applications in a manner that covers a broad list of methods. We have included methods such as Runge–Kutta and midpoint ODE methods, explicit, implicit and Crank–Nicholson FDM, trapezoid, and Adams–Bashford time stepping on top of a spatial FEM realization. We also see FEM both on rectangular and triangular partitions and three variations of collocation method, spectral collocation in one spatial dimension, Gaussian collocation or OSC in one and two dimensions and discontinuous collocation in 2D using a triangular partition. Of course each application can be approached from more than one point of view.

We have mostly stayed away from 3D. Most interesting 3D applications require more computing power than a single processor computer can provide. Currently, nearly all academic institutions have access to high performance computing. Soon we may see a high performance computer on every desktop. However, there is little conceptual difference between two or higher dimensions. Hence, we make only occasional reference to higher dimensional techniques.

In Part 1, we make special effort to lead the reader through the multi-step FEM process. It is somewhat controversial whether a student can be expected to carry out an FEM on the first go. We feel this is achievable provided the student is handed data files for the elements and nodes and provided the context is sufficiently simple. In addition, we contend that reaching this milestone is an essential step toward grasping the topic. Even if the student sees only the simplest case, everything afterward can be understood as a modification or extension.

Also in Part 1, we pay special attention to visualizing the computed results. We are convinced that this is the most effective way to communicate the results of a study. In this regard, it is critical that the researcher maintains clear focus on the purpose of the project when preparing the output.

In Part 2, we first look at FDM. We begin with the Lax Equivalence Theorem. Subsequently, we look at the special issues associated to implementations of FDM for elliptical, parabolic and hyperbolic PDE. As all transient processes are resolved via time stepping and all time stepping is resolved using finite differences, it is essential to begin the theory here.

The most complex procedure is FEM. It is the gold standard of PDE simulation techniques. We begin with a chapter that gives a detailed description of the technique. Here, we discuss the details of the geometric model, the assembly process and the application of boundary values. The convergence theorem for a class of elliptical PDE is the most mathematically demanding part of the book. This requires that we detour into Sobolev spaces. In this regard, we have included some of the basic results while others are omitted as they would lead us too far afield. We include the Lax–Milgram theorem and the Bramble–Hilbert lemma as two milestones along this path. However, we omit much of the Sobolev embedding theory.

Our last major topic is the theory of collocation method. Here, we look at three varieties, the Gaussian collocation or OSC, the spectral version and finally an FEM type that supports triangular domain