

# Preface

In many areas in the sciences, in particular the natural and engineering sciences, modeling and simulation have established themselves as a third pillar supporting the acquisition of knowledge: Previously, the understanding, prediction, or optimization of the behavior of processes and systems had to be based on either experiments or theoretical analyses. Today, however, we are offered the elegant possibility of conducting “experiments on the computer.” Completely new fields have been developed—either in terms of specializations within classical fields or as independent fields on the interface of existing ones. They all live on the cross-disciplinary interaction between efficient methods (mostly from mathematics or computer science) with exciting application fields and models that are not at all restricted to the natural and engineering sciences, for example, financial mathematics. To this end, the naming convention that we use nowadays suggests the slight differences in emphases: “Scientific Computing” stresses mathematical (in particular numerical) aspects, whereas “High-Performance Computing (HPC)” and “Advanced Computing” both stress computer science aspects. In the former case, HPC, the focus is given to supercomputers, while Advanced Computing is based on an integrative approach to include algorithms, computers, data, and software. Nomenclature such as “Computational Sciences,” “Computational Science and Engineering,” or “Computational Engineering,” on the other hand, indicates that the main interest lies within the subject of simulation.

Despite both the wide spectrum of application areas and the high bandwidth of employed methods—analytical and approximate, numerical and discrete, deterministic and stochastic, originating from mathematics (differential equations, etc.) or from computer science (fuzzy logic, Petri nets, etc.)—modeling and simulation are based on a consistent, systematic approach that is recognized ever more frequently in the relevant courses. In fact, this current book resulted from lecture notes from courses in “Foundations of modeling and simulation” and “Modeling and simulation,” resp., taught by the first two authors several times at the Universität Stuttgart and the Technische Universität München. While primarily tied in with the computer science curriculum, both courses also address students of mathematics as well as students in the technical or natural sciences. It is quite typical, even

inevitable, for each student to be somewhat familiar with the material while simultaneously being embraced with something new.

Because our interest is in modeling and simulation as a systematic approach, material that is supposedly familiar will be presented in a new light while previously hidden connections will be revealed and the eye will be trained to recognize not only the particular solution approach but also the underlying systematic approach—an essential intention of this book. In this context and of major importance: Our goal is not to provide an introduction to the basic use of existing tools, however widespread and powerful they may be, but rather to provide a point of entry into the exciting world of building better tools.

Considering the complexity of the topic it would be absurd to claim, or even to expect, a complete treatment in either breadth or depth. Therefore, while this book touches on some very interesting and relevant applications that differ quite a bit with respect to the methodical approach taken, the selection of topics naturally reflects the personal preferences and experiences of the authors. But then the fundamental similarities existing between the different approaches will be highlighted since these often remain invisible if the topic of modeling and simulation is approached through only a single application domain. The simulation pipeline, beginning with the derivation of the model up to its validation, is a prominent example. Consequent to this and part of the maxim of this book is the repeated concern regarding “a little bit of everything, but nothing in detail” that can be levied against such courses or book concepts. This book is about a first encounter with models and simulations, about gaining an impression of the diversity of tools employed from mathematics and computer science, and about the diversity of problem settings. We will discuss fluid dynamics, but we cannot nor would we want to provide the same level of detail given in a book on computational fluid dynamics; we will mention numerical techniques without listing all of their variants and discussing all of their properties as it is expected from a book on numerical analysis; and all scenarios will be greatly simplified, which typically results in models that are a bit less connected to reality.

We do not want to train the readers of this book to become specialists in individual topics, but rather provide an overview to students in computer science, mathematics, or the natural or engineering sciences—and of course increase their appetite for more.

A further challenge is the balance between modeling and simulation—here to be taken in the more literal meaning of the word, i.e., the part implying the calculation or solution of the models. For example, we will discuss models without losing track of their origins and the goals of the modeling—the simulation. Conversely, we will discuss numerical methods without the models appearing out of the blue.

It is our opinion that a concentration on breadth as well as the dovetailing of connections is very important, even if it is reached at the expense of depth in the individual topics—however, this book is neither exclusively on mathematical modeling nor exclusively on numerical analysis.

There are at least two different possibilities for the structure of this book. One may organize the material based on the employed methodology which would, for example, lead to chapters on models with graphs, models with ordinary differential

equations, or models with partial differential equations. The advantage is methodical rigor. However, certain topics such as traffic simulation would appear multiple times which hinders a comparative consideration and evaluation of alternative approaches.

