Introduction

This book describes aspects of mathematical modeling, analysis, computer simulation, and visualization that are widely used in the mathematical sciences and engineering.

Scientists often use ordinary language models to describe observations of physical and biological phenomena. These are precise where data are known and appropriately imprecise otherwise. Ordinary language modelers carve away chunks of the unknown as they collect more data. On the other hand, mathematical modelers formulate minimal models that produce results similar to what is observed. This is the Ockham's razor approach, where simpler is better, with the caution from Einstein that "Everything should be made as simple as possible, but not simpler."

The success of mathematical models is difficult to explain. The same tractable mathematical model describes such diverse phenomena as when an epidemic will occur in a population or when chemical reactants will begin an explosive chain-branched reaction, and another model describes the motion of pendulums, the dynamics of cryogenic electronic devices, and the dynamics of muscle contractions during childbirth.

Ordinary language models are necessary for the accumulation of experimental knowledge, and mathematical models organize this information, test logical consistency, predict numerical outcomes, and identify mechanisms and parameters that characterize them.

Often mathematical models are quite complicated, but simple approximations can be used to extract important information from them. For example, the mechanisms of enzyme reactions are complex, but they can be described by a single differential equation (the Michaelis–Menten equation [14]) that identifies two useful parameters (the saturation constant and uptake velocity) that are used to characterize reactions. So this modeling and analysis identifies what are the critical data to collect. Another example is Semenov's theory of explosion limits [128], in which a single differential equation can be extracted from over twenty chemical rate equations modeling chain-branched reactions to describe threshold combinations of pressure and temperature that will result in an explosion.

Mathematical analysis includes geometrical forms, such as hyperbolic structures, phase planes, and isoclines, and analytical methods that derive from calculus and involve iterations, perturbations, and integral transforms. Geometrical methods are elegant and help us visualize dynamical processes, but analytical methods can deal with a broader range of problems, for example, those including random perturbations and forcing over unbounded time horizons. Analytical methods enable us to calculate precisely how solutions depend on data in the model.

As humans, we occupy regions in space and time that are between very small and very large and very slow and very fast. These intermediate space and time scales are perceptible to us, but mathematical analysis has helped us to perceive scales that are beyond our senses. For example, it is very difficult to "understand" electric and magnetic fields. Instead, our intuition is based on solutions to Maxwell's equations. Fluid flows are quite complicated and usually not accessible to experimental observations, but our knowledge is shaped by the solutions of the Navier–Stokes equations. We can combine these multiple time and space scales together with mathematical methods to unravel such complex dynamics. While realistic mathematical models of physical or biological phenomena can be highly complicated, there are mathematical methods that extract simplifications to highlight and elucidate the underlying process. In some cases, engineers use these representations to design novel and useful things.

We also live with varying levels of logical rigor in the mathematical sciences that range from complete detailed proofs in sharply defined mathematical structures to using mathematics to probe other structures where its validity is not known.

The mathematical methods presented and used here grew from several different scientific sources. Work of Newton and Leibniz was partly rigorous and partly speculative. The Göttingen school of Gauss, Klein, Hilbert, and Courant was carried forward in the U.S. by Fritz John, James Stoker, and Kurt Friedrichs, and they and their students developed many important ideas that reached beyond rigorous differential equation models and studied important problems in continuum mechanics and wave propagation. Russian and Ukrainian workers led by Liapunov, Bogoliubov, Krylov, and Kolmogorov developed novel approaches to problems of bifurcation and stability theory, statistical physics, random processes, and celestial mechanics. Fourier's and Poincaré's work on mathematical physics and dynamical systems continues to provide new directions for us, and the U.S.

mathematicians G. D. Birkhoff and N. Wiener and their students have contributed to these topics as well. Analytical and geometrical perturbation and iteration methods were important to all of this work, and all involved different levels of rigor.

Computer simulations have enabled us to study models beyond the reach of mathematical analysis. For example, mathematical methods can provide a language for modeling and some information, such as existence, uniqueness, and stability, about their solutions. And then well executed computer algorithms and visualizations provide further qualitative and quantitative information about solutions. The computer simulations presented here describe and illustrate several critical computer experiments that produced important and interesting results.

