

Introduction To Computational Science Modeling And Simulation For The Sciences Second Edition

Modeling and computing is becoming an essential part of the analysis and design of an engineered system. This is also true of "geotechnical systems", such as soil foundations, earth dams and other soil-structure systems. The general goal of modeling and computing is to predict and understand the behaviour of the system subjected to a variety of possible conditions/scenarios (with respect to both external stimuli and system parameters), which provides the basis for a rational design of the system. The essence of this is to predict the response of the system to a set of external forces. The modelling and computing essentially involve the following three phases: (a) Idealization of the actual physical problem, (b) Formulation of a mathematical model represented by a set of equations governing the response of the system, and (c) Solution of the governing equations (often requiring numerical methods) and graphical representation of the numerical results. This book will introduce these phases. MATLAB® codes and MAPLE® worksheets are available for those who have bought the book. Please contact the author at mbulker@itu.edu.tr or canulker@gmail.com. Kindly provide the invoice number and date of purchase.

Overview -- Fundamental considerations -- System dynamics problems with rate proportional to amount -- Force and motion -- Simulation techniques -- System dynamics models with interactions -- Additional dynamic systems projects -- Data-driven models -- Monte Carlo simulations -- Random walk simulations -- Diffusion -- High performance computing -- Additional cellular automata projects.

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Biologists, climate scientists, and economists all rely on models to move their work forward. In this book, Stephen M. Downes explores the use of models in these and other fields to introduce readers to the various philosophical issues that arise in scientific modeling. Readers learn that paying attention to models plays a crucial role in appraising scientific work. This book first presents a wide range of models from a number of different scientific disciplines. After assembling some illustrative examples, Downes demonstrates how models shed light on many perennial issues in philosophy of science and in philosophy in general. Reviewing the range of views on how models represent their targets introduces readers to the key issues in debates on representation, not only in science but in the arts as well. Also, standard epistemological questions are cast in new and interesting ways when readers confront the question, "What makes for a good (or bad) model?" All examples from the sciences and positions in the philosophy of science are presented in an accessible manner. The book is suitable for undergraduates with minimal experience in philosophy and an introductory undergraduate experience in science. Key features: The book serves as a highly accessible philosophical introduction to models and modeling in the sciences, presenting all philosophical and scientific issues in a nontechnical manner. Students and other readers learn to practice philosophy of science by starting with clear examples taken directly from the sciences. While not comprehensive, this book introduces the reader to a wide range of views on key issues in the philosophy of science.

Introduction to Modeling and Simulation with MATLAB and Python is intended for students and professionals in science, social science, and engineering that wish to learn the principles of computer modeling, as well as basic programming skills. The book content focuses on meeting a

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set of basic modeling and simulation competencies that were developed as part of several National Science Foundation grants. Even though computer science students are much more expert programmers, they are not often given the opportunity to see how those skills are being applied to solve complex science and engineering problems and may also not be aware of the libraries used by scientists to create those models. The book interleaves chapters on modeling concepts and related exercises with programming concepts and exercises. The authors start with an introduction to modeling and its importance to current practices in the sciences and engineering. They introduce each of the programming environments and the syntax used to represent variables and compute mathematical equations and functions. As students gain more programming expertise, the authors return to modeling concepts, providing starting code for a variety of exercises where students add additional code to solve the problem and provide an analysis of the outcomes. In this way, the book builds both modeling and programming expertise with a "just-in-time" approach so that by the end of the book, students can take on relatively simple modeling example on their own. Each chapter is supplemented with references to additional reading, tutorials, and exercises that guide students to additional help and allows them to practice both their programming and analytical modeling skills. In addition, each of the programming related chapters is divided into two parts – one for MATLAB and one for Python. In these chapters, the authors also refer to additional online tutorials that students can use if they are having difficulty with any of the topics. The book culminates with a set of final project exercise suggestions that incorporate both the modeling and programming skills provided in the rest of the volume. Those projects could be undertaken by individuals or small groups of students. The companion website at

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<http://www.intromodeling.com> provides updates to instructions when there are substantial changes in software versions, as well as electronic copies of exercises and the related code. The website also offers a space where people can suggest additional projects they are willing to share as well as comments on the existing projects and exercises throughout the book. Solutions and lecture notes will also be available for qualifying instructors.

