MATHEMATICAL MODELING WITH COMPUTERS

Samuel L.S. Jacoby
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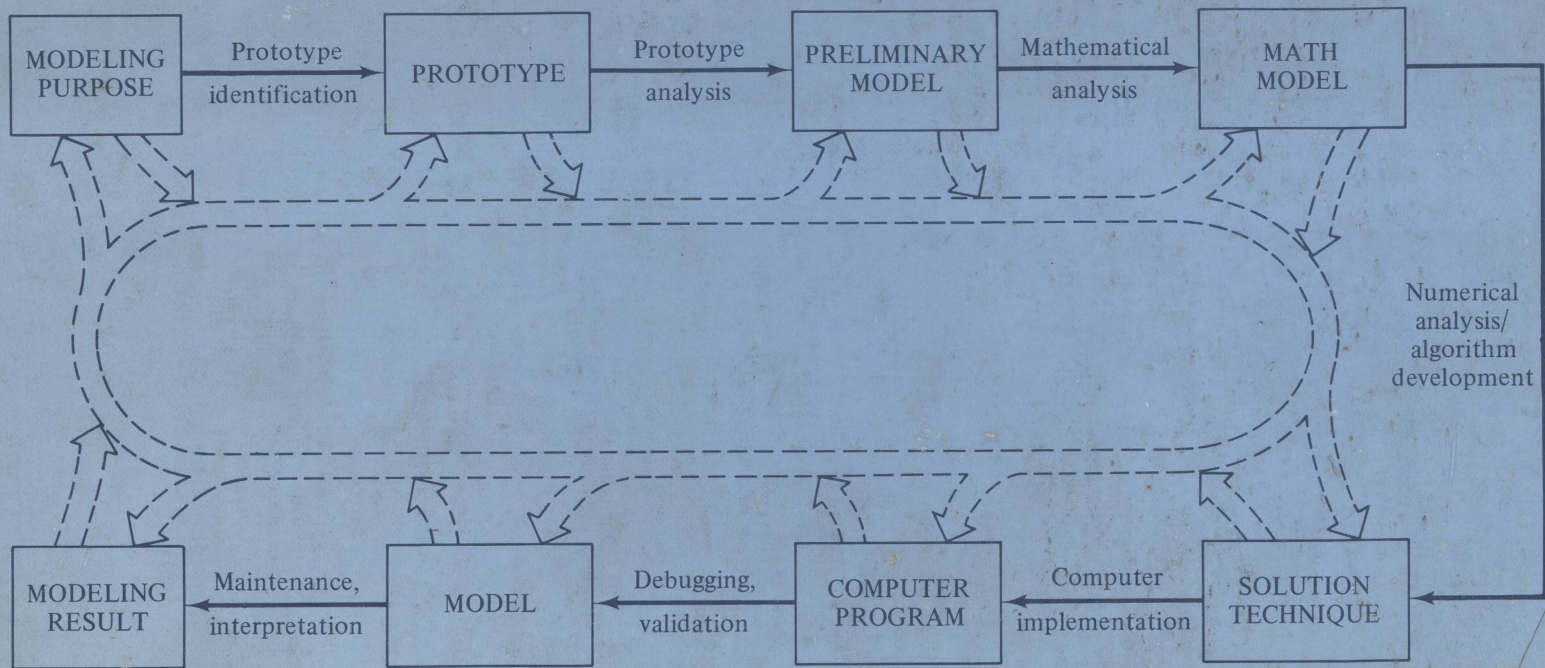

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Mathematical Modeling with Computers

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To our wives,
Michal Jacoby and Krystyna Kowalik

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Mathematical Modeling with Computers

Preface

A *mathematical model* is an approximate representation, in mathematical terms, of a concept, an object, a system, or a process. The model behaves, in some sense, like the prototype. We use the term *prototype* here to mean anything the model represents. Mathematical models are used by scientists, engineers, operations researchers, and managers to study the behavior and operation of many different prototypes. Mathematical modeling started as an aid in scientific research and in engineering design projects. More recently, interest has focused on modeling related to operations research, natural resources, and environmental and urban development studies. Today, medical, social, and economic problems are also being studied with the help of mathematical models. The use of mathematical models has expanded in parallel with the continuing development of computers and of computational techniques.

Existing modeling experience is described in hundreds of technical papers about particular modeling projects. Several of the model-building and modeling steps are discussed in papers and books on subjects such as numerical analysis and computer programming. There is however no general book that covers *all* the steps of mathematical model building and modeling with computers, and that provides guidance and tools for those engaged in these activities. The objective of this book is to serve this need.