Analysis and computer simulations of mathematical models are important parts of understanding physical and biological phenomena. The knowledge created in modeling, analysis, simulation, and visualization contributes to revealing the secrets they embody.

The first two chapters present background material for later topics in the book, and they are not intended to be complete presentations of Linear Systems (Chapter 1) and Dynamical Systems (Chapter 2). There are many excellent texts and research monographs dealing with these topics in great detail, and the reader is referred to them for rigorous developments and interesting applications. In fact, to keep this book to a reasonable size while still covering the wide variety of topics presented here, detailed proofs are not usually given, except in cases where there are minimal notational investments and the proofs give readily accessible insight into the meaning of the theorem. For example, I see no reason to present the details of proofs for the Implicit Function Theorem or for the main results of Liapunov's stability theory. Still, these results are central to this book. On the other hand, the complete proofs of some results, like the Averaging Theorem for Difference Equations, are presented in detail.

The remaining chapters of this book present a variety of mathematical methods for solving problems that are sorted by behavior (e.g., bifurcation, stability, resonance, rapid oscillations, and fast transients). However, interwoven throughout the book are topics that reappear in many different, often surprising, incarnations. For example, the cusp singularity and the property of stability under persistent disturbances arise often. The following list describes cross-cutting mathematical topics in this book.

1. *Perturbations.* Even the words used here cause some problems. For example, *perturb* means to throw into confusion, but its purpose here is to relate to a simpler situation. While the perturbed problem is confused, the unperturbed problem should be understandable. Perturbations usually involve the identification of parameters, which unfortunately is often misunderstood by students to be perimeters from their studies of geometry. Done right, parameters should be dimensionless numbers that result from the model, such as ratios of eigenvalues of linear problems. Parameter iden-

tification in problems might involve difficult mathematical preprocessing in applications. However, once this is done, basic perturbation methods can be used to understand the perturbed problem in terms of solutions to the unperturbed problem. Basic perturbation methods used here are Taylor's method for approximating a smooth function by a polynomial and Laplace's method for the approximation of integral formulas. These lead to the implicit function theorem and variants of it, and to matching, averaging, and central-limit theorems. Adaptations of these methods to various other problems are described here. Two particularly useful perturbation methods are the method of averaging and the quasistatic-state approximation. These are dealt with in detail in Chapters 7 and 8, respectively.

2. *Iterations.* Iterations are mathematical procedures that begin with a state vector and change it according to some rule. The same rule is applied to the new state, and so on, and a sequence of iterates of the rule results. Fra Fibonacci in 1202 introduced a famous iteration that describes the dynamics of an age-structured population. In Fibonacci's case, a population was studied, geometric growth was deduced, and the results were used to describe the compounding of interest on investments.

Several iterations are studied here. First, Newton's method, which continues to be the paradigm for iteration methods, is studied. Next, we study Duffing's iterative method and compare the results with similar ones derived using perturbation methods. Finally, we study chaotic behavior that often occurs when quite simple functions are iterated. There has been a controversy of sorts between iterationists and perturbationists; each has its advocates and each approach is useful.

3. *Chaos.* The term was introduced in its present connotation by Yorke and Li in 1976 [101, 48]. It is not a precisely defined concept, but it occurs in various physical and religious settings. For example, Boltzmann used it in a sense that eventually resulted in ergodic theories for dynamical systems and random processes, and Poincaré had a clear image of the chaotic behavior of dynamical systems that occurs when stable and unstable manifolds cross. The book of Genesis begins with chaos, and philosophical discussions about it and randomness continue to this day. For the most part, the word chaos is used here to indicate behavior of solutions to mathematical models that is highly irregular and usually unexpected. We study several problems that are known to exhibit chaotic behavior and present methods for uncovering and describing this behavior. Related to chaotic systems are the following:

a. Almost periodic functions and generalized Fourier analysis [11, 140].

b. Poincaré's stroboscopic mappings, which are based on snapshots of a solution at fixed time intervals—"Chaos, illumined by flashes of lightning" [from Oscar Wilde in another context] [111].

c. Fractals, which are space filling curves that have been studied since Weierstrass, Hausdorff, Richardson, and Peano a century ago and more recently by Mandelbrodt [107].

d. Catastrophes, which were introduced by René Thom [133] in the 1960s.

e. Fluid turbulence that occurs in convective instabilities described by Lorenz and Keller [104].

f. Irregular ecological dynamics studied by Ricker and May [48].

g. Random processes, including the Law of Large Numbers and ergodic and other limit theorems [82].

