Preface

What is Mathematical Modelling?

In order to explain the purpose of modelling, it is helpful to start by asking: *what is a mathematical model*? One answer was given by Rutherford Aris [4]:

> A model is a set of mathematical equations that … provide an adequate description of a physical system.

Dissecting the words in his description, "*a physical system*" can be broadly interpreted as any real-world problem—natural or man-made, discrete or continuous and can be deterministic, chaotic, or random in behaviour. The context of the system could be physical, chemical, biological, social, economic or any other setting that provides observed data or phenomena that we would like to quantify. Being "*adequate*" sometimes suggests having a minimal level of quality, but in the context of modelling it describes equations that are good enough to provide sufficiently accurate predictions of the properties of interest in the system without being too difficult to evaluate.

Trying to include every possible real-world effect could make for a complete description but one whose mathematical form would likely be intractable to solve. Likewise, over-simplified systems may become mathematically trivial and will not provide accurate descriptions of the original problem. In this spirit, Albert Einstein supposedly said, *"Everything should be made as simple as possible, but not simpler"* [107], though ironically this is actually an approximation of his precise statement [34].

Many scientists have expressed views about the importance of modelling and the limitations of models. Some other notable examples are:

- In the opening of his foundational paper on developmental biology, Alan Turing wrote *"This [mathematical] model will be a simplification and an idealisation, and consequently a falsification. It is to be hoped that the features retained for discussion are those of greatest importance ..."* [100]
- George Box wrote *"...all models are wrong, but some are useful."* [17]

- Mark Kac wrote *"Models are, for the most part, caricatures of reality, but if they are good, they portray some features of the real world."* [55]

Useful models strike a balance between such extremes and provide valuable insight into phenomena through mathematical analysis. Every proposed model for a problem should include a description of how results will be obtained—a solution strategy. This suggests an operational definition:

> **model**: a useful, practical description of a real-world problem, capable of providing systematic mathematical predictions of selected properties

Models allow researchers to assess balances and trade-offs in terms of levels of calculational details versus limitations on predictive capabilities.

Concerns about models being "wrong" or "false" or "incomplete" are actually criticisms of the levels of physics, chemistry or other scientific details being included or omitted from the mathematical formulation. Once a well-defined mathematical problem is set up, its mathematical study can be an important step in understanding the original problem. This is particularly true if the model predicts the observed behaviours (a positive result). However, even when the model does not work as expected (a negative result), it can lead to a better understanding of which (included or omitted) effects have significant influence on the system's behaviour and how to further improve the accuracy of the model.

While being mindful of the possible weaknesses, the positive aspects of models should be praised,

> Models are expressions of the hope that aspects of complicated systems can be described by simpler underlying mathematical forms.

Exact solutions can be found for only a very small number of types of problems; seeking to extend systems beyond those special cases often makes the exact solutions unusable. Modelling can provide more viable and robust approaches, even though they may start from counterintuitive ideas, *"... simple, approximate solutions are more useful than complex exact solutions"* [15].

Mathematical models also allow for the exploration of conjectures and hypothetical situations that cannot normally be de-coupled or for parameter ranges that might not be easily accessible experimentally or computationally. Modelling lets us qualitatively and quantitatively dissect problems in order to evaluate the importance of their various parts, which can lead to the original motivating problem becoming a building block for the understanding of more complex systems. Good models provide the flexibility to be systematically developed allowing more accurate answers to be obtained by solving extensions of the model's mathematical equations. In summary, our description of the process is

> **modelling**: a systematic mathematical approach to formulation, simplification and understanding of behaviours and trends in problems.

Levels of Models

Mathematical models can take many different forms spanning a wide range of types and complexity,

$$\boxed{\text{“\textit{Toy}” problems}} \quad \le \quad \text{Math Models} \quad \le \quad \boxed{\text{Complete systems}}$$

At the upper end of complexity are models that are equivalent to the full first-principles scientific description of all of the details involved in the entire problem. Such systems may consist of dozens or even hundreds of equations describing different parts of the problem; computationally intensive numerical simulations are often necessary to investigate the full system.

At the other end of the spectrum are improvised or phenomenological “toy” problems[1] that may have some conceptual resemblance to the original system but have no obvious direct derivation from that problem. These might be only a few equations or just some geometric relations. They are the mathematical modelling equivalents of an “artistic impression” motivated or inspired by the original problem. Their value is that they may provide a simple “proof of concept” prototype for how to describe a key element of the complete system.

Both extremes have drawbacks: intractable calculations in one extreme, and imprecise qualitative results at the other. Mathematical models exist in-between and try to bridge the gap by offering a process for using identifiable assumptions to reduce the full system down to a simpler form, where analysis, calculations and insights are more achievable, but without losing the accuracy of the results and the connection to the original problem.

Classes of Real World Problems

The kinds of questions being considered play an important role in how the model for the problem should be constructed. There are three broad types of questions:

(i) Evaluation questions [also called *Forward problems*]: Given all needed information about the system, can we quantitatively predict its other properties and how the system will function? Examples: What is the maximum attainable speed of this car? How quickly will this disease spread through the population of this city?

(ii) Detection questions [*Inverse problems*] [8]: If some information about a “black box” system is not directly available, can you “reverse engineer” those missing parameters? Examples: How can we use data from CAT scans to

[1] Sometimes also described as *ad hoc* or *heuristic* models.

estimate the location of a tumour? Can we determine the damping of an oscillator from the decay of its time series data?