Introduction to Computational Models with Python explains how to implement computational models using the flexible and easy-to-use Python programming language. The book uses the Python programming language interpreter and several packages from the huge Python Library that improve the performance of numerical computing, such as the Numpy and Scipy m

"For the neuroscientist or psychologist who cringes at the sight of mathematical formulae and whose eyes glaze over at terms like differential equations, linear algebra, vectors, matrices, Bayes' rule, and Boolean logic, this book just might be the therapy needed." - Anjan Chatterjee, Professor of Neurology, University of Pennsylvania "Anderson provides a gentle introduction to computational aspects of psychological science, managing to respect the reader's intelligence while also being completely unintimidating. Using carefully-selected computational demonstrations, he guides students through a wide array of important approaches and tools, with little in the way of prerequisites...I recommend it with enthusiasm." - Asohan Amarasingham, The City University of New York This unique, self-contained and accessible textbook provides an introduction to computational modelling neuroscience accessible to readers with little or no background in computing or mathematics. Organized into thematic sections, the book spans from modelling integrate and firing neurons to playing the game Rock, Paper, Scissors in ACT-R. This non-

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technical guide shows how basic knowledge and modern computers can be combined for interesting simulations, progressing from early exercises utilizing spreadsheets, to simple programs in Python. Key Features include: Interleaved chapters that show how traditional computing constructs are simply disguised versions of the spread sheet methods. Mathematical facts and notation needed to understand the modelling methods are presented at their most basic and are interleaved with biographical and historical notes for context. Numerous worked examples to demonstrate the themes and procedures of cognitive modelling. An excellent text for postgraduate students taking courses in research methods, computational neuroscience, computational modelling, cognitive science and neuroscience. It will be especially valuable to psychology students.

Taking a novel, more appealing approach than current texts, *An Integrated Introduction to Computer Graphics and Geometric Modeling* focuses on graphics, modeling, and mathematical methods, including ray tracing, polygon shading, radiosity, fractals, freeform curves and surfaces, vector methods, and transformation techniques. The author begins with fractals, rather than the typical line-drawing algorithms found in many standard texts. He also brings the turtle back from obscurity to introduce several major concepts in computer graphics. Supplying the mathematical foundations, the book covers linear algebra topics, such as vector geometry and algebra, affine and projective spaces, affine maps, projective transformations, matrices, and quaternions. The main graphics areas explored include reflection and refraction, recursive ray tracing, radiosity, illumination models, polygon shading, and hidden surface procedures. The book also discusses geometric modeling, including planes, polygons, spheres, quadrics, algebraic and parametric curves and surfaces, constructive solid geometry,

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boundary files, octrees, interpolation, approximation, Bezier and B-spline methods, fractal algorithms, and subdivision techniques. Making the material accessible and relevant for years to come, the text avoids descriptions of current graphics hardware and special programming languages. Instead, it presents graphics algorithms based on well-established physical models of light and cogent mathematical methods.

Computational Frameworks: Systems, Models and Applications provides an overview of advanced perspectives that bridges the gap between frontline research and practical efforts. It is unique in showing the interdisciplinary nature of this area and the way in which it interacts with emerging technologies and techniques. As computational systems are a dominating part of daily lives and a required support for most of the engineering sciences, this book explores their usage (e.g. big data, high performance clusters, databases and information systems, integrated and embedded hardware/software components, smart devices, mobile and pervasive networks, cyber physical systems, etc.). Provides a unique presentation on the views of frontline researchers on computational systems theory and applications in one holistic scope Cover both computational science and engineering Bridges the gap between frontline research and practical efforts

This advanced textbook provides an introduction to the basic methods of computational physics.

Accessible text features over 100 reality-based examples pulled from the science, engineering, and operations research fields. Prerequisites: ordinary differential equations, continuous probability.

Numerous references. Includes 27 black-and-white

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figures. 1978 edition.

