Kai Velten

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Mathematical Modeling and Simulation

Introduction for Scientists and Engineers

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Cover

Simulated soil moisture isosurfaces in an asparagus ridge (details are explained in the text). Computer simulation performed by the author.

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The purpose of computing is insight, not numbers.
R.W. Hamming [242]

Preface

"Everyone is an artist" was a central message of the famous twentieth century artist Joseph Beuys. "Everyone models and simulates" is a central message of this book. Mathematical modeling and simulation is a fundamental method in engineering and science, and it is absolutely valid to say that everybody uses it (even those of us who are not aware of doing so). The question is not whether to use this method or not, but rather how to use it effectively.

Today we are in a situation where powerful desktop PCs are readily available to everyone. These computers can be used for any kind of professional data analysis. Even complex structural mechanical or fluid dynamical simulations which would have required supercomputers just a few years ago can be performed on desktop PCs. Considering the huge potential of modeling and simulation to solve complex problems and to save money, one should thus expect a widespread and professional use of this method. Particularly in the field of engineering, however, complex problems are often still treated largely based on experimental data. The amount of money spent on experimental equipment sometimes seems proportional to the complexity and urgency of the problems that are solved, and simple spreadsheet calculations are used to explore the information content of such expensive data. As this book will show, mathematical models and simulations help to reduce experimental costs not only by a partial replacement of experiments by computations, but also by a better exploration of the information content of experimental data.

This book is based on the author's modeling and simulation experience in the fields of science and engineering and as a consultant. It is intended as a first introduction to the subject, which may be easily read by scientists, engineers and students at the undergraduate level. The only mathematical prerequisites are some calculus and linear algebra – all other concepts and ideas will be developed in the course of the book. The reader will find answers to basic questions such as: What is a mathematical model? What types of models do exist? Which model is appropriate for a particular problem? How does one set up a mathematical model? What is simulation, parameter estimation, validation? The book aims to be a practical guide, enabling the reader to setup simple mathematical models on his own and to interpret his own and other people's results critically. To achieve

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this, many examples from various fields such as biology, ecology, economics, medicine, agricultural, chemical, electrical, mechanical and process engineering are discussed in detail.

The book relies exclusively upon open-source software, which is available to everybody free of charge. The reader is introduced into *CAELinux*, *Calc*, *Code-Saturne*, *Maxima*, *R*, and *Salome-Meca*, and the entire book software – including 3D CFD and structural mechanics simulation software – can be used based on a (free) CAELinux-Live-DVD that is available in the Internet (works on most machines and operating systems, see Appendix A).

While software is used to solve most of the mathematical problems, it is nevertheless attempted to put the reader mathematically on firm ground as much as possible. Trap-doors and problems that may arise in the modeling process, in the numerical treatment of the models or in their interpretation are indicated, and the reader is referred to the literature whenever necessary.

The book is organized as follows. Chapter 1 explains the principles of mathematical modeling and simulation. It provides definitions and illustrative examples of the important concepts as well as an overview of the main types of mathematical models. After a treatment of phenomenological (data-based) models in Chapter 2, the rest of the book introduces the most important classes of mechanistic (process-oriented) models (ordinary and partial differential equation models in Chapters 3 and 4, respectively).

Although it is possible to write a book like this on your own, it is also true that it is impossible to write a book like this on your own . . . I am indebted to a great number of people. I wish to thank Otto Richter (TU Braunschweig), my first teacher in mathematical modeling; Peter Knabner (U Erlangen), for an instructive excursion into the field of numerical analysis; Helmut Neunzert and Franz-Josef Pfreundt (TU and Fraunhofer-ITWM Kaiserslautern), who taught me to apply mathematical models in the industry; Helmut Kern (FH Wiesbaden), for blazing a trail to Geisenheim; Joël Cugnoni (EPFL Lausanne), for our cooperation and an adapted version of CAELinux (great idea, excellent software); Anja Tschörtner, Cornelia Wanka, Alexander Grossmann, H.-J. Schmitt and Uwe Krieg from Wiley-VCH; and my colleagues and friends Marco Günther, Stefan Rief, Karlheinz Spindler, and Aivars Zemitis for proofreading.

I dedicate this book to Birgid, Benedikt, Julia, and Theresa for the many weekends and evenings they patiently allowed me to work on this book, to the Sisters of the Ursuline Order in Geisenheim and Straubing, and, last but not least, to my parents and to my brothers Axel and Ulf, to Bettina and Brigi and, of course, to Felix, for their support and encouragment through so many years.

