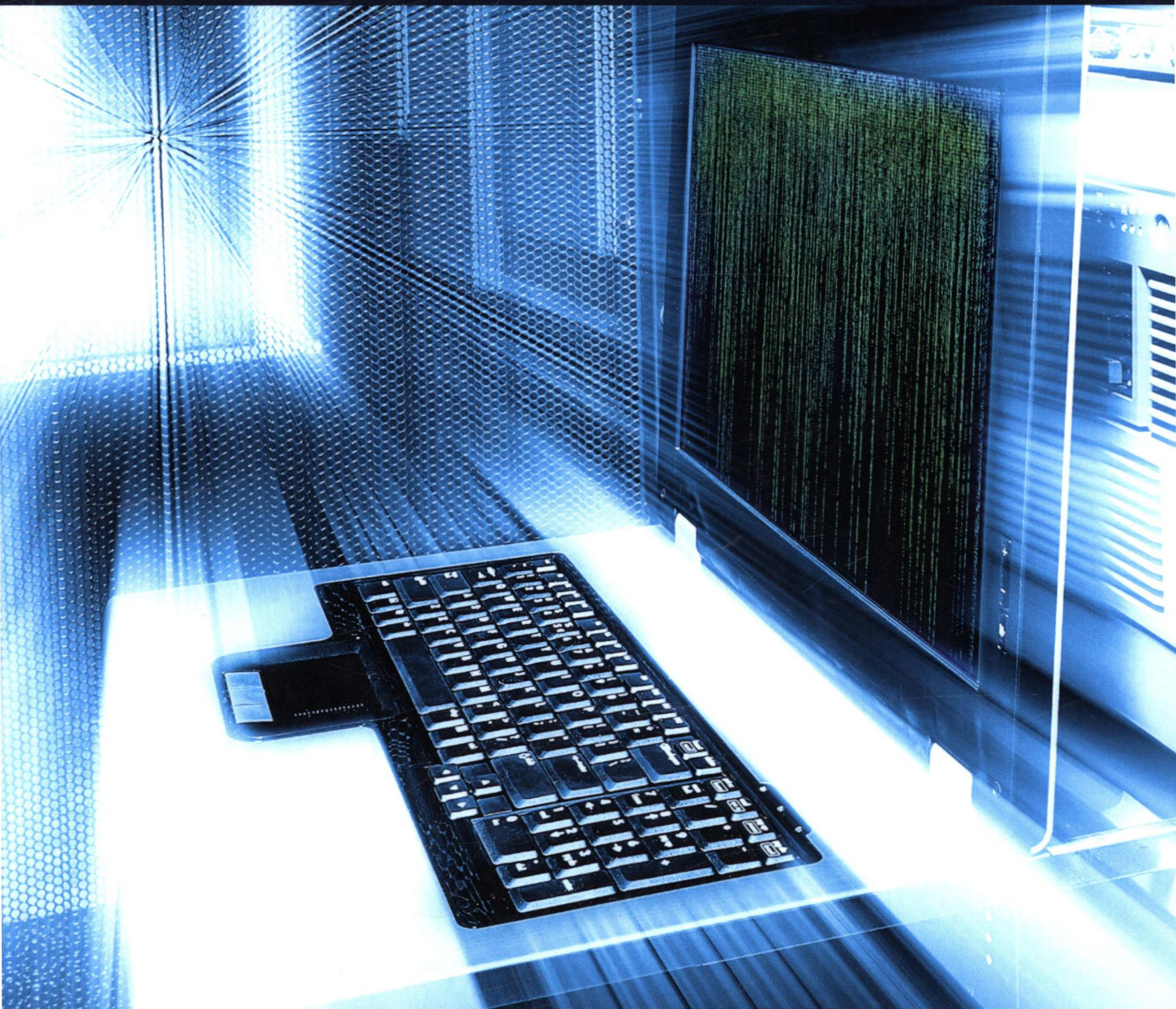
Computational Techniques for Process Simulation and Analysis Using MATLAB®



Niket S. Kaisare

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Computational Techniques for Process Simulation and Analysis Using MATLAB®

MATLAB® has become one of the prominent languages used in research and industry. Mathworks, the makers of MATLAB®, describe it as "the language of technical computing". The focus of this book will be to highlight the use of MATLAB® in technical computing; or more specifically, in solving problems in Process Simulations. This book aims to bring a practical approach to expounding theories: both numerical aspects of stability and convergence, as well as linear and nonlinear analysis of systems.