Computational Economics: A concise introduction is a comprehensive textbook designed to help students move from the traditional and comparative static analysis of economic models, to a modern and dynamic computational study. The ability to equate an economic problem, to formulate it into a mathematical model and to solve it computationally is becoming a crucial and distinctive competence for most economists. This vital textbook is organized around static and dynamic models, covering both macro and microeconomic topics, exploring the numerical techniques required to solve those models. A key aim of the book is to enable students to develop the ability to modify the models themselves so that, using the MATLAB/Octave codes provided on the book and on the website, students can demonstrate a complete understanding of computational methods. This textbook is innovative, easy to read and highly focused, providing students of economics with the skills needed to understand the essentials of using numerical methods to solve economic problems. It also provides more technical readers with an easy way to cope with economics through modelling and simulation. Later in the book, more elaborate economic models and advanced numerical methods are introduced which will prove valuable to those in more advanced study. This book is ideal for all

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students of economics, mathematics, computer science and engineering taking classes on Computational or Numerical Economics.

The new edition of an introductory text that teaches students the art of computational problem solving, covering topics ranging from simple algorithms to information visualization. This book introduces students with little or no prior programming experience to the art of computational problem solving using Python and various Python libraries, including PyLab. It provides students with skills that will enable them to make productive use of computational techniques, including some of the tools and techniques of data science for using computation to model and interpret data. The book is based on an MIT course (which became the most popular course offered through MIT's OpenCourseWare) and was developed for use not only in a conventional classroom but in in a massive open online course (MOOC). This new edition has been updated for Python 3, reorganized to make it easier to use for courses that cover only a subset of the material, and offers additional material including five new chapters. Students are introduced to Python and the basics of programming in the context of such computational concepts and techniques as exhaustive enumeration, bisection search, and efficient approximation algorithms. Although it covers such traditional topics as computational complexity

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and simple algorithms, the book focuses on a wide range of topics not found in most introductory texts, including information visualization, simulations to model randomness, computational techniques to understand data, and statistical techniques that inform (and misinform) as well as two related but relatively advanced topics: optimization problems and dynamic programming. This edition offers expanded material on statistics and machine learning and new chapters on Frequentist and Bayesian statistics.

Introduction to Computational Modeling Using C and Open-Source Tools presents the fundamental principles of computational models from a computer science perspective. It explains how to implement these models using the C programming language. The software tools used in the book include the Gnu Scientific Library (GSL), which is a free software library of C functions, and the versatile, open-source GnuPlot for visualizing the data. All source files, shell scripts, and additional notes are located at science.kennesaw.edu/~jgarrido/comp_models The book first presents an overview of problem solving and the introductory concepts, principles, and development of computational models before covering the programming principles of the C programming language. The author then applies programming principles and basic numerical techniques, such as polynomial evaluation,

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regression, and other numerical methods, to implement computational models. He also discusses more advanced concepts needed for modeling dynamical systems and explains how to generate numerical solutions. The book concludes with the modeling of linear optimization problems.

Emphasizing analytical skill development and problem solving, this book helps you understand how to reason about and conceptualize the problems, generate mathematical formulations, and computationally visualize and solve the problems. It provides you with the foundation to understand more advanced scientific computing, including parallel computing using MPI, grid computing, and other techniques in high-performance computing.

Created to help scientists and engineers write computer code, this practical book addresses the important tools and techniques that are necessary for scientific computing, but which are not yet commonplace in science and engineering curricula. This book contains chapters summarizing the most important topics that computational researchers need to know about. It leverages the viewpoints of passionate experts involved with scientific computing courses around the globe and aims to be a starting point for new computational scientists and a reference for the experienced. Each contributed chapter focuses on a specific tool or skill, providing the content needed to provide a working knowledge

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of the topic in about one day. While many individual books on specific computing topics exist, none is explicitly focused on getting technical professionals and students up and running immediately across a variety of computational areas.