Geisenheim, May 2008 *Kai Velten*

Contents

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1 Principles of Mathematical Modeling

We begin this introduction to mathematical modeling and simulation with an explanation of basic concepts and ideas, which includes definitions of terms such as *system, model, simulation, mathematical model,* reflections on the objectives of mathematical modeling and simulation, on characteristics of "good" mathematical models, and a classification of mathematical models. You may skip this chapter at first reading if you are just interested in a hands-on application of specific methods explained in the later chapters of the book, such as regression or neural network methods (Chapter 2) or differential equations (DEs) (in Chapters 3 and 4). Any professional in this field, however, should of course know about the principles of mathematical modeling and simulation. It was emphasized in the preface that everybody uses mathematical models – "even those of us who are not aware of doing so". You will agree that it is a good idea to have an idea of what one is doing...

Our starting point is the complexity of the problems treated in science and engineering. As will be explained in Section 1.1, the difficulty of problems treated in science and engineering typically originates from the complexity of the systems under consideration, and models provide an adequate tool to break up this complexity and make a problem tractable. After giving general definitions of the terms *system, model,* and *simulation* in Section 1.2, we move on toward mathematical models in Section 1.3, where it is explained that mathematics is *the* natural modeling language in science and engineering. Mathematical models themselves are defined in Section 1.4, followed by a number of example applications and definitions in Sections 1.5 and 1.6. This includes the important distinction between phenomenological and mechanistic models,which has been used as the main organization principle of this book (see Section 1.6.1 and Chapters 2–4). The chapter ends with a classification of mathematical models and Golomb's famous "Don'ts of mathematical modeling" in Sections 1.7 and 1.8.

1.1 A Complex World Needs Models

Generally speaking, engineers and scientists try to understand, develop, or optimize "systems". Here, "system" refers to the object of interest, which can be a part of

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nature (such as a plant cell, an atom, a galaxy etc.) or an artificial technological system (see Definition 1.2.3 below). Principally, everybody deals with systems in his or her everyday life in a way similar to the approach of engineers or scientists. For example, consider the problem of a table which is unstable due to an uneven floor. This is a technical system and everybody knows what must be done to solve the problem: we just have to put suitable pieces of cardboard under the table legs. Each of us solves an abundant number of problems relating to simple technological systems of this kind during our lifetime. Beyond this, there is a great number of really difficult technical problems that can only be solved by engineers. Characteristic of these more demanding problems is a high complexity of the technical system. We would simply need no engineers if we did not have to deal with complex technical systems such as computer processors, engines, and so on. Similarly, we would not need scientists if processes such as the photosynthesis of plants could be understood as simply as an unstable table. The reason why we have scientists and engineers, virtually their right to exist, is the complexity of nature and the complexity of technological systems.

Note 1.1.1 (The complexity challenge) It is the genuine task of scientists and engineers to deal with complex systems, and to be effective in their work, they most notably need specific methods to deal with complexity.

The general strategy used by engineers or scientists to break up the complexity of their systems is the same strategy that we all use in our everyday life when we are dealing with complex systems: simplification. The idea is just this: if something is complex, make it simpler. Consider an everyday life problem related to a complex system: A car that refuses to start. In this situation, everyone knows that a look at the battery and fuel levels will solve the problem in most cases. Everyone will do this automatically, but to understand the problem solving strategy behind this, let us think of an alternative scenario. Assume someone is in this situation for the first time. Assume that "someone" was told how to drive a car, that he has used the car for some time, and now he is for the first time in a situation in which the car does not start. Of course, we also assume that there is no help for miles around! Then, looking under the hood for the first time, our "someone" will realize that the car, which seems simple as long as it works well, is quite a complex system. He will spend a lot of time until he will eventually solve the problem, even if we admit that our "someone" is an engineer. The reason why each of us will solve this problem much faster than this "someone" is of course the simple fact that this situation is not new to us. We have experienced this situation before, and from our previous experience we know what is to be done. Conceptually, one can say that we have a simplified picture of the car in our mind similar to Figure 1.1. In the moment when we realize that our car does not start, we do not think of the car as the complex system that it really is, that is, we do not think of this conglomerate of valves, pistons, and all the kind of stuff that can be found under the hood; rather, we have this simplified picture of the car in our mind. We know that this simplified

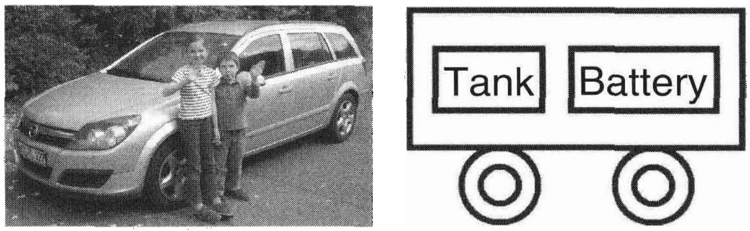

Fig. 1.1 Car as a real system and as a model.

picture is appropriate in this given situation, and it guides us to look at the battery and fuel levels and then to solve the problem within a short time.

