Kai Velten

Mathematical Modeling and Simulation

Introduction for Scientists and Engineers

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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 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*

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 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 that similar investigations have been performed in the past, and one should of course try to profit from the experiences made by others that are described in the literature. Beyond this, the system analysis step usually involves a lot of discussions and meetings that bring together people from different disciplines who can answer your questions regarding the system. These discussion will usually show that new data are needed for a better understanding of the system and for the validation of the models in the validation step of the above scheme. Hence, the definition of an experimental program is also another typical part of the systems analysis step.

The *modeling step* will also involve the identification of appropriate software that can solve the equations of the mathematical model. In many cases, it will be possible to use standard software such as the software tools discussed in the next chapters. Beyond this, it may be necessary to write your own software in cases where the mathematical model involves nonstandard equations. An example of this case is the modeling of the press section of paper machines, which involves highly convection-dominated diffusion equations that cannot be treated by standard software with sufficient precision, and which hence need specifically tailored numerical software [5].

In the *validation step*, the model results will be compared with experimental data. These data may come from the literature, or from experiments that have been specifically designed to validate the model. Usually, a model is required to fit the data not only quantitatively, but also qualitatively in the sense that it reproduces the general shape of the data as closely as possible. See Section 3.2.3.4 for an example of a qualitative misfit between a model and data. But, of course, even a model that perfectly fits the data quantitatively and qualitatively may fail the validation step of the above scheme if it cannot be used to solve the problem that is to be solved, which is the most important criterion for a successful validation.

The modeling and simulation scheme (Note 1.2.3) focuses on the essential steps of modeling and simulation, giving a rather simplified picture of what really happens in a concrete modeling and simulation project. For different fields of application, you may find a number of more sophisticated descriptions of the modeling and simulation process in books such as [6–9]. An important thing that you should note is that a real modeling and simulation project will very rarely go straight through the steps of the above scheme; rather, there will be a lot of interaction between the individual steps of the scheme. For example, if the validation step fails, this will bring you back to one of the earlier steps in a *loop-like structure*: you may then improve your model formulation, reanalyze the system, or even redefine your problem formulation (if your original problem formulation turns out to be unrealistic).

Note 1.2.4 (Start with simple models!) To find the best model in the sense of Note 1.2.2, start with the simplest possible model and then generate a sequence of increasingly complex model formulations until the last model in the sequence passes the validation step.

1.2.3 Simulation

So far we have given a definition of the term *model* only. The above modeling and simulation schemes involve other terms, such as *system* and *simulation*, which we may view as being implicitly defined by their role in the above scheme. Can this be made more precise? In the literature, you will find a number of different definitions, for example of the term *simulation*. These differences can be explained by different interests of the authors. For example, in a book with a focus on the so-called *discrete event simulation* which emphasizes the development of a system over time, simulation is defined as "the imitation of the operation of a real-world process or system over time" [6]. In general terms, simulation can be defined as follows:

Definition 1.2.2 (Simulation) *Simulation* is the application of a model with the objective to derive strategies that help solve a problem or answer a question pertaining to a system.

Note that the term *simulation* originates from the Latin word "simulare", which means "to pretend": in a simulation, the model pretends to be the real system. A similar definition has been given by Fritzson [7] who defined simulation as "an experiment performed on a model". Beyond this, the above definition is a *teleological* (purpose-oriented) definition similar to Definition 1.2.1 above, that is, this definition again emphasizes the fact that simulation is always used to achieve some goal. Although Fritzson's definition is more general, the above definition reflects the real use of simulation in science and engineering more closely.