This book is intended to be a post-graduate level textbook for Numerical Methods, Simulation and Analysis of Process Systems and Computational Programming Lab. The book is split into three sections, which are laid out with a "Process Analysis" viewpoint. Thus, Section I covers dynamics and linear system analysis, Section II covers solving nonlinear equations, including Differential Algebraic Equations (DAE); and Section III covers function approximation and optimization for modeling of data.

Key Points:

- Concise coverage of numerical methods for solving process analysis and simulation problems using MATLAB®.
- Analysis of transient behavior of linear and nonlinear systems.
- Discusses coding hygiene, and practical aspects of simulation using MATLAB®.
- Treatment of process dynamics, linear stability, nonlinear analysis, and function approximation through contemporary examples.
- Focus on simulation using MATLAB® to solve ODEs and PDEs that are frequently encountered in process systems.

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To Pradnya for her unending love, patience, and support
and
To my parents, Komal and Satish Kaisare

Preface

STUDENTS TODAY ARE EXPECTED to know one or more of the several computing or simulation tools as part of their curriculum, due to their widespread use in the industry. MATLAB® has become one of the prominent languages used in research and industry. MATLAB is a numerical computing environment that is based on a MATLAB scripting language. MathWorks, the makers of MATLAB, describe it as "the language of technical computing." The focus of this book will be to highlight the *use* of MATLAB in technical computing or, more specifically, in solving problems in the *analysis and simulation of processes* of interest to engineers.

This is intended to be an intermediate-level book, geared toward postgraduate students, practicing engineers, and researchers who use MATLAB. It provides advanced treatment of topics relevant to modeling, simulation, and analysis of dynamical systems. Although this is not an introductory MATLAB or numerical techniques textbook, it may however be used as a companion book for introductory courses. For the sake of completeness, a primer on MATLAB as well as introduction to some numerical techniques is provided in the Appendices. Since mid-2000s,we have always used MATLAB in electives in IIT Madras. The popularity of MATLAB among students led us to start a *core* undergraduate (sophomore) and a postgraduate (first-year masters) laboratory. Since 2016, I have started teaching a massive open online course (MOOC) on MATLAB programming on the NPTEL platform.* The first two years of this course had over 10,000 enrolled students. Needless to say, MATLAB has become an important tool in teaching and research. The focus of all the above courses is to introduce students to MATLAB as a numerical methods tool. Some of the students who complete these courses inquire about the next-level courses that would help them *apply* MATLAB skills to solve engineering problems. This book may also be used for this purpose. In introductory courses, a significant amount of time is spent in developing the background for numerical methods itself. In our effort to make the treatment general and at a beginner's level, we eschew real-world examples in favor of abstracted ones. For example, we would often introduce a second-order ODE using a generic formulation, such as $y'' + ay' + b(y-c) = 0$. A sophomore who hasn't taken a heat transfer course may not yet appreciate a "heating in a rod" problem. An intermediate-level text means that it is more valuable to use a real example, such as $T'' + r^{-1}T' + \beta(T - T_a) = 0$. The utility of such

* NPTEL stands for National Programme for Technology Enhanced Learning and is a Government of India–funded initiative to bring high-quality engineering and science courses on an online (MOOC) platform to enhance students' learning.

an approach cannot be understated, since it allows the freedom to introduce some of the complexity that engineers, scientists, and researchers face in their work.