This is exactly the strategy used by engineers or scientists when they deal with complex systems. When an engineer, for example, wants to reduce the fuel consumption of an engine, then he will not consider that engine in its entire complexity. Rather, he will use simplified descriptions of that engine, focusing on the machine parts that affect fuel consumption. Similarly, a scientist who wants to understand the process of photosynthesis will use simplified descriptions of a plant focusing on very specific processes within a single plant cell. Anyone who wants to understand complex systems or solve problems related to complex systems needs to apply appropriate simplified descriptions of the system under consideration. This means that anyone who is concerned with complex systems needs models, since simplified descriptions of a system are models of that system by definition.

Note 1.1.2 (Role of models) To break up the complexity of a system under consideration, engineers and scientists use simplified descriptions of that system (i.e. models).

1.2 Systems, Models, Simulations

In 1965, Minsky gave the following general definition of a model [1, 2]:

Definition 1.2.1 (Model) To an observer B, an object A* is a *model* of an object A to the extent that B can use A* to answer questions that interest him about A.

Note 1.2.1 (Formal definitions) Note that Definition 1.2.1 is a *formal definition* in the sense that it operates with terms such as *object* or *observer* that are not defined in a strict axiomatic sense similar to the terms used in the definitions of standard mathematical theory. The same remark applies to several other definitions in this book, including the definition of the term *mathematical model* in Section 1.4. Definitions of this kind are justified for practical reasons, since they allow us to talk about the formally defined terms in a concise way. An example is Definition 2.5.2 in Section 2.5.5, a concise formal definition of the term *overfitting*, which uses several of the previous formal definitions.

The application of Definition 1.2.1 to the car example is obvious – we just have to identify B with the car driver, A with the car itself, and A* with the simplified tank/battery description of the car in Figure 1.1.

1.2.1 Teleological Nature of Modeling and Simulation

An important aspect of the above definition is the fact that it includes the purpose of a model, namely, that the model helps us to answer questions and to solve problems. This is important because particularly beginners in the field of modeling tend to believe that a good model is one that mimics the part of reality that it pertains to as closely as possible. But as was explained in the previous section, modeling and simulation aims at simplification, rather than at a useless production of complex copies of a complex reality, and hence, the contrary is true:

Note 1.2.2 (The best model) The best model is the simplest model that still serves its purpose, that is, which is still complex enough to help us understand a system and to solve problems. Seen in terms of a simple model, the complexity of a complex system will no longer obstruct our view, and we will virtually be able to look through the complexity of the system at the heart of things.

The entire procedure of modeling and simulation is governed by its purpose of problem solving – otherwise it would be a mere l'art pour l'art. As [3] puts it, "modeling and simulation is always goal-driven, that is, we should know the purpose of our potential model before we sit down to create it". It is hence natural to define fundamental concepts such as the term *model* with a special emphasis on the purpose-oriented or *teleological nature of modeling and simulation*. (Note that teleology is a philosophical discipline dealing with aims and purposes, and the term *teleology* itself originates from the Greek word *telos*, which means end or purpose [4].) Similar teleological definitions of other fundamental terms, such as *system*, *simulation*, and *mathematical model* are given below.

1.2.2 Modeling and Simulation Scheme

Conceptually, the investigation of complex systems using models can be divided into the following steps:

Note 1.2.3 (Modeling and simulation scheme)

Definitions
- Definition of a problem that is to be solved or of a question that is to be answered
- Definition of a system, that is, a part of reality that pertains to this problem or question

Systems Analysis
- Identification of parts of the system that are relevant for the problem or question

Modeling
- Development of a model of the system based on the results of the systems analysis step

Simulation
- Application of the model to the problem or question
- Derivation of a strategy to solve the problem or answer the question

Validation
- Does the strategy derived in the simulation step solve the problem or answer the question for the real system?

The application of this scheme to the examples discussed above is obvious: in the *car example*, the problem is that the car does not start and the car itself is the system. This is the "definitions" step of the above scheme. The "systems analysis" step identifies the battery and fuels levels as the relevant parts of the system as explained above. Then, in the "modeling" step of the scheme, a model consisting of a battery and a tank such as in Figure 1.1 is developed. The application of this model to the given problem in the "simulation" step of the scheme then leads to the strategy "check battery and fuel level". This strategy can then be applied to the real car in the "validation" step. If it works, that is, if the car really starts after refilling its battery or tank, we say that the model is valid or validated. If not, we probably need a mechanic who will then look at other parts of the car, that is, who will apply more complex models of the car until the problem is solved.

In a real modeling and simulation project, the *systems analysis step* of the above scheme can be a very time-consuming step. It will usually involve a thorough evaluation of the literature. In many cases, the literature evaluation will show