1.2.4 System

Regarding the term *system*, you will again find a number of different definitions in the literature, and again some of the differences between these definitions can be explained by the different interests of their authors. For example, [10] defines a system to be "a collection of entities, for example, people or machines, that act and interact together toward the accomplishment of some logical end". According to [11], a system is "a collection of objects and relations between objects". In the context of mathematical models, we believe it makes sense to think of a "system" in very general terms. Any kind of object can serve as a system here if we have a question relating to that object and if this question can be answered using mathematics. Our view of systems is similar to a definition that has been given by [12] (see also the discussion of this definition in [3]): " A system is whatever is distinguished as a system." [3] gave another definition of a "system" very close to our view of systems here: "A system is a potential source of data". This definition emphasizes the fact that a system can be of scientific interest only if there is some communication between the system and the outside world, as it will be discussed below in Section 1.3.1. A definition that includes the teleological principle discussed above has been given by Fritzson [7] as follows:

Definition 1.2.3 (System) A *system* is an object or a collection of objects whose properties we want to study.

1.2.5 Conceptual and Physical Models

The model used in the car example is something that exists in our minds only. We can write it down on a paper in a few sentences and/or sketches, but it does not have any physical reality. Models of this kind are called *conceptual models* [11]. Conceptual models are used by each of us to solve everyday problems such as the car that refuses to start. As K.R. Popper puts it, ‘‘all life is problem solving’’, and conceptual models provide us with an important tool to solve our everyday problems [13]. They are also applied by engineers or scientists to simple problems or questions similar to the car example. If their problem or question is complex enough, however, they rely on experiments, and this leads us to other types of models. To see this, let us use the modeling and simulation scheme (Note 1.2.3) to describe a possible procedure followed by an engineer who wants to reduce the fuel consumption of an engine: In this case, the problem is the reduction of fuel consumption and the system is the engine. Assume that the systems analysis leads the engineer to the conclusion that the fuel injection pump needs to be optimized. Typically, the engineer will then create some experimental setting where he can study the details of the fuel injection process.

Such an experimental setting is then a model in the sense that it will typically be a very simplified version of that engine, that is, it will typically involve only a few parts of the engine that are closely connected with the fuel injection process. In contrast to a conceptual model, however, it is not only an idea in our mind but also a real part of the physical world, and this is why models of this kind are called *physical models* [11]. The engineer will then use the physical model of the fuel injection process to derive strategies – for example, a new construction of the fuel injection pump – to reduce the engine’s fuel consumption, which is the simulation step of the above modeling and simulation scheme. Afterwards, in the validation step of the scheme, the potential of these new constructions to reduce fuel consumption will be tested in the engine itself, that is, in the real system. Physical models are applied by scientists in a similar way. For example, let us think of a scientist who wants to understand the photosynthesis process in plants. Similar to an engineer, the scientist will set up a simplified experimental setting – which might be some container with a plant cell culture – in which he can easily observe and measure the important variables, such as CO_2, water, light, and so on. For the same reasons as above, anything like this is a physical model. As before, any conclusion drawn from such a physical model corresponds to the simulation step of the above scheme, and the conclusions need to be validated by data obtained from the real system, that is, data obtained from real plants in this case.

1.3
Mathematics as a Natural Modeling Language

1.3.1
Input–Output Systems

Any system that is investigated in science or engineering must be observable in the sense that it produces some kind of output that can be measured (a system that would not satisfy this minimum requirement would have to be treated by theologians rather than by scientists or engineers). Note that this observability condition can also be satisfied by systems where nothing can be measured directly, such as black holes, which produce measurable gravitational effects in their surroundings. Most systems investigated in engineering or science do also accept some kind of input data, which can then be studied in relation to the output of the system (Figure 1.2a). For example, a scientist who wants to understand photosynthesis will probably construct experiments where the carbohydrate production of a plant is measured at various levels of light, CO_2, water supply, and so on. In this case, the plant cell is the system; the light, CO_2, and water levels are the input quantities; and the measured carbohydrate production is the output quantity. Or, an engineer who wants to optimize a fuel injection pump will probably change the construction of that pump in various ways and then measure the fuel consumption resulting from these modified constructions. In this case, the fuel injection pump is the system, the construction parameters changed by the engineer are the input parameters and the resulting fuel consumption is the output quantity.

Note 1.3.1 (Input–output systems) Scientists or engineers investigate "input–output systems", which transform given input parameters into output parameters.

