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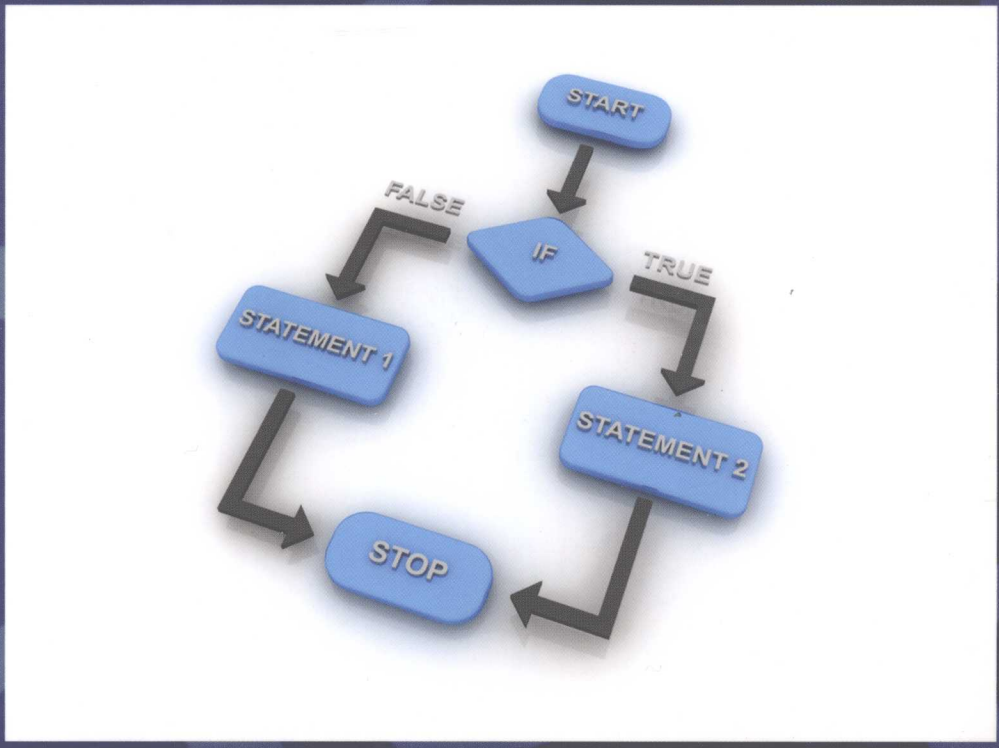
Introduction to Elementary Computational Modeling

Essential Concepts, Principles, and Problem Solving



José M. Garrido

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Preface

Computational science is an emerging area (or discipline) that includes concepts, principles, and methods from applied mathematics and algorithmic design and computer programming; these are applied in various areas of science and engineering to solve large-scale scientific problems. A *computational model* is a computer implementation of the solution to a (scientific) problem for which a mathematical representation has been formulated. Developing a computational model includes formulating the mathematical representation and implementing it by applying computer science concepts, principles and methods. Computational modeling is the foundational component of computational science and focuses on reasoning about problems using *computational thinking* and developing models for problem solving.

The primary goal of this book is to introduce readers to the basic principles of computational modeling at the level of fundamental concepts. Emphasis is on reasoning about problems, conceptualizing the problem, elementary mathematical modeling, and their computational solution that involves computing results and visualization.

The book emphasizes analytical skill development and problem solving rather than programming language syntax and explains simple pseudo-code, simple algorithm design, and MATLAB®, Octave, and FreeMat programming. MATLAB is a widely used scientific software tool; Octave and FreeMat are freely available software tools compatible with MATLAB.

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Although computational models require high-performance computing to solve large and complex scientific problems, this book presents only the elementary notions of computational models. For beginning undergraduate students (of science and engineering), the goal is to provide relevant material for

easy understanding of computational models and their development, as early as possible in their studies. Therefore, the book takes an "early introduction" approach to computational models by providing the readers with a strong foundation in computational modeling by applying elementary mathematical concepts and basic principles, methods, and techniques of computer science.

The book consists of two parts. Part I presents the basic concepts and principles of computational models. In this part, the book discusses basic modeling and techniques for designing and implementing problem solutions, independent of software and hardware tools. Standard pseudo-code constructs and flowcharts are explained and applied in designing models for various case studies. These are implemented using only the minimum necessary knowledge of MATLAB, a widely used scientific software tool, and Octave, a freely available tool that is compatible with MATLAB. Part II of the book presents the elementary mathematical modeling principles and more detailed computer implementation of models with programming constructs using MATLAB and Octave. Examples and case studies demonstrate the computation and visualization of computational models.

The basic syntax constructs of MATLAB and Octave are presented gradually and the various programming principles are explained in an incremental manner for the actual implementation of computational models. This book avoids presenting too much syntax of the programming language at the beginning, which usually results in unnecessary difficulty for the student in understanding the underlying concepts in problem solution and programming.

There are very few books on the basic treatment of computational models; this book and its associated models were designed as teaching materials. The book is aimed at beginning college students in computer science, mathematics, statistics, science, and engineering. The main features of the book are the following:

- Explanation of the basic concepts and principles of computational models are explained.
- Discussion of the models is based on elementary mathematical models, at the level of pre-calculus.
- Emphasis on modularity and abstraction that help in dealing with large and complex models. These concepts are introduced early in Chapters 1 and 2.
- Discussion of the design of algorithmic solutions to problems using standard flowcharts and pseudo-code.
- Implementation of the problem solutions and the corresponding models in MATLAB and Octave.

The material in this book is adequate at the beginning undergraduate level, a CS0 course or a CS1 course. As mentioned previously, the material can also be used in other undergraduate curricula, e.g., mathematics, engineering, and the other sciences. Because of the level of mathematics used, the book can also be utilized for a course in college preparation at the high school level.

This book will be extremely helpful to readers who have never programmed before and the book can help improve the overall approach in teaching/learning programming principles by emphasizing more problem solving, abstraction, algorithm design with pseudo-code, and basic programming before teaching/learning more advanced programming principles with standard programming languages such as Java, C++, Ada, and others.

I acknowledge the help provided through discussions with some of my colleagues, namely Dr. Ben Setzer and Dr. Dick Gayler. I also acknowledge and give special thanks to Professor Rich Schlesinger for writing Chapter 1.

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About the Author

José M. Garrido is professor of computer science in the Department of Computer Science, Kennesaw State University, Georgia. He holds a Ph.D. from George Mason University in Fairfax, Virginia, an M.S.C.S also from George Mason University, an M.Sc. from the University of London, and B.S. in electrical engineering from the Universidad de Oriente, Venezuela.

Dr. Garrido's research interest is on object-oriented modeling and simulation, multi-disciplinary computational modeling, formal specification of real-time systems, language design and processors, modeling systems performance, and software security. Dr. Garrido developed the Psim3, PsimJ, and PsimJ2 simulation packages for C++ and Java. He has recently developed the OOSimL, the Object-Oriented Simulation Language (with partial support from NSF).

Dr. Garrido has published several papers on modeling and simulation, and on programming methods. He has also published six textbooks on object-oriented simulation and operating systems.

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