Such a disadvantage is avoided if the material is organized by subject areas in which one models and simulates—by comparison, this has the effect of turning the above advantages into disadvantages and vice versa. We decided for the second alternative after considering that the resulting structure would be more plausible and attractive especially to the beginner. Furthermore, the important message concerning the existence of more than one possible model and more than one applicable apparatus from mathematics or computer science might be delivered better through the second approach.

Chapter 1 provides an introduction into the topics of modeling and simulation. It begins with a presentation of the simulation pipeline and the simulation cycle, resp. Next, we discuss general questions concerning mathematical models—e.g., concerning their derivation, analysis of their properties, existence and uniqueness of solutions, model hierarchies and model reduction—and the transition into a simulation process. Chapter 2 concisely provides the methodical tools that are subsequently required from the various areas of mathematics and computer science. Once more we have to choose one out of the several possible strategies—ranging from the uncompromising (and room saving) “this and that is all assumed to be known” approach up to the caring (and exceeding the scope of any textbook) “all that is needed will be explained” approach. We opted for a compromise: a brief summary of elementary mathematics, discrete mathematics, linear algebra, analysis, stochastics, statistics, and numerics. Hence, all the essentials are included, however, not in epic breadth. Most of the topics should, in more or less detail, be material of the introductory or bachelor level courses in the respective fields of study. However, we will provide numerous references so that possible gaps can be filled efficiently. To facilitate the classification and to support a selective reading of this book, we will always begin the application scenarios with explicit links to the required tools.

The subsequent chapters are grouped by topics into four parts and treat different areas exemplarily in which models and model-based simulation are employed to a large extent.

Part I is devoted to the topic “Gaming—deciding—planning.” Here, we discuss problem settings in the areas of game theory (Chap. 3), decision theory (Chap. 4), scheduling (Chap. 5), as well as mathematical finance (Chap. 6).

Part II covers modeling and simulation in the area of the transportation system—an area which is well suited to illustrate the diversities of problem settings, approaches, and employed tools. Here, we first introduce a macroscopic simulation of road traffic using simple models based on differential equations (Chap. 7). In contrast, the classical microscopic approach is based on cellular automata (Chap. 8). A completely different approach is offered in stochastic traffic simulation in which queuing systems provide the central descriptive tool (Chap. 9).

Part III treats scenarios from the wide field of dynamical systems. The first respective insight is given by the classic topic of population dynamics (Chap. 10). Control engineering will serve as an example to cover the conventional approaches

for the control of technical systems, e.g., multibody systems or fuzzy control systems (Chap. 11). This part is concluded by a brief excursion into the world of chaos (Chap. 12).

Part IV, the final part, discusses topics with a strong connection to physics—topics which typically lead to computationally intense simulations and thus are closely linked to high-performance computers. We will discuss molecular dynamics as the representative from particle methods (Chap. 13) and then continue with two representatives from models based on partial differential equations, namely heat conduction (Chap. 14) and fluid dynamics (Chap. 15). The concluding scenario, the modeling and calculation of realistic global illumination, illustrates the use of physically motivated models and simulation in computer science, or more precisely, in computer graphics (Chap. 16).

As mentioned before, this book is also suited for a selective treatment in courses or for selective self-study of topics of interest. Combined with the introductory Chap. 1 as well as the respective prerequisites of Chap. 2, each part presents a self-contained unit and can be studied as such or covered in a class, resp.

As always, quite a few have contributed to this book. We owe special thanks to our colleagues in the department—for critical comments, helpful hints, and some of the figures—as well as to the students of the previously mentioned courses who naturally contributed through their questions and comments to this final version of the book.

Last but not least, we have the pleasure to see the end product of an endeavor that gives us the English edition of our book. The translation was worked in parallel with, and is the counterpart of, the second edition that is in German. As with any production of scale, there are many helping hands that have our gratitude: This book was the idea of Dr. Martin Peters from Springer and it was his enthusiasm that convinced us to begin the project. Once started, it was the Springer team that provided the foundation for a successful partnership. But, perhaps most important for a translated work are the translators—we are deeply grateful to Professor Sabine Le Borne (Hamburg University of Technology) and Professor Richard Le Borne (Tennessee Technological University). They managed to preserve our style which is characterized through our attempt to never become too dry and sterile even when immersed in a topic that might appear as such.

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Stuttgart, Germany  
Munich, Germany  
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H.-J. Bungartz  
S. Zimmer, D. Pflüger  
M. Buchholz

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Bungartz, H.-J.; Zimmer, S.; Buchholz, M.; Pflüger, D.

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