Note that there are of course situations where scientists are looking at the system itself and not at its input–output relations, for example when a botanist just wants

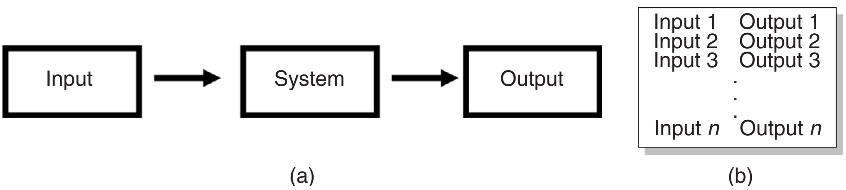

Fig. 1.2 (a) Communication of a system with the outside world. (b) General form of an experimental data set.

to describe and classify the anatomy of a newly discovered plant. Typically, however, such purely descriptive studies raise questions about the way in which the system works, and this is when input–output relations come into play. Engineers, on the other hand, are always concerned with input–output relations since they are concerned with technology. The Encyclopedia Britannica defines technology as "the application of scientific knowledge to the practical aims of human life". These "practical aims" will usually be expressible in terms of a system output, and the tuning of system input toward optimized system output is precisely what engineers typically do, and what is in fact the genuine task of engineering.

1.3.2
General Form of Experimental Data

The experimental procedure described above is used very generally in engineering and in the (empirical) sciences to understand, develop, or optimize systems. It is useful to think of it as a means to explore *black boxes*. At the beginning of an experimental study, the system under investigation is similar to such a "black box" in the sense that there is some uncertainty about the processes that happen inside the system when the input is transformed into the output. In an extreme case, the experimenter may know only that "something" happens inside the system which transforms input into output, that is, the system may be really a black box. Typically, however, the experimenter will have some hypotheses about the internal processes, which he wants to prove or disprove in the course of his study. That is, experimenters typically are concerned with systems as gray boxes which are located somewhere between black and white boxes (more details in Section 1.5).

Depending on the hypothesis that the experimenter wants to investigate, he confronts the system with appropriate input quantities, hoping that the outputs produced by the system will help prove or disprove his hypothesis. This is similar to a question-and-answer game: the experimenter poses questions to the system, which is the input, and the system answers to these questions in terms of measurable output quantities. The result is a data set of the general form shown in Figure 1.2b. In rare cases, particularly if one is concerned with very simple systems, the internal processes of the system may already be evident from the data set itself. Typically, however, this experimental question-and-answer game is similar to the questioning of an oracle: we know there is some information about the system in the data set, but it depends on the application of appropriate ideas and methods if one wants to uncover the information content of the data and, so to speak, shed some light into the black box.

1.3.3
Distinguished Role of Numerical Data

Now what is an appropriate method for the analysis of experimental datasets? To answer this question, it is important to note that in most cases experimental data are numbers and can be quantified. The input and output data of Figure 1.2b will typically consist of columns of numbers. Hence, it is natural to think of a system in mathematical terms. In fact, a system can be naturally seen as a mathematical function, which maps given input quantities x into output quantities $y = f(x)$ (Figure 1.2a). This means that if one wants to understand the internal mechanics of a system ''black box'', that is, if one wants to understand the processes inside the real system that transform input into output, a natural thing to do is to translate all these processes into mathematical operations. If this is done, one arrives at a simplified representation of the real system in mathematical terms. Now remember that a simplified description of a real system (along with a problem we want to solve) is a model by definition (Definition 1.2.1). The representation of a real system in mathematical terms is thus a mathematical model of that system.

Note 1.3.2 (Naturalness of mathematical models) Input–output systems usually generate numerical (or quantifiable) data that can be described naturally in mathematical terms.