The book is a guide for builders and users of computer-implemented mathematical models. It is structured according to the stages of the mathematical model-building and modeling process which include: prototype identification and statement of the modeling problem; mathematical model definition and analysis; mathematical problem analysis; reformulation and solution development; computer program design and development; and model validation, adjustment, and use. To focus the subject matter, we

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present brief surveys of types and purposes of models and of types and elements of mathematical models. In addition, necessary and sufficient conditions for mathematical model usefulness are proposed, explored, and related to the model-building stages.

The book spans the whole process of mathematical model building and modeling, starting with the modeling objective and prototype definition and concluding with modeling and interpretation of results. Topics are discussed in the order in which the steps are normally carried out. However, the depth of coverage is not uniform because more emphasis and details are given for subjects not covered elsewhere. For the subjects not treated in great detail in this book, the reader is referred to articles and books from which he can get the information he will need. Thus this book, supplemented by the readily available reference material, is intended to be a study of and handbook or guide for mathematical model building and modeling with digital computers.

Chapter 1 includes a brief introduction to modeling, in general, and to mathematical models, in particular. Types, purposes, and conditions for usefulness of models are described and a survey is given of types and elements of mathematical models. A final section includes a description of the stages of mathematical model building and modeling, starting with prototype and modeling purpose definition and concluding with interpretation of modeling results. The iterative nature of the model-building process is emphasized. Model-building project management considerations are also discussed.

The subject of Chapter 2 is the analytical stage of model building. The chapter starts with the methodology for the identification and definition of the prototype and the modeling objective and problem; then we discuss mathematical model definition and analysis of the modeling problem, and the development of a solution technique for this problem. The discussion is illustrated with three case studies: steady, two-dimensional flow, nonlinear network flow, and a large-scale nonlinear optimization of a complex system operation.

Chapter 3 is concerned with computer implementation of the model. In it we explain the systematic design and development of computer programs and their construction, testing, and maintenance as the modeler's working tool. The nonlinear network flow model developed in Chapter 2 is used in Chapter 3 to illustrate the basic steps of the method proposed for computer program design.

Chapter 4 includes a discussion of model validation and "fine tuning," its use for modeling and interpretation of modeling results. We consider how to best use the model and how to obtain the most effective and efficient modeling strategy. The discussion then turns to the relation between modeling output and prototype behavior. This includes interpretation of the modeling results and error analysis. As in the other chapters, this discussion is illustrated with examples.

The Appendix includes a discussion on the development and use of numerical simulation models. References to related literature are given in the Appendix, as well as in each chapter.

We have worked in mathematical modeling for almost two decades and have participated in many model building and modeling projects. In this book we have drawn on our experience to present the subject to students of modeling and to future model builders and users. It is hoped that the examples and methodology presented will be helpful to workers in the many different scientific and technological disciplines in which our readers may be interested and will make a contribution to the success of their modeling projects. To facilitate this, the book is as general as we could make it, with examples drawn from many areas. The level of presentation is geared to senior undergraduate or junior graduate students, or to practitioners with some background in applied mathematics and some computer experience. Teachers who use this book as a text are referred to an article by Bonder [1973] (see references at the end of Chapter 1), which discusses educational requirements and deficiencies in the area of modeling.

The approach recommended in this text and the examples used reflect our experience with the subject. This experience could not have been gained without the help and contribution of our colleagues at Boeing Computer Services. First and foremost of these is Mr. Claude R. Gagnon, our collaborator on the projects described in Sections 2.3 and 2.4. He also read the manuscript and provided many helpful comments and suggestions. Dr. H. Blair Burner prepared Chapter 3, "Computer Implementation of the Model." We wish to acknowledge also the patience and efficiency of Mrs. Roberta A. Gillespie, Mrs. Carmel M. Neibergs and Mrs. Lucille G. Wirak in preparing the typed manuscript. Many thanks go to the management of Boeing Computer Services for supporting our mathematical modeling activities and our writing of this book.

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Chapter 1

Introduction to Mathematical Modeling

1.1 INTRODUCTION

A *model* is an imitation or an approximate representation of a prototype. The term *prototype* is used here to mean a concept, an object, a system or a process. Model behavior is in some sense similar to that of the prototype. Model uses derive from this similarity. Models are used to study, plan, design, or to control the prototype. In most cases modeling reduces cost, risk, and flow time of these tasks. Frequently, modeling is the only way to accomplish these tasks because the prototype may be unavailable or unusable for this purpose. Models are used by artists, architects, engineers, designers, planners, operations researchers, economists, managers, scientists, and many others.