The value of using real-world examples was highlighted during my experience in industrial R&D, where we used MATLAB extensively. We needed to interface with cross-functional teams: engineering, implementation, and software development teams. Individuals came from a wide range of backgrounds. These interactions exposed me to a new experience: Your work must be understood by people with very different backgrounds, who may not speak the same technical language. The codes had to bridge the "language barrier" spoken in different teams, and the codes were to be combined with a reasonably intuitive interface. I have tried to adopt some of these principles in this book, without moving too far from the more common pedagogy in creating such a book.

Thus, a practically *oriented text* that caters to an intermediate-level audience is my objective in writing this book.

ORIGIN OF THIS BOOK

There are several excellent books on numerical techniques for engineers. Laurene Forsell's book, *Numerical Methods Using MATLAB*, provides a MATLAB-based approach to learning numerical techniques. The books on numerical techniques by Chapra and Canale and by S.K. Gupta are excellent undergraduate textbooks, which introduce undergraduates to this subject for the first time. Thus, their focus is conceptual understanding of numerical techniques themselves. While undergraduate teaching is in good stead, a textbook that covers *core* requirements for a balanced postgraduate curriculum is missing. Such a book will also be useful to practicing engineers, scientists, and researchers who use MATLAB.

This book is borne out of my experience in teaching a postgraduate course called *Process Analysis and Simulation*, postgraduate lab in *Process Simulation*, and theory of computational techniques. They provide the first-year postgraduates the basis to tackle research problems in their theses. The former course takes a balanced focus on modeling, simulation, and analysis of chemical process systems, while the process simulation lab gives them a numerical methods perspective. Postgraduate-level books, such as the evergreen *Numerical Recipes* by Press et al., are rather advanced and focused on numerical methods. On the other hand, the book by Strogatz on nonlinear dynamics or other similar books are not general enough for the needs of an audience interested in simulations. A "bridge" book, which assumes some familiarity with undergraduate material, but still covers the basics, is missing.

Having said this, I do not intend this to be a postgraduate numerical methods text. This book aims to introduce students and practitioners to simulation and analysis of process systems in MATLAB. We often find it difficult to connect the numerical tool to the physical analysis of a system. This book intends to bring in a strong process simulation treatment to linear stability and nonlinear analysis.

Thus, this book intends to bring a practical approach to expounding theories: both numerical aspects of stability and convergence, as well as linear and nonlinear analysis of systems. The "process" is the focus. Numerical methods are introduced insofar as is essential to make a judicious choice of algorithms for simulation and analysis.

PREREQUISITES

Since this is a postgraduate-level text, some familiarity with an undergraduate-level numerical techniques or an equivalent course is assumed, though we will review all the relevant concepts at the appropriate stage. So, the students are not expected to remember the details or nuances of "Newton-Raphson" or "Runge-Kutta" methods, but this book is not the first time they hear these terms.

Some familiarity with coding (MATLAB, Fortran, C++, Python, or any language) will be useful, but not a prerequisite. MATLAB primer is provided in the Appendix for first-time users of MATLAB. Finally, with respect to writing MATLAB code, I focus on "doing it right the first time" approach—by bringing in good programming practices that I have learnt over the years. Things like commenting and structuring your code, scoping of variables, etc., are also covered, not as an afterthought but as an integral part of the discussion. However, these are dealt with more informally than a "programming language" course.

HOW THIS BOOK IS LAID OUT

This book derives examples from three different courses I have taught: (i) Numerical Methods, (ii) Process Analysis and Simulation, and (iii) Computational Programming Lab. It is structured so that it may be used for any of the three courses. Each chapter deals with one approach to solving computational problems (e.g., ODEs, PDEs, nonlinear equations, etc.), culminating in case studies that utilize the concepts discussed in the chapter.