With an emphasis on problem solving, this book introduces the basic principles and fundamental concepts of computational modeling. It emphasizes reasoning and conceptualizing problems, the elementary mathematical modeling, and the implementation using computing concepts and principles. Examples are included that demonstrate the computation and visualization of the implemented models. The author provides case studies, along with an overview of computational models and their development. The first part of the text presents the basic concepts of models and techniques for designing and implementing problem solutions. It applies standard pseudo-code constructs and flowcharts for designing models. The second part covers model implementation with basic programming constructs using MATLAB®, Octave, and FreeMat. Aimed at beginning students in computer science, mathematics, statistics, and engineering, *Introduction to Elementary Computational Modeling: Essential Concepts, Principles, and Problem Solving* focuses on fundamentals, helping the next generation of scientists and engineers hone their problem solving

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Introduction to Mathematical Modeling and Computer Simulations is written as a textbook for readers who want to understand the main principles of Modeling and Simulations in settings that are important for the applications, without using the profound mathematical tools required by most advanced texts. It can be particularly useful for applied mathematicians and engineers who are just beginning their careers. The goal of this book is to outline Mathematical Modeling using simple mathematical descriptions, making it accessible for first- and second-year students.

Teach Your Students Both the Mathematics of Numerical Methods and the Art of Computer Programming Introduction to Computational Linear Algebra presents classroom-tested material on computational linear algebra and its application to numerical solutions of partial and ordinary differential equations. The book is designed for senior undergraduate stud

This textbook provides an introduction to the growing interdisciplinary field of computational science. It combines a foundational development of numerical methods with a variety of illustrative applications spread across numerous areas of science and engineering. The intended audience is the undergraduate who has completed introductory coursework in mathematics and computer science.

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Students gain computational acuity by authoring their own numerical routines and by practicing with numerical methods as they solve computational models. This education encourages students to learn the importance of answering: How expensive is a calculation, how trustworthy is a calculation, and how might we model a problem to apply a desired numerical method? The text is written in two parts. Part I provides a succinct, one-term inauguration into the primary routines on which a further study of computational science rests. The material is organized so that the transition to computational science from coursework in calculus, differential equations, and linear algebra is natural. Beyond the mathematical and computational content of Part I, students gain proficiency with elemental programming constructs and visualization, which are presented in MATLAB syntax. The focus of Part II is modeling, wherein students build computational models, compute solutions, and report their findings. The models purposely intersect numerous areas of science and engineering to demonstrate the pervasive role played by computational science. This book covers the essentials of Computational Science and gives tools and techniques to solve materials science problems using molecular dynamics (MD) and first-principles methods. The new edition expands upon the density functional theory (DFT) and how the original DFT has

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advanced to a more accurate level by GGA+U and hybrid-functional methods. It offers 14 new worked examples in the LAMMPS, Quantum Espresso, VASP and MedeA-VASP programs, including computation of stress-strain behavior of Si-CNT composite, mean-squared displacement (MSD) of ZrO₂-Y₂O₃, band structure and phonon spectra of silicon, and Mo-S battery system. It discusses methods once considered too expensive but that are now cost-effective. New examples also include various post-processed results using VESTA, VMD, VTST, and MedeA.

This book is a definitive reference source for the growing, increasingly more important, and interdisciplinary field of computational cognitive modeling, that is, computational psychology. It combines breadth of coverage with definitive statements by leading scientists in this field. Research in computational cognitive modeling explores the essence of cognition and various cognitive functionalities through developing detailed, process-based understanding by specifying computational mechanisms, structures, and processes. Given the complexity of the human mind and its manifestation in behavioral flexibility, process-based computational models may be necessary to explicate and elucidate the intricate details of the mind. The key to understanding cognitive processes is often in fine details. Computational models provide

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algorithmic specificity: detailed, exactly specified, and carefully thought-out steps, arranged in precise yet flexible sequences. These models provide both conceptual clarity and precision at the same time. This book substantiates this approach through overviews and many examples.