In a mathematical model the representation of the prototype is symbolic, in mathematical terms including variables, parameters, and relationships such as equations and inequalities. Mathematical models frequently have to be implemented on analog, digital, or hybrid computers to make possible the data handling and calculations involved in modeling studies. Generally then, mathematical model building or adaptation and computer implementation precedes mathematical modeling studies or experiments. This book is about building and using mathematical models on computers. This process starts with the prototype: a concept, an object, a system, or a process, and a set of questions about its behavior under certain, given conditions. The objective of the process is to build a model and to use it in modeling studies to answer these questions.

A great body of mathematical modeling experience has been accumulated in the last two decades. This experience is related to the development and increased use of computers. Much of the mathematical modeling effort during this period focused on problems of the physical sciences and engineering. Mathematical models of anything from a water distribution network to the human pancreas gland have been built and studied. More recently interest has shifted to biological, medical, natural and energy resources problems, and urban development (see Gold [1977] or Brewer [1973] for example). It is also becoming increasingly apparent that mathematical modeling has the potential to make a significant contribution to the understanding and the solution of social problems (e.g., Hawkes [1973]) and to behavioral science (e.g., Lehman [1977]). It appears that the experience gained in modeling of prototypes from the physical sciences and engineering will be applicable in modeling of other prototypes in the future. Currently we are indeed witnessing a substantial diffusion of mathematical modeling methods from the so-called hard sciences (such as physics and engineering) to the socio-economic and life sciences. Eventually, socio-economic and biological processes may be accurately described by quantitative models, making possible a better understanding of these very complex phenomena.

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Examples of books covering and/or illustrating certain aspects of mathematical model building and modeling include: Alexander and Bailey [1962], Andrews [1976], Bauer [1973], Bender [1978], Blackwell [1968], Dahl, et al. [1972], Emshoff and Sisson [1970], Furman [1972], Lehman [1977], Machol [1965], Smith [1968], Smith, et al. [1970], Vemuri [1978], Williams [1978], and Wolberg [1971].

The remainder of Chapter 1 introduces the reader to modeling and focuses on mathematical models. Section 1.2 is about types, purposes and conditions for usefulness of models. Section 1.3 contains a survey of types and elements of mathematical models. Section 1.4 includes a description of the process of model building, computer implementation and use. The stages of this process are justified in terms of conditions for model usefulness developed in Section 1.2.

1.2 TYPES, PURPOSES, AND USEFULNESS OF MODELS

"God created man in His image, in the image of God He created him" (Genesis 1:27). For Rabbi Shelomo Yitzhaki (Rashi), the famous 11th-century commentator, this attribution of a human image to God was unthinkable. His interpretation of the phrase "His image" was: "In the mold which was made for man . . . made in a mold like a coin which is stamped." The creator, one might say in modern terms, used a mold to make man, a mold which had been made especially for this purpose. All other creatures were created simply by divine command, whereas the creation of man is one of the first recorded uses of modeling. Modeling has been used ever since for many creative purposes.

Models may replace a phenomenon in an unfamiliar field by one in a field with which the model user is better acquainted. With models, phenomena can be simplified, relevant properties can be extracted, and effects can be scaled up or down in space or time, to obtain an appropriate level of detail and ease of modeling experimentation. Models enable one to carry out experiments under more favorable conditions than would be possible with the prototype. In many instances these experiments cannot be carried out with the prototype. In fact modeling can, and often does, proceed even when the prototype is only a preliminary concept or design. And in general, it frequently is simpler to study its behavior through a model. The effect of changes, for example, can be studied on the model without actually implementing these changes in the prototype. Theoretical models are useful in explaining phenomena and also as a basis for physical and mathematical models. In general, modeling facilitates the achievement of many different purposes at reduced cost, risk and flow time. Current uses of modeling include observation and explanation, planning, engineering design, planning and design optimization, performance analysis, operational control, and scientific research. Different types and purposes of models are further discussed in this section. Table 1.2.1 summarizes what prototype information is available and what information results from modeling for different purposes. Table 1.2.2 indicates which model types are suitable for different purposes.

