# Introduction to Mathematical Modeling and Computer Simulations

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CRC Press
Taylor & Francis Group
Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an **informa** business
A CHAPMAN & HALL BOOK

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742



Printed on acid-free paper
Version Date: 20180112

International Standard Book Number-13: 978-1-138-19765-7 (Hardback)



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# *Preface*

*"Philosophy is written in that great book which ever lies before our eyes - I mean the universe - but we cannot understand it if we do not first learn the language and grasp the symbols, in which it is written. This book is written in the mathematical language, and the symbols are triangles, circles and other geometrical figures, without whose help it is impossible to comprehend a single word of it; without which one wanders in vain through a dark labyrinth"*

Galileo Galilei

To learn or not to learn mathematics? Such Shakespearean questions are posed by engineers. Perhaps, to learn linear algebraic systems for numerical methods but rather not to learn advanced integrals because they can be calculated by computer. A mathematician can pay too much attention to existence of the integral. For an engineer, the existence of the integral means for instance, existence of the mass of a given body. One can imagine the engineer's opinion about a mathematician who discusses an object without mass. An engineer can think that "a mathematician discusses strange surface integrals instead of the integrals needed to calculate the heat flux through the surfaces". However, it turns out that the engineer is interested in the same integrals[1]. Now, one can imagine what a mathematician thinks about an engineer. This book is written, in particular, to avoid such misleading declarations from both sides.

Development of new technologies, new materials and technological objects requires theoretical mathematical descriptions of new objects and study of their behavior. Engineers then have to make frequently expensive and long experiments, which are sometimes dangerous. It is possible to gather a small set of a data and further to extend the results by the use of Mathematical Modeling. So, mathematical and computer calculations can be considered as a continuation of the physical experiments[2]. Consider, for instance, creation of new composites. Let an engineer note that a new substance added to a material makes it better for certain purposes. A problem of describing this phenomenon then arises. Does the temperature impact on new material? What is the optimal concentration of the admixture? Many answers can be obtained not by hard experimental works, but by Mathematical Modeling. Let a new composite consist of 10 different substances which can be embedded in

[1] it is a true story

[2] V.I. Arnold [8]: "Mathematics is the part of physics where experiments are cheap."

material with various concentrations. In order to optimize the properties of the composite let an engineer try the concentrations 7%, 10% and 13% of each component. Then the experimental problem to determine the optimal composite is reduced to the investigation of $3^9 = 19683$ samples. At the same time one can use the known formulae for the effective properties and quickly obtain the results.

This textbook is intended for readers who want to understand the main principles of Modeling and Simulations in settings that are important for the applications without using profound mathematical tools required by most advanced texts. It can be useful for beginning applied mathematicians and engineers who use Mathematical Modeling. Our goal is to outline Mathematical Modeling using simple mathematical description that make it accessible for first- and second-year students (undergraduate courses for bachelor's degrees). This book consists of three parts. Part I "General Principles and Methods" is an elementary introduction to Mathematical Modeling based on the introductory mathematical courses. We think that this is the main part which should be worked out by a beginner in Applied Mathematics and other sciences addressed to Mathematical Modeling. There are general principles, methods and tricks of Mathematical Modeling used in different sciences. For instance, it is useful to introduce a linear operator in general form and later to describe linear models of econometrics. The didactic principle of primary introduction of examples and further of a theory narrows down applications of Mathematical Modeling. In this book, the linear operator is not rigorously introduced in a general space but it is outlined for further applications. In econometrics, it is better first to study the Method of Least Squares as minimizing a quadratic function and after to learn economical terms. In engineering, first it is preferable to study the vector calculus and after to describe topics from fluid and solid mechanics. Such an approach facilitates understanding special topics. Universality of Mathematical Modeling and the corresponding equations helps to understand such formally different phenomena as the behavior of solids and liquids for engineers, credit and debit for economists, etc.

Part II contains the fundamental mathematical methods and examples used in Mathematical Modeling. Parts I and II are written in such a simple form that it can be presented to second-year students at the undergraduate level familiar with calculus and elementary ordinary differential equations. I suppose that Parts I and II can be considered as an introductory course to general problems of Mathematical Modeling, in particular, to Industrial Mathematics. Other examples from engineering, economics, computer sciences, biology are widely presented in the books [3], [13], [31], [32], [33], [38], [39], [40], [43], [48], [49], [61].

Part III concerns vector calculus. The main attention is paid to computer implementation of the main calculus operators. Further, initial and boundary value problems are discussed for the heat equation. This part can be considered as an example of constructive methods applied to ordinary and partial differential equations suitable for students at the graduate level. There are many nice textbooks devoted to such problems [16], [31], [41], [52] where the fundamental mathematical methods such as separation of variables, discrete and integral transforms etc., can be combined with the computer approach presented here.

The main point of this book is thewide use of computer for numerical and symbolic computations, and for graphic presentations. We suggest using the computer while reading this book, especially the one with the package *Mathematica*® (see courses in the books [60, 56, 28, 30, 43, 27]). Other software packages can be used but special codes should be prepared then. One may read this book without using any computer code, but many features of Mathematical Modeling could be lost. So, it is better to pay one hour to *Mathematica* to apply at least simple operators and completely use the material presented in this book. Use of *Mathematica* is caused by its possibilities to apply symbolic computations. Frequently, methods of Applied Mathematics are reduced by users to numerical packages without addressing to the corresponding mathematical description that can lead to missing of the important features of the considered real-life problem. We use symbolic computations to demonstrate advanced possibilities of computer simulations. Other alternatives to *Mathematica* are available. We use also MATLAB and insert in the book MATLAB-boxes containing codes and necessary descriptions [19, 29].

Besides necessary formal theoretical presentation, we try to explain "how to do it" revealing secrets and tricks used in practical applications. Informal advice presented as "principles" facilitates understanding the interdisciplinary approaches applied to real-life problems. An important feature of this book is the inclusion of exercises considered as projects with computer implementation. A lot of interesting projects with codes are selected at *http:// demonstrations.wolfram.com/*. They can be also used for a course on Mathematical Modeling and Computer Simulations.

Partially, this book is based on the textbook [46] written in Polish (open access at *http://mityu.up.krakow.pl/publication/*).

Kraków, *Vladimir Mityushev, Natalia Rylko and Wojciech Nawalaniec*
December 2017