This book delivers a comprehensive and insightful account of applying mathematical modelling approaches to very large biological systems and networks—a fundamental aspect of computational systems biology. The book covers key modelling paradigms in detail, while at the same time retaining a simplicity that will appeal to those from less quantitative fields. Key Features: A hands-on approach to modelling Covers a broad spectrum of modelling, from static networks to dynamic models and constraint-based models Thoughtful exercises to test and enable understanding of concepts State-of-the-art chapters on exciting new developments, like community modelling and biological circuit design Emphasis on coding and software tools for systems biology Companion website featuring lecture videos, figure slides, codes, supplementary exercises, further reading, and appendices:

<https://ramanlab.github.io/SysBioBook/> An Introduction to Computational Systems Biology: Systems-Level Modelling of Cellular Networks is highly multi-disciplinary and will appeal to biologists, engineers, computer scientists, mathematicians and

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Computational science is a rapidly growing multidisciplinary field concerned with the design, implementation, and use of mathematical models to analyze and solve real-world problems. It is an area of science that spans many disciplines and which involves the development of models and allows the use of computers to perform simulations or numerical analysis to understand problems that are computational and theoretical. Computational Science and its Applications provides an opportunity for readers to develop abilities to pose and solve problems that combine insights from one or more disciplines from the natural sciences with mathematical tools and computational skills. This requires a unique combination of applied and theoretical knowledge and skills. The topics covered in this edited book are applications of wavelet and fractals, modeling by partial differential equations on flat structure as well as on graphs and networks, computational linguistics, prediction of natural calamities and diseases like epilepsy seizure, heart attack, stroke, biometrics, modeling through inverse problems, interdisciplinary topics of physics, mathematics, and medical science, and modeling of terrorist attacks and human behavior. The focus of this book is not to educate computer specialists, but to provide readers with a solid understanding of basic science as well as an integrated knowledge on

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how to use essential methods from computational science. Features: Modeling of complex systems Cognitive computing systems for real-world problems Presentation of inverse problems in medical science and their numerical solutions Challenging research problems in many areas of computational science This book could be used as a reference book for researchers working in theoretical research as well as those who are doing modeling and simulation in such disciplines as physics, biology, geoscience, and mathematics, and those who have a background in computational science. This open access book offers an initial introduction to programming for scientific and computational applications using the Python programming language. The presentation style is compact and example-based, making it suitable for students and researchers with little or no prior experience in programming. The book uses relevant examples from mathematics and the natural sciences to present programming as a practical toolbox that can quickly enable readers to write their own programs for data processing and mathematical modeling. These tools include file reading, plotting, simple text analysis, and using NumPy for numerical computations, which are fundamental building blocks of all programs in data science and computational science. At the same time, readers are introduced to the fundamental concepts of programming, including

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variables, functions, loops, classes, and object-oriented programming. Accordingly, the book provides a sound basis for further computer science and programming studies.

An introduction to scientific computing for differential equations Introduction to Computation and Modeling for Differential Equations provides a unified and integrated view of numerical analysis, mathematical modeling in applications, and programming to solve differential equations, which is essential in problem-solving across many disciplines, such as engineering, physics, and economics. This book successfully introduces readers to the subject through a unique "Five-M" approach: Modeling, Mathematics, Methods, MATLAB, and Multiphysics. This approach facilitates a thorough understanding of how models are created and preprocessed mathematically with scaling, classification, and approximation, and it also illustrates how a problem is solved numerically using the appropriate mathematical methods. The book's approach of solving a problem with mathematical, numerical, and programming tools is unique and covers a wide array of topics, from mathematical modeling to implementing a working computer program. The author utilizes the principles and applications of scientific computing to solve problems involving: Ordinary differential equations Numerical methods for Initial Value Problems (IVPs) Numerical methods

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for Boundary Value Problems (BVPs) Partial Differential Equations (PDEs) Numerical methods for parabolic, elliptic, and hyperbolic PDEs Mathematical modeling with differential equations Numerical solution Finite difference and finite element methods Real-world examples from scientific and engineering applications including mechanics, fluid dynamics, solid mechanics, chemical engineering, electromagnetic field theory, and control theory are solved through the use of MATLAB and the interactive scientific computing program Comsol Multiphysics. Numerous illustrations aid in the visualization of the solutions, and a related Web site features demonstrations, solutions to problems, MATLAB programs, and additional data. Introduction to Computation and Modeling for Differential Equations is an ideal text for courses in differential equations, ordinary differential equations, partial differential equations, and numerical methods at the upper-undergraduate and graduate levels. The book also serves as a valuable reference for researchers and practitioners in the fields of mathematics, engineering, and computer science who would like to refresh and revive their knowledge of the mathematical and numerical aspects as well as the applications of scientific computation.