These and many other useful and interesting aspects of chaos are described here.

4. *Oscillations.* Oscillators play fundamental roles in our lives—"discontented pendulums that we are" [R.W. Emerson]. For example, most of the cells in our bodies live an oscillatory life in an oscillating chemical environment. The study of pendulums gives great insight into oscillators, and we focus a significant effort here in studying pendulums and similar physical and electronic devices.

One of the most interesting aspects of oscillators is their tendency to synchronize with other nearby oscillators. This had been observed by musicians dating back at least to the time of Aristotle, and eventually it was addressed as a mathematical problem by Huygens in the 17th century and Korteweg around 1900 [142]. This phenomenon is referred to as phase locking, and it now serves as a fundamental ingredient in the design of communications and computer-timing circuits. Phase locking is studied here for a variety of different oscillator populations using the rotation vector method. For example, using the VCON model of a nerve cell, we model neural networks as being flows on high-dimensional tori. Phase locking occurs when the flow reduces to a knot on the torus for the original and all nearby systems.

5. *Stability.* The stability of physical systems is often described using energy methods. These methods have been adapted to more general dynamical systems by Liapunov and others. Although we do study linear and Liapunov stability properties of systems here, the most important stability concept used here is that of *stability under persistent disturbances.* This idea explains why mathematical results obtained for minimal models can often describe behavior of systems that are operating in noisy environments. For example, think of a metal bowl having a lowest point in it. A marble placed in the bowl will eventually move to the minimum point. If the bowl is now dented with many small craters or if small holes are put in it, the marble will still move to near where the minimum of the original bowl had been, and the degree of closeness can be determined from the size of the dents and holes. The dents and the holes introduce irregular

disturbances to the system, but the dynamics of the marble are similar in both the simple (ideal) bowl and the imperfect (realized) bowl.

Stability under persistent disturbances is sometimes confused with structural stability. The two are quite different. Structural stability is a concept introduced to describe systems whose behavior does not change when the system is slightly perturbed. Hyperbolic structures are particularly important examples of this. However, it is the changes in behavior when a system is slightly perturbed that are often the only things observable in experiments: Did something change? Stability under persistent disturbances carries through such changes. For example, the differential equation

$$\dot{x} = ax - x^3 + \varepsilon f(t),$$

where f is bounded and integrable, ε is small, and a is another parameter, occurs in many models. When $\varepsilon = 0$ and a increases through the value $a = 0$, the structure of static state solutions changes dramatically: For $a < 0$, there is only one (real) static state, $x = 0$; but for $a > 0$ there are three: $x = \pm\sqrt{a}$ are stable static states, and $x = 0$ is an unstable one. This problem is important in applications, but it is not structurally stable at $a = 0$. Still, there is a Liapunov function for a neighborhood of $x = 0, a = 0, \varepsilon = 0$, namely, $V(x) = x^2$. So, the system is stable under persistent disturbances. Stability under persistent disturbances is based on results of Liapunov, Malkin, and Massera that we study here.

6. *Computer simulation.* The two major topics studied in this book are mathematical analysis and computer simulation of mathematical models. Each has its uses, its strengths, and its deficiencies. Our mathematical analysis builds mostly on perturbation and iteration methods: They are often difficult to use, but once they are understood, they can provide information about systems that is not otherwise available. Understanding them for the examples presented here also lays a basis for one to use computer packages such as Mathematica, Matlab or Maple to construct perturbation expansions. Analytical methods can explain regular behavior of noisy systems, they can simplify complicated systems with fidelity to real behavior, and they can go beyond the edges of practical computability in dealing with fast processes (e.g., rapid chemical reactions) and small quantities (e.g., trace-element calculations).