Most models fall in one of the two broad categories of physical and symbolic models. A model is said to be a *physical* (or *material*) *model* whenever the modeling representation is physical and tangible, with model elements made of materials and hardware. Examples of physical models include iconic models, hardware scale models, and analog computer models. A model is said to be a *symbolic* (or *formal*) *model* whenever the modeling

Table 1.2.1 Prototype Information Available for and Resulting from Modeling

PROTOTYPE INFORMATION	MODELING PURPOSE					
	OBSERVATION AND EXPLANATION	PLANNING AND DESIGN	PLANNING AND DESIGN OPTIMIZATION	PERFORMANCE ANALYSIS	OPERATIONAL CONTROL	RESEARCH
Preliminary concept, design or plan	Available	Available	Available	Available	Available	Available
Well-defined system, object or process	Resulting	Available and resulting	Available and resulting	Available	Available	Resulting
Components, configuration and fixed parameters	Resulting	Available and resulting	Available and resulting	Available	Available	Resulting
Adjustable parameters	Resulting	Available and resulting	Resulting	Available	Resulting	Resulting
Environment, circumstances, operating conditions	Available	Available	Available	Available	Available	Available
Purpose mission, appearance, behavior, performance	Available and resulting	Available	Available	Resulting	Available	Available

Table 1.2.2 Types of Models and Their Suitability for Different Modeling Purposes

	MODEL TYPE	MODELING PURPOSE: OBSERVATION AND EXPLANATION	PLANNING AND DESIGN	PLANNING AND DESIGN OPTIMIZATION	PERFORMANCE ANALYSIS	OPERATIONAL CONTROL	RESEARCH
PHYSICAL	Iconic	×	×				
	Hardware: scale	×	×		×		×
	Hardware: analog	×	×		×	×	×
SYMBOLIC	Verbal/logical/drawing	×	×				
	Mathematical	×	×	×	×	×	×

representation is theoretical, or symbolic, with model elements consisting of a symbolic statement of certain structural or behavioral aspects of the prototype. Examples of symbolic models include drawings, verbalizations, logical and mathematical models and their digital computer implementations. We should remark at this point that the distinction between physical and symbolic models is not always clear. In reality symbolic models may use materials and hardware such as computers. Physical models, on the other hand, are frequently based on symbolic representations of the prototype. As an illustration of this, consider for example a set of mathematical relationships representing an engineering system which may be the basis for a physical scale model, an analog computer model (physical), or a digital computer model (symbolic).

Perhaps the simplest physical models are *iconic* models. They provide a visual representation of certain aspects of the prototype, but can be manipulated only in a limited fashion. Their use is therefore restricted mainly to static prototype studies such as architecture of buildings or sculptures. Other physical models constitute simplified representations of their prototypes, representations of those prototype properties which have been selected for study. Frequently the physical model performs the same function as the prototype in a scaled version. Such scaling can be up or down and in space, in material properties or in time.

Scale models constitute perhaps the largest class of physical models. Ship models used in towing tanks to study drag are an example of geometrically scaled models. Other fluid-flow models combine geometric and fluid property scaling. An example of time scaling in a model is the use of drosophila insects, whose reproductive cycle is short, to study heredity. Time scaling is not always possible. This is one of the major disadvantages of those physical models which perform the same, or similar, function as their prototype. Hardware scale models are frequently expensive to build and to use. They are not very flexible and therefore not suited to represent many aspects of the prototype and of its behavior. A hardware model of the fuel pipe network on an airplane, for example, cannot be subjected to all the forces and accelerations that its prototype may experience in real life. Scale models sometimes therefore represent a distorted operation of their prototype because of modeling law limitations. On the other hand, hardware scale models have many advantages including ease of communication and of validation of the modeling results, again primarily if they perform the same function as their prototype. In some cases (e.g., wind tunnel models), due to their small size and the relative expense and difficulty of other modeling approaches, the hardware scale models are the most cost-effective way to achieve the modeling purpose.

Hardware *analog* computer models constitute another large class of physical models, used for observation, planning and design, performance analysis, operational control, and research. These models are built of electric circuit elements such as resistances, amplifiers, integration networks, potentiometers, etc. Prototype attributes are represented in analog computers by analogous physical magnitudes or by electric signals. Analog models have some of the advantages of mathematical models such as flexibility, scalability, and the ability to compress modeling flow time. Hardware components used in special-purpose analog computers can be reused for other modeling purposes. Disadvantages of analog models include insufficient modeling accuracy for some applications and poor cost effectiveness. To overcome these disadvantages, digital computers have been put into increasing use as simulators of analog computers. A multitude of languages has been developed for general-purpose modeling, which makes digital computers look to the user like analog computers. This approach makes a very cost-effective tool available to the traditional users of hardware analog models. More detail about these languages is provided in the Appendix.

Examples of very simple symbolic models include geographic or topographic maps and plans of buildings and machines. These types of logical models or drawings could be termed *symbolic scale* models. The advantages and the disadvantages of these simple symbolic models are very much like those of the iconic models. They are simple and inexpensive to make, can only be manipulated in a limited way, but are very useful for the purpose of

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