I have split the book into three sections, which are laid out with a "Process Analysis" viewpoint: Section I covers system dynamics and linear system analysis; Section II covers solving nonlinear equations, including differential algebraic equations (DAEs); and Section III covers function approximation and optimization for modeling of data. The following table summarizes the various chapters in the book:

Basics	Chapter 1 Introduction	Appendix A MATLAB® Primer		
Appendices		Appendix B Differentiation	Appendix C Linear Equations	Appendix E Integration
Section I. **Dynamics**	Chapter 2 Linear Algebra	Chapter 3 ODE-IVP	Chapter 4 Transient PDEs	Chapter 5 Simulation
Section II. **Equations**	Chapter 6 Nonlinear Equations	Chapter 7 Special Methods (ODE-BVP/PDE)	Chapter 8 Implicit Methods (DAEs)	Chapter 9 Nonlinear Analysis
Section III. **Data Fitting**	Appendix D Interpolation	Chapter 10 Regression		

LAYOUT FOR PROCESS ANALYSIS

The layout of this book is largely based on the postgraduate-level process simulation and analysis course. The material I cover in this course is chronologically as laid out in the book. The course starts with an introduction to the role of simulation and analysis in engineering, and a primer on MATLAB. Thereafter, I introduce concepts in linear algebra (Chapter 2), ODEs (Chapter 3), and solving hyperbolic and parabolic PDEs (Chapter 4). Problems in either linear analysis or dynamical simulations (Chapter 5) typically form mid-term projects for students. The second part of the course also follows a similar structure, with nonlinear equations (Chapter 6), ODE-BVPs and elliptic PDEs (Chapter 7), and DAEs (Chapter 8) providing the adequate background for end-semester projects involving nonlinear analysis and bifurcation (Chapter 9). I have added Chapter 10 (Parameter Estimation) for the sake of completion.

LAYOUT FOR NUMERICAL METHODS

This book may also be used for an advanced numerical methods course. In such a case, I suggest treating the material column-wise. This course may start with the first row to cover the basics (Introduction, MATLAB Primer, Differentiation, Integration, and Linear Equations). Thereafter, Chapter 2 and Chapter 6 may be covered, to equip students to solve linear and nonlinear equations. Chapters 3 and 7 cover ODE-IVP and ODE-BVP, respectively, followed by Parameter Estimation (Chapter 10). A four-credit course may also cover PDEs (Chapter 4). Typically, Chapters 5 and 9 will be beyond the scope of such a course.

LAYOUT FOR NUMERICAL DIFFERENTIAL EQUATIONS

The shaded chapters (Chapters 3, 4, 5, 7, 8, and 9), along with appendices on numerical differentiation and integration, can form a numerical differential equations course.

FOR PRACTICING ENGINEER OR NEW RESEARCHER

A practicing engineer or researcher can embark on a self-guided journey through case studies and examples covered in this book. This includes not only the case studies analyzed in Chapters 5 and 9 but also the ones discussed in other chapters (penultimate section in the other chapters).

Author

Dr. Niket S. Kaisare is currently an associate professor in the Department of Chemical Engineering at IIT Madras. He received his PhD in chemical engineering from Georgia Institute of Technology, working in the area of model-based advanced process control. He then joined the Department of Chemical Engineering at the University of Delaware, where he worked on multiscale modeling of reacting flows in microreactors, as a postdoctoral researcher. After this, he joined IIT Madras as assistant professor in 2007. While in IIT Madras, he taught several courses in process analysis and simulation, computational techniques, process simulation laboratory, and advanced control theory. MATLAB was used extensively in most of these courses. He has also taught an online course called "MATLAB Programming for Numerical Computations" as a part of NPTEL (National Programme for Technology Enhanced Learning). This course was popular, with more than ten thousand students enrolling in it.

He spent three years, from mid-2011 to 2014, in industrial R&D. During this stint, he worked on numerous simulation problems related to modeling of vehicle catalytic convertors, cryogenic hydrogen storage, monitoring and control of oil and gas wells, and automation engineering. As a part of the R&D team, he used MATLAB extensively and spent a significant part of his time interfacing with engineering and development teams.

He has extensive experience working in MATLAB and FORTRAN as well as simulation softwares Fluent and Comsol. He also has good working experience with various other simulation tools, such as Aspen-Plus/Unisim, Gaussian, and Abacus. His current research program is focused on "multiscale modeling, analysis, and control of catalytic microreactors for energy- and fuel-processing applications."

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