Chapter 1

Theme and Contents of this Book

Observations of events in the world require that they must proceed in space and time. A goal of science is to identify phenomena believed to be of interest and subsequently establish predictive rules of their causes and consequences. In many areas of scientific theory the mathematical language of this program is that of differential equations. Solutions of these equations serve to describe how the elements of one or more phenomena proceed due to mutual interactions between the elements and with the external world. An 18th century ideal was that solution of Newton's differential equations of motion, given the forces between all the particles in the world, would answer any and all questions. This, of course, is technologically impossible. But even if it were, it would be a Pyrrhic victory, for while such solutions would tell us how all the particles move in space and time, one could not apriori distingish where some of the particles are participants in, say, a chemical reaction, a population migration. a wind current, an eye color or in fact any boundable situation. To do so requires the construction of contracted descriptions of qualitatively identifiable objects which are adjudged to interact with each other and with external influences. The mathematics of such contracted descriptions are in many cases a small number of differential equations.

The principle aim of this book is to explore selected nonlinear ordinary differential equations, describing evolution in time, and nonlinear partial differential equations describing evolution in space and time, which have proven pivotal to understanding many phenomena in nature. The unifying theme is that these equations are foundational in that in almost all cases the ideas behind them and the equations themselves have become extended into areas beyond their original intent. Of course, while there are many such equations, the present selection reflects the interests and activities of the authors as well as a belief in their importance. The invention of these equations is a matter of history and ingenuity extending over 100 years. The intent here is to explore their salient analytical properties and consequences. Their age should not belie their importance, since whole fields of research have sprung from them. In many cases a given equation has remained fallow for many years before being rediscovered and its importance recognized. Most of them saw the light of day before the computer age but their rediscovery around our time, with the added power of computation, makes a formal presentation of these equations for the student and interested researcher irresistible. Many of the chapters are concerned with a few key equations. This is supplemented by considerations of related differential equations which have been developed as model extensions of the key equations. The latter equations serve to either extend the range of applicability or to provide more insight into the structure of the key equations. The rationale for the equations are given and approximate solutions are explored using a combination of analytical techniques and computer study.

There are many books which treat nonlinear dynamics from equally many points of view, selection of subject matters and style of presentation. These considerations have prompted our hope that, for the student, a given subject is provided in a sufficiently transparent manner to encourage further exploration in the direction of the chapter. For the researcher no doubt many will find chapters in their area of expertise very simple but there may be subjects in other chapters which will stimulate interest and further study with the aid of the references. To provide a guide through this book, a summary of each chapter is below.

Chapter 2. Processes in Closed and Open Systems: Thermodynamics sets the stage for chemical reactions and provides the frame for handling equilibria or near equilibrium systems. Closed systems are common in chemistry and biochemistry laboratory experiments:

A reaction is started and then progresses towards equilibrium without further intervention by the experimenter. Gibbs free energy is the appropriate thermodynamic potential for the usual conditions of constant pressure and temperature. Open systems are required to keep reaction away from equilibrium. This is achieved in various flow reactors where the materials consumed by the reaction are replenished by an influx of stock solution. Effective nonlinearities leading to multistability, oscillations, or deterministic chaos are introduced into chemical reaction networks through autocatalytic reaction steps. The nature of the nonlinearity – quadratic, cubic, or higher degree – determines the qualitative behavior of the reaction system as it is reflected by the bifurcation diagrams.