This simple idea, that is, the mapping of the internal mechanics of real systems into mathematical operations, has proved to be extremely fruitful to the understanding, optimization, or development of systems in science and engineering. The tremendous success of this idea can only be explained by the naturalness of this approach – mathematical modeling is simply the best and most natural thing one can do if one is concerned with scientific or engineering problems. Looking back at Figure 1.2a, it is evident that mathematical structures emanate from the very heart of science and engineering. Anyone concerned with systems and their input–output relations is also concerned with mathematical problems – regardless of whether he likes it or not and regardless of whether he treats the system appropriately using mathematical models or not. The success of his work, however, depends very much on the appropriate use of mathematical models.

1.4 Definition of Mathematical Models

To understand mathematical models, let us start with a general definition. Many different definitions of mathematical models can be found in the literature. The differences between these definitions can usually be explained by the different scientific interests of their authors. For example, Bellomo and Preziosi [14] define a mathematical model to be a set of equations which can be used to compute the time-space evolution of a physical system. Although this definition suffices for the problems treated by Bellomo and Preziosi, it is obvious that it excludes a great number of mathematical models. For example, many economical or sociological problems cannot be treated in a time-space framework or based on equations only. Thus, a more general definition of mathematical models is needed if one wants to cover all kinds of mathematical models used in science and engineering. Let us start with the following attempt of a definition:

A mathematical model is a set of mathematical statements $M = \{\Sigma_1, \Sigma_2, \ldots, \Sigma_n\}$.

Certainly, this definition covers all kinds of mathematical models used in science and engineering as required. But there is a problem with this definition. For example, a simple mathematical statement such as $f(x) = e^x$ would be a mathematical model in the sense of this definition. In the sense of Minsky's definition of a model (Definition 1.2.1), however, such a statement is not a model as long as it lacks any connection with some system and with a question we have relating to that system. The above attempt of a definition is incomplete since it pertains to the word "mathematical" of "mathematical model" only, without any reference to purposes or goals. Following the philosophy of the teleological definitions of the terms *model*, *simulation*, and *system* in Section 1.2, let us define instead:

Definition 1.4.1 (Mathematical Model) A mathematical model is a triplet (S, Q, M) where S is a system, Q is a question relating to S, and M is a set of mathematical statements $M = \{\Sigma_1, \Sigma_2, \ldots, \Sigma_n\}$ which can be used to answer Q.

Note that this is again a formal definition in the sense of Note 1.2.1 in Section 1.2. Again, it is justified by the mere fact that it helps us to understand the nature of mathematical models, and that it allows us to talk about mathematical models in a concise way. A similar definition was given by Bender [15]: "A mathematical model is an abstract, simplified, mathematical construct related to a part of reality and created for a particular purpose." Note that Definition 1.4.1 is not restricted to physical systems. It covers psychological models as well that may deal with essentially metaphysical quantities, such as thoughts, intentions, feelings, and so on. Even mathematics itself is covered by the above definition. Suppose, for example, that S is the set of natural numbers and our question Q relating to S is whether there are infinitely many prime numbers or not. Then, a set (S, Q, M) is a mathematical model in the sense of Definition 1.4.1 if M contains the statement "There are infinitely many prime numbers" along with other statements which prove this statement. In this sense, the entire mathematical theory can be viewed as a collection of mathematical models.

The notation (S, Q, M) in Definition 1.4.1 emphasizes the chronological order in which the constituents of a mathematical model usually appear. Typically, a system is given first, then there is a question regarding that system, and only then a mathematical model is developed. Each of the constituents of the triplet (S, Q, M) is an indispensable part of the whole. Regarding M, this is obvious, but S and Q are important as well. Without S, we would not be able to formulate a question Q; without a question Q, there would be virtually "nothing to do" for the mathematical model; and without S and Q, the remaining M would be no more than "l'art pour l'art''. The formula $f(x) = e^x$, for example, is such a purely mathematical ''l'art pour l'art'' statement as long as we do not connect it with a system and a question. It becomes a mathematical model only when we define a system S and a question Q relating to it. For example, viewed as an expression of the exponential growth period of plants (Section 3.10.4), $f(x) = e^x$ is a mathematical model which can be used to answer questions regarding plant growth. One can say it is a genuine property of mathematical models to be more than ''l'art pour l'art'', and this is exactly the intention behind the notation (S, Q, M) in Definition 2.3.1. Note that the definition of mathematical models by Bellomo and Preziosi [14] discussed above appears as a special case of Definition 1.4.1 if we restrict S to physical systems, M to equations, and only allow questions Q which refer to the space-time evolution of S.