Computer simulation replaces much of the work formerly done by mathematicians (often as graduate students), and sophisticated software packages are increasing simulation power. Simulations illustrate solutions of a mathematical model by describing a sample trajectory, or sample path, of the process. Sample paths can be processed in a variety of ways—plotting, calculating ensemble statistics, and so on. Simulations do not describe the dependence of solutions on model parameters, nor are their stability, accuracy, or reliability always assured. They do not deal well with chaotics or unexpected catastrophes—irregular or unexpected rapid changes in a solution—and it is usually difficult to determine when chaos lurks nearby.

Mathematical analysis makes possible computer simulations; conversely, computer simulations can help with mathematical analysis. New computer-based methods are being derived with parallelization of computations, simplification of models through automatic preprocessing, and so on, and the future holds great promise for combined work of mathematical and computer-based analysis. There have been many successes to date, for example the discovery and analysis of solitons.

The material in this book is not presented in order of increasing difficulty. The first two chapters provide background information for the last six chapters, where oscillation, iteration, and perturbation techniques and examples are developed. We begin with three examples that are useful throughout the rest of the book. These are electrical circuits and pendulums. Next, we describe linear systems and spectral decomposition methods for solving them. These involve finding eigenvalues of matrices and deducing how they are involved in the solution of a problem. In the second chapter we study dynamical systems, beginning with descriptions of how periodic or almost periodic solutions can be found in nonlinear dynamical systems using methods ranging from Poincaré and Bendixson's method for two differential equations to entropy methods for nonlinear iterations. The third chapter presents stability methods for studying nonlinear systems. Particularly important for later work is the method of stability under persistent disturbances.

The remainder of the book deals with methods of approximation and simulation. First, some useful algebraic and topological methods are described, followed by a study of implicit function theorems and modifications and generalizations of them. These are applied to several bifurcation problems. Then, regular perturbation problems are studied, in which a small parameter is identified and the solutions are constructed directly using the parameter. This is illustrated by several important problems in nonlinear oscillations, including Duffing's equation and nonlinear resonance.

In Chapter 7 the method of averaging is presented. This is one of the most interesting techniques in all of mathematics. It is closely related to Fourier analysis, to the Law of Large Numbers in probability theory, and to the dynamics of physical and biological systems in oscillatory environments. We describe here multitime methods, Bogoliubov's transformation, and integrable systems methods.

Finally, the method of quasistatic-state approximations is presented. This method has been around in various useful forms since 1900, and it has been called by a variety of names—the method of matched asymptotic expansions being among the most civil. It has been derived in some quite complicated ways and in some quite simple ones. The approach taken here is of quasistatic manifolds, which has a clear geometric flavor that can aid intuition. It combines the geometric approach of Hadamard with the analytical methods of Perron to construct stable and unstable manifolds for systems that might involve irregular external forcing.

In rough terms, averaging applies when a system involves rapid oscillations that are slowly modulated, and quasistatic-state approximations are used when solutions decay rapidly to a manifold on which motions are slower. When problems arise where both kinds of behavior occur, they can often be unraveled. But there are many important problems where neither of these methods apply, including diffraction by crossed wires in electromagnetic theory, stagnation points in fluid flows, flows in domains with sharp corners, and problems with intermittent rapid time scales.

I have taught courses based on this book in a variety of ways depending on the time available and the background of the students. When the material is taught as a full year course for graduate students in mathematics and engineering, I cover the whole book. Other times I have taken more advanced students who have had a good course in ordinary differential equations directly to Chapters 4, 5, 6, 7, and 8. A one quarter course is possible using, for example, Chapters 1, 7, and 8. For the most part Chapters 1 and 2 are intended as background material for the later chapters, although they contain some important computer simulations that I like to cover in all of my presentations of this material. A course in computer simulations could deal with sections from Chapters 2, 4, 7, and 8. The exercises also contain several simulations that have been interesting and useful.

The exercises are graded roughly in increasing difficulty in each chapter. Some are quite straightforward illustrations of material in the text, and others are quite lengthy projects requiring extensive mathematical analysis or computer simulation. I have tried to warn readers about more difficult problems with an asterisk where appropriate.

Students must have some degree of familiarity with methods of ordinary differential equations, for example, from a course based on Coddington and Levinson [24], Hale [58], or Hirsch and Smale [68]. They should also be competent with matrix methods and be able to use a reference text such as Gantmacher [46]. Some familiarity with *Interpretation of Dreams* [45] has also been found to be useful by some students.

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