(iii) Design questions [*Control and optimisation problems*]: Can we create a solution that best meets a proposed goal? Examples: What shape paper airplane flies the furthest? How should a pill be coated to release its drug at a constant rate over an entire day?

There are many routes available to attack such questions that are typically treated in different areas of study. This book will introduce methods for addressing some problems of the forms (i) and (iii) in the context of continuous systems and differential equations.

Stages of the Modelling Process

The modelling process can sometimes start from a creative and inspired toy problem and then seeks to validate the model's connection to the original problem. However, this approach requires having a lot of previous experience with and background knowledge on the scientific area and/or relevant mathematical techniques in order to generate the new model. In this book, we follow the more systematic approach of starting with some version of the complete scientific problem statement and then using mathematical techniques to obtain reduced models that can be simplified to a manageable level of computational difficulty.

The modelling process has two stages, consisting of setting up the problem and then solving it:

- In the *formulation phase*, the problem is described using basic principles or governing laws and assumed relations taken from some branches of knowledge, such as physics, biology, chemistry, economics, geometry, probability or others. Then all side-conditions that are needed to completely define the problem must be identified: geometric constraints, initial conditions, material properties, boundary conditions and design parameter values. Finally, the properties of interest, how they are to be measured, relevant variables, coordinate systems and a system of units must all be decided on.
- Then[2], in the *solution phase*, mathematical modelling provides approaches to reformulating the original problem into a more convenient structure from which it can be reduced into solvable parts that can ultimately be re-assembled to address the main questions of interest for the problem.

In some cases, the reformulated problem may seem to only differ from the original system at a notational level, but these changes can be essential for separating out different effects in the system. At the simplest level, "problem reduction" consists of

[2] Assuming that the problem cannot be easily solved analytically or computed numerically, and hence does not need modelling.

obtaining so-called *asymptotic approximations* of the solution, but for more challenging problems, this will also involve approaches for transforming the problem into different forms that are more tractable for analysis or computation.

The techniques described here are broadly applicable to many branches of engineering and applied science: biology, chemistry, physics, the geosciences and mechanical engineering, to name a few. To keep examples compact and accessible, we present concise reviews of background from different fields when needed (including population biology and chemical reactions in Chap. 1, fluid dynamics in Chap. 2 and classical mechanics in Chap. 3), but we seek to maintain focus on the modelling techniques and the properties of solutions that can be obtained. We direct interested readers to books that present more detailed case studies of problems needing more extensive background in specific application areas [8, 27, 37, 38, 51, 69, 96].

The structure of this book follows the description of the modelling process described above:

- Part I: Formulation of models
  This part consists of four chapters that present fundamental approaches and exact methods for formulating different classes of problems:
  1. Rate equations: simple models for properties evolving in time
  2. Transport equations: models involving structural changes
  3. Variational principles: models based on optimisation of properties
  4. Dimensional analysis: determination of the number of essential system parameters
- Part II: Solution techniques
  This part presents methods for obtaining approximate solutions to some of the classes of problems introduced in Part I.
  5. Similarity solutions: determining important special solutions of PDEs using scaling analysis
  6. Perturbation methods: exploiting limiting parameters to obtain expansions of solutions
  7. Boundary layers: constructing solutions having non-uniform spatial structure
  8. Long-wave asymptotics: reduction of problems on slender domains
  9. Weakly-nonlinear oscillators: predicting cumulative changes over large numbers of oscillations
  10. Fast/slow dynamical systems: separating effects acting over different timescales
  11. Reduced models: obtaining essential properties from simplified versions of partial differential equation problems
- Part III: Case studies: some applications illustrating uses of techniques from Parts I and II.

While this book cannot be an exhaustive introduction to all types of mathematical models, we seek to develop intuition from the ground-up on formulating equations and methods of solving models expressible in terms of differential equations.

The book is written in a concise and self-contained form that should be well-suited for an advanced undergraduate or beginning graduate course or independent study. Students should have a background in calculus and basic differential equations. Each chapter provides references to sources that can provide more detail on topics that readers wish to pursue in greater depth. We note that the examples and exercises are an important part of the book and will introduce readers to many classic models that have become important milestones in applied mathematics for illustrating important or universal solution structures. Some of these highlights include:

- The Burgers equation (Chaps. 2, 4, 5)
- The shallow water equations (Chaps. 2, 4, 6)
- The porous medium equation (Chaps. 5, 8, 11)
- The Korteweg de Vries (KdV) equation (Chaps. 8, 9)
- The Fredholm alternative theorem (Chap. 9)
- The van der Pol equation (Chaps. 9, 10)
- The Michaelis–Menten reaction rate model (Chap. 10)
- The Turing instability mechanism (Chap. 11)
- Taylor dispersion (Chap. 11)

Solutions are provided to many exercises. Readers are encouraged to work through the exercises in order to gain a deeper understanding of the techniques presented.

Durham, NC, USA Thomas Witelski
Tokyo, Japan Mark Bowen
June 2015

Springer

http://www.springer.com/978-3-319-23041-2

Methods of Mathematical Modelling
Continuous Systems and Differential Equations
Witelski, Th.; Bowen, M.
2015, XVIII, 305 p. 50 illus., 45 illus. in color., Softcover
ISBN: 978-3-319-23041-2