This unique book provides a comprehensive introduction to computational mathematics, which forms an essential

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part of modern numerical algorithms and scientific computing. It uses a theorem-free approach with just the right balance between mathematics and numerical algorithms. It covers all major topics in computational mathematics with a wide range of carefully selected numerical algorithms, ranging from the root-finding algorithms, numerical integration, numerical methods of partial differential equations, finite element methods, optimization algorithms, stochastic models, to nonlinear curve-fitting and swarm optimization. Especially suitable for undergraduates and graduates in computational mathematics, numerical algorithms, and scientific computing, it can be used as a textbook and/or reference book.

Emphasising essential methods and universal principles, this textbook provides everything students need to understand the basics of simulating materials behaviour. All the key topics are covered from electronic structure methods to microstructural evolution, appendices provide crucial background material, and a wealth of practical resources are available online to complete the teaching package. Modelling is examined at a broad range of scales, from the atomic to the mesoscale, providing students with a solid foundation for future study and research. Detailed, accessible explanations of the fundamental equations underpinning materials modelling are presented, including a full chapter summarising essential mathematical background. Extensive appendices, including essential background on classical and quantum mechanics, electrostatics, statistical thermodynamics and linear elasticity, provide the

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background necessary to fully engage with the fundamentals of computational modelling. Exercises, worked examples, computer codes and discussions of practical implementations methods are all provided online giving students the hands-on experience they need.

Scientific computing is the study of how to use computers effectively to solve problems that arise from the mathematical modeling of phenomena in science and engineering. It is based on mathematics, numerical and symbolic/algebraic computations and visualization. This book serves as an introduction to both the theory and practice of scientific computing, with each chapter presenting the basic algorithms that serve as the workhorses of many scientific codes; we explain both the theory behind these algorithms and how they must be implemented in order to work reliably in finite-precision arithmetic. The book includes many programs written in Matlab and Maple – Maple is often used to derive numerical algorithms, whereas Matlab is used to implement them. The theory is developed in such a way that students can learn by themselves as they work through the text. Each chapter contains numerous examples and problems to help readers understand the material “hands-on”.

Learn How to Program Stochastic Models Highly recommended, the best-selling first edition of Introduction to Scientific Programming and Simulation Using R was lauded as an excellent, easy-to-read introduction with extensive examples and exercises. This second edition continues to introduce scientific

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programming and stochastic modelling in a clear, An easy-to-read introduction to the concepts associated with the creation of optimization models for production planning starts off this book. These concepts are then applied to well-known planning models, namely mrp and MRP II. From this foundation, fairly sophisticated models for supply chain management are developed. Another unique feature is that models are developed with an eye toward implementation. In fact, there is a chapter that provides explicit examples of implementation of the basic models using a variety of popular, commercially available modeling languages.

This textbook provides a comprehensive and reader-friendly introduction to the field of computational social science (CSS). Presenting a unified treatment, the text examines in detail the four key methodological approaches of automated social information extraction, social network analysis, social complexity theory, and social simulation modeling. This updated new edition has been enhanced with numerous review questions and exercises to test what has been learned, deepen understanding through problem-solving, and to practice writing code to implement ideas. Topics and features: contains more than a thousand questions and exercises, together with a list of acronyms and a glossary; examines the similarities and differences between computers and social systems; presents a focus on automated information extraction; discusses the measurement, scientific laws, and generative theories of social complexity in CSS; reviews the methodology of social simulations, covering both variable- and object-

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oriented models.

A Concise Introduction to Computation Models and Computability Theory provides an introduction to the essential concepts in computability, using several models of computation, from the standard Turing Machines and Recursive Functions, to the modern computation models inspired by quantum physics. An in-depth analysis of the basic concepts underlying each model of computation is provided. Divided into two parts, the first highlights the traditional computation models used in the first studies on computability: - Automata and Turing Machines; - Recursive functions and the Lambda-Calculus; - Logic-based computation models. and the second part covers object-oriented and interaction-based models. There is also a chapter on concurrency, and a final chapter on emergent computation models inspired by quantum mechanics. At the end of each chapter there is a discussion on the use of computation models in the design of programming languages.