Note 1.4.1 (More than ''l'art pour l'art'') The system and the question relating to the system are indispensable parts of a mathematical model. It is a genuine property of mathematical models to be more than mathematical ''l'art pour l'art''.

Let us look at another famous example that shows the importance of Q. Suppose we want to predict the behavior of some mechanical system S. Then the appropriate mathematical model depends on the problem we want to solve, that is, on the question Q. If Q is asking for the behavior of S at moderate velocities, classical (Newtonian) mechanics can be used, that is, $M = \{$*equations of Newtonian mechanics*$\}$. If, on the other hand, Q is asking for the behavior of S at velocities close to the speed of light, then we have to set $M = \{$*equations of relativistic mechanics*$\}$ instead.

1.5 Examples and Some More Definitions

Generally speaking, one can say we are concerned with mathematical models in the sense of Definition 1.4.1 whenever we perform computations in our everyday life, or whenever we apply the mathematics we have learned in schools and universities. Since everybody computes in his everyday life, everybody uses mathematical models, and this is why it was valid to say that ''everyone models and simulates'' in the preface of this book. Let us look at a few examples of mathematical models now, which will lead us to the definitions of some further important concepts.

Note 1.5.1 (Everyone models and simulates) Mathematical models in the sense of Definition 1.4.1 appear whenever we perform computations in our everyday life.

Suppose we want to know the *mean age of some group of people*. Then, we apply a mathematical model (S, Q, M) where S is that group of people, Q asks for their mean age, and M is the mean value formula $\overline{x} = \left(\sum_{i=1}^{n} x_i\right)/n$. Or, suppose we want to know the mass X of some substance in the cylindrical tank of Figure 1.3, given

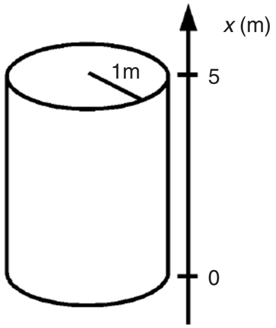

Fig. 1.3 Tank problem.

a constant concentration c of the substance in that tank. Then, a multiplication of the tank volume with c gives the mass X of the substance, that is,

$$X = 5\pi c \tag{1.1}$$

This means we apply a model (S, Q, M) where S is the tank, Q asks for the mass of the substance, and M is Equation 1.1. An example involving more than simple algebraic operations is obtained if we assume that the *concentration c in the tank* of Figure 1.3 depends on the height coordinate, x. In that case, Equation 1.1 turns into

$$X = \pi \cdot \int_0^5 c(x)\, dx \tag{1.2}$$

This involves an integral, that is, we have entered the realms of calculus now.

Note 1.5.2 (Notational convention) Variables such as X and c in Equation 1.1, which are used without further specification are always assumed to be real numbers, and functions such as $c(x)$ in Equation 1.2 are always assumed to be real functions with suitable ranges and domains of definition (such as $c : [0, 5] \to \mathbb{R}_+$ in the above example) unless otherwise stated.

In many mathematical models (S, Q, M) involving calculus, the question Q asks for the optimization of some quantity. Suppose for example we want to *minimize the material consumption* of a cylindrical tin having a volume of 1 l. In this case,

$$M = \{\pi r^2 h = 1, A = 2\pi r^2 + 2\pi r h \to \min\} \tag{1.3}$$

can be used to solve the problem. Denoting by r and h the radius and height of the tin, the first statement in Equation 1.3 expresses the fact that the tin volume is 1 l. The second statement requires the surface area of the tin to be minimal, which is equivalent to a minimization of the metal used to build the tin. The mathematical