Chapter 3. Dynamics of Molecular Evolution: Multiplication in biology can be traced down to the copying process of genetic information of organisms which is stored in nucleic acids, DNA or RNA. This copying process called replication is a special form of autocatalysis: A nucleic acid molecule acts as template and the synthesis of the copy completes a single strand to a double helix making use of digit complementarity. Replication under the condition of constant population size gives rise to ODEs called replicator equations, which encapsulate essential features of evolutionary processes. Two mechanisms of template induced autocatalysis are analyzed and discussed in terms of the ODEs provided by chemical reaction kinetics: (i) autocatalytic formation of oligonucleotides and (ii) replication of RNA molecules. Replication under non-equilibrium conditions of a flow reactor leads to selection and provides access to Darwinian evolution experiments in the test tube. Mutation is an inevitable consequence of finite accuracy in copying molecules and provides the basis for optimization through replication, variation, and selection. Error propagation sets an upper limit for mutation rates in form of an error threshold: If error rates are too high genetic information cannot be transmitted stably to future generations. Evolution by variation and selection is the result of a quadratic nonlinearity in the sense of chapter 2. Higher order nonlinearities in replicator equations may be introduced by different molecular mechanisms like recombination in sexual reproduction or catalysis of replication. The results of these higher order nonlinear terms are diverse scenarios known from other nonlinear differential equations: multistability, oscillations, and deterministic chaos. Relevant for biology is the possibility to suppress competition through selection by means of higher order autocatalytic terms as it is observed, for example, in various forms of symbioses.

Chapter 4. Relaxation Oscillations: Relaxation oscillations occur when there are periodic transitions between two or more dynamical states of vastly differing lifetimes. They occur in mechanical, electronic, laser and animal systems. The prototypic equation for analysis is the van der Pol equation and a closely related simplification of it, the Stoker-Haag equation. As application it will be shown to provide a predictive model for current induced oscillations displayed by neurons. Analysis of harmonically forced relaxation oscillations provides entry to entrainment and multiperiodic phenomena.

Chapter 5. Order and Chaos: Although not achievable in practice science assumed that in principle, given sufficient computational power and ingenuity, solution of unambiguously defined differential equations would provide precise prediction for the time course of the events described by these equations. The centerpiece of this chapter is the Lorenz equations which demonstrated that this ideal even in principle is impossible under certain situations. Considered here is a discussion of relationships between prediction inherent to stable orbits and the unpredictability of chaos demonstrated by the Lorenz equations. The discussion is initiated by analysis of a very simple mathematical representation, the logistic map, which is not a differential equation but a compact mathematical prescription which highlights the coexistence of order and chaos. This provides the stage for discussion of paramount ordered and chaotic features demonstrated by computer solutions to the Lorenz equations. An autocatalytic reaction network, discussed within the more general framework of molecular evolution in Chapter 3, is considered here as demonstration that small autocatalytic networks under certain conditions can exhibit not only complicated multiple periodic but chaotic behavior as well. This is a chemical example of distinct regions of order and chaos as modulated control parameters which carry the system from one region to another. A final example considers the equations for the Chua circuit. This circuit, which can be built with off-the shelf components, has provided a transparent basis for generation of aperiodic and chaotic signals. The descriptive equations display a dynamics which feature an additive property in the progression from simple periodicity to multiple periodicity and progressing to chaos.

Chapter 6. Reaction Diffusion Dynamics: Undiminished pulse fronts occur in chemical and biological signals. The prototype is the Fisher equation originally proposed to account for the spatial spread of a favored gene in a population. Approximate analytic solutions are developed that illustrate the details of these pulses. The same methods are applied to biased migration and nonlinear convection. A second form of solution predicts the existence of spatial inhomogeneities driven by diffusion. This leads to a discussion and application of the Turing theory of spatial pattern formation. The Turing postulates serve to explain cellular development and morphogenesis on a chemical level: diffusion provides the driving mechanism to destabilize a homogeneous chemical situation and transform it into heterogeneous spatial patterns. The discussion includes mathematical analysis of spatial steady state chemical pattern formations.

Chapter 7. Solitons: While chaos is a dynamical situation where orbits of predictable motion lose their stability, solitons represent the opposite extreme of structural integrity. If chaos demonstrates unpredictable meanderings the soliton demonstrates objects of such rigidity that two encountering solitons can merely pass through each other and emerge unscathed or alternatively scatter upon collision as particles. They were first observed as non dispersable water waves. The existence of these wave was confirmed on the basis of hydrodynamics by Kortewg and de Vries whose equation bearing their names is the initial focus of this chapter. The Korteweg-de Vries equation represents a dynamical balance between dispersion and nonlinear localization. As such they can be derived within the framework of classical mechanics. The model is of an assembly of identical particles arranged on a lattice with nonlinear forces between adjacent particles. The chapter starts with an introduction to lattice dynamics leading to the Korteweg-deVries equation. A discussion and graphical presentation is made of solutions to this equation. If one introduces a periodic potential into the lattice dynamics, the sine-Gordon equation is produced in which dispersion and localization can be embedded in a single mathematical package. This facilitates assigning to the sine-Gordon soliton a particle-like mass and energy where the size of the effective mass is dictated by the strength of the nonlinear interactions. Solutions to the sine-Gordon equation demonstrate collisions between "solitons" and "anti-solitons." The Burgers equation is briefly discussed which, in contrast to the Korteweg-deVries equation, is a dissipative equation which predicts shock waves produced by turbulence.