This book presents computer programming as a key method for solving mathematical problems. There are two versions of the book, one for MATLAB and one for Python. The book was inspired by the Springer book TCSE 6: A Primer on Scientific Programming with Python (by Langtangen), but the style is more accessible and concise, in keeping with the needs of engineering students. The book outlines the shortest possible path from no previous experience with programming to a set of skills that allows the students to write simple programs for solving common mathematical problems with numerical methods in engineering and science courses.

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The emphasis is on generic algorithms, clean design of programs, use of functions, and automatic tests for verification.

A comprehensive and hands-on introduction to the core concepts, methods, and applications of agent-based modeling, including detailed NetLogo examples. The advent of widespread fast computing has enabled us to work on more complex problems and to build and analyze more complex models. This book provides an introduction to one of the primary methodologies for research in this new field of knowledge. Agent-based modeling (ABM) offers a new way of doing science: by conducting computer-based experiments. ABM is applicable to complex systems embedded in natural, social, and engineered contexts, across domains that range from engineering to ecology. An Introduction to Agent-Based Modeling offers a comprehensive description of the core concepts, methods, and applications of ABM. Its hands-on approach—with hundreds of examples and exercises using NetLogo—enables readers to begin constructing models immediately, regardless of experience or discipline. The book first describes the nature and rationale of agent-based modeling, then presents the methodology for designing and building ABMs, and finally discusses how to utilize ABMs to answer complex questions. Features in each chapter include step-by-step guides to developing models in the main text; text boxes with additional information and concepts; end-of-chapter explorations; and references and lists of relevant reading. There is also an accompanying website with all the models and code.

Computational science is an exciting new field at the intersection of the sciences, computer science, and mathematics because much scientific investigation now involves computing as well as theory and experiment. This

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textbook provides students with a versatile and accessible introduction to the subject. It assumes only a background in high school algebra, enables instructors to follow tailored pathways through the material, and is the only textbook of its kind designed specifically for an introductory course in the computational science and engineering curriculum. While the text itself is generic, an accompanying website offers tutorials and files in a variety of software packages. This fully updated and expanded edition features two new chapters on agent-based simulations and modeling with matrices, ten new project modules, and an additional module on diffusion. Besides increased treatment of high-performance computing and its applications, the book also includes additional quick review questions with answers, exercises, and individual and team projects. The only introductory textbook of its kind—now fully updated and expanded Features two new chapters on agent-based simulations and modeling with matrices Increased coverage of high-performance computing and its applications Includes additional modules, review questions, exercises, and projects An online instructor's manual with exercise answers, selected project solutions, and a test bank and solutions (available only to professors) An online illustration package is available to professors

Computational Materials Engineering is an advanced introduction to the computer-aided modeling of essential material properties and behavior, including the physical, thermal and chemical parameters, as well as the mathematical tools used to perform simulations. Its emphasis will be on crystalline materials, which includes all metals. The basis of Computational Materials Engineering allows scientists and engineers to create virtual simulations of material behavior and properties, to better understand how a particular material works and performs and then use that knowledge to design improvements for particular material

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applications. The text displays knowledge of software designers, materials scientists and engineers, and those involved in materials applications like mechanical engineers, civil engineers, electrical engineers, and chemical engineers. Readers from students to practicing engineers to materials research scientists will find in this book a single source of the major elements that make up contemporary computer modeling of materials characteristics and behavior. The reader will gain an understanding of the underlying statistical and analytical tools that are the basis for modeling complex material interactions, including an understanding of computational thermodynamics and molecular kinetics; as well as various modeling systems. Finally, the book will offer the reader a variety of algorithms to use in solving typical modeling problems so that the theory presented herein can be put to real-world use. Balanced coverage of fundamentals of materials modeling, as well as more advanced aspects of modeling, such as modeling at all scales from the atomic to the molecular to the macro-material Concise, yet rigorous mathematical coverage of such analytical tools as the Potts type Monte Carlo method, cellular automata, phase field, dislocation dynamics and Finite Element Analysis in statistical and analytical modeling

Mathematics of Computing -- Numerical Analysis.

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