Chapter 8. Neuron Pulse Propagation: The fundamental unit of neural behavior, and thereby the structural pivot of neurobiology, is the neuron. The interconnections between millions of neurons forming neural networks provide the machinery of neural phenomena. A single neuron functions by transmitting electrochemical signals called action potentials. The definitive elaboration of by what mechanism an action potential is produced, as well as its shape and speed, was provided by the experimental and theoretical work of Hodgkin and Huxley. Their results are encapsulated in the Hodgkin-Huxley equations which form the centerpiece of this chapter. The action potential propagates in space and time along the neural axon and by clamping the axon these equations account for neural relaxation oscillations with properties similar to those discussed in Chapter 4. Here, however, is the added feature of the role of diffusion in concert with the electrochemical mechanisms of sodium and potassium ion channels. The description of this collaboration requires the four dimensional Hodgkin-Huxley equations. First introduced is a formal mathematical simplification, the FitzHugh-Nagumo equations, which allow analytical discussion of neural pulse properties of speed, shape and height. This provides an introduction to the subsequent discussion of the Hodgkin-Huxley equations whose intricacies can be tamed in two ways. First, some of the complicated mathematical structures of the ion gating functions which drive the neural pulse can be simplified. Secondly, to close approximation the gating functions are not independent and therefore can be interrelated. This reduces the mathematical complexity of the Hodgkin-Huxley equations to facilitate prediction of the pulse speed and height as functions of the temperature.

Chapter 9. Time Reversal, Dissipation and Conservation: This chapter is intended as a reprise providing opportunity to more critically discuss some key concepts underlying descriptions of dynamical systems. Some events in time appear unidirectional such as the progression of a pulse front or soliton, some appear repetitious such as current induced relaxation oscillations displayed by neurons or chemical patterns which can arise due to Turing instabilities, some appear cyclical as autocatalytic networks, some may or may not show periodic behavior or alternatively multiperiodic or chaotic behavior. Overriding these many possibilities is that all the descriptive equations are either reversible in time or they are not. Correspondingly certain quantities are invariant, that is conserved, or they are not. The presence of diffusion removes time reversal and in its simplest manifestation tends to drive a system to homogeneity. Yet, time-directed diffusion equations featuring nonlinearities can produce heterogeneous structures. Oppositely time reversible equations can demonstrate what appear to be irreversible behavior. Chaos which upsets predictability was discussed in terms of equations which are inherently irreversible in time, outside the framework of Newtonian mechanics. Within the Newtonian framework are included two surprises. First,the Fermi-Pasta-Ulam equations anticipated to show the establishment of equipartition of energy from some initial condition do not, but rather exhibit time reversible behavior. This result provided a foundation for derivation of the solitonic Korteweg-deVries equation. Secondly, the Hénon-Heiles equations constructed according to Newtonian mechanics demonstrate that regions of predictable order and Hamiltonian chaos can coexist in time reversible dynamics.

Except for Chapter 9, the other chapters are reasonably independent: the reading of one is not a requirement for the reading of another. On the other hand there are formal connections between concepts or between two or more equations in different chapters in many cases. This is hardly surprising, emphasizing that even amid this diversity resides recurring patterns of human constructions which have lead to the existence of these equations. Finally, the level of mathematics presumes some knowledge of linear differential equations and in particular of fixed point analysis. An attempt has been made, on the other hand, to explicitly summarize what is used in linear theory during the course of the discussions of nonlinear dynamics.