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Large-Scale Networks in Engineering and Life Sciences

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ISSN 2164-3679 ISSN 2164-3725 (electronic)
Modeling and Simulation in Science, Engineering and Technology
ISBN 978-3-319-08436-7 ISBN 978-3-319-08437-4 (eBook)
DOI 10.1007/978-3-319-08437-4
Springer Heidelberg New York Dordrecht London

Library of Congress Control Number: 2014953776

Mathematics Subject Classification (2010): 34A26, 92C42, 94C05, 90B10, 90C27

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

Modeling, analysis, and control of complex large-scale systems are becoming increasingly important. Large-scale systems are often the result of networked interactions among an ample number of subsystems. Examples of large-scale networked systems include biochemical reaction networks, communication networks such as mobile phone networks and the Internet, complex chemical production processes, neural networks, fish and bird swarms, and circuit networks in microprocessors. The objective of the 2011 summer school *Large-Scale Networks in Engineering and Life Sciences* of the International Max Planck Research School Magdeburg was to provide insights and tools for modeling, analysis, optimization, and control of large-scale networks in life sciences and engineering. The chapters provided in this book are based on the lectures given during this summer school. They cover a wide range of applications and focus on mathematical modeling of the different network structures in these areas. Thus, this book complements recent monographs on the theory of networks such as "Networks: An Introduction" by Newman (Cambridge University Press, 2010) and "The Structure of Complex Networks" by Estrada (Oxford University Press, 2011) or the edited volume "Network Science. Complexity in Nature and Technology" by Estrada, Fox, and Higham (Springer, 2010).

The chapters in this book are mostly self-contained introductions to network modeling in various areas. They can be read independently and may serve as the basis for a seminar series or, in combination with the introductory texts mentioned above, as course supplements for a course on Network Theory and Applications. We hope the book will be useful for graduate students or beginners in the respective fields with a solid mathematical background, but also as a compendium for network researchers. Since different fields employ different techniques as outlined below, we expect that fruitful ideas can result from studying how other disciplines approach network structures.

Basically, the book can be partitioned into four parts. The first part, consisting only of Chap. 1, treats the mathematical theory of (bio)-chemical reaction networks. It can also serve as a self-contained introduction into the geometric theory of ordinary differential equations. Two different applications of network theory in electrical engineering areas are the topic of Chaps. 2 and 3; these can be considered as the second part. Optimization of and on networks is a fundamental issue in discrete mathematics and is treated in the fourth chapter, which can be considered again as a part on its own. The last three chapters discuss biological networks from different view points and together form a fourth part of the book.

In the following, we provide a brief introduction to the individual chapters of this book. Chapter 1 by Flockerzi gives an “Introduction to the Geometric Theory of Ordinary Differential Equations with Applications to Chemical Processes”. Though providing the fundamentals of the geometric theory of differential equations in a general setting, it is tailored to applications to (bio-)chemical reaction networks and chemical separation processes. Thus, quite often, the ordinary differential equations under investigation are derived from underlying partial differential equations as in the search for solutions of quasi-linear partial differential equations by the method of characteristics. The *geometric theory* addresses invariant and integral manifolds, e.g., center manifolds for bifurcation problems and slow invariant manifolds for networks with slow and fast variables and/or processes. In applications, the associated reduction methods are based on suitable quasi-stationary approximations of such (slow) invariant manifolds. Several model problems illustrate applications of the derived methods to different instances of chemical reaction networks.

In the second chapter, Reis introduces “Circuit Modelling with Differential–Algebraic Equations”. Electrical circuits underlie most electronic devices in everyday life, ranging from computers to tablets and cell phones to car electronics. Mathematical models of these circuits are based on graph and network theory and are the core of circuit and device simulation in industrial design processes. The chapter provides a basic and self-contained introduction to the mathematical description of electrical circuits consisting of resistances, capacitances, inductances, as well as voltage and current sources. The standard methods for the modeling of circuits by differential–algebraic equations—“modified nodal analysis” and “modified loop analysis”—are presented, and a detailed analysis of the mathematical properties of these equations is included.

The third chapter by Egerstedt, de la Croix, and Kingston on “Interacting with Networks of Mobile Agents” discusses the design of control, communication, and coordination strategies for multi-agent networks, a central issue in current research in systems and control theory. Applications of distributed, mobile agent systems or “swarms” include, but are by no means limited to, multi-agent robotics, distributed sensor networks, interconnected manufacturing chains, and data networks. The question discussed is how humans can control or influence the behavior of the swarm. Lagrangian and Eulerian models are proposed to model the movements of the agents. Both of them are amenable to human manipulation. Interaction of the agents are modeled by graphs/networks, and controllability and manipulability notions for the human-swarm interaction are introduced, based on which control strategies are developed.

Chapter 4 “Combinatorial Optimization: The Interplay of Graph Theory, Linear and Integer Programming Illustrated on Network Flow” by Wagler deals with combinatorial optimization which is the main mathematical discipline dealing with optimizing networks. It uses basic elements from graph theory, geometry, linear and integer programming. The network flow problem is used as a running example to illustrate the concepts and methods introduced. It does not require prior knowledge in advanced optimization techniques. Basic introductions into linear programming, including the simplex method, and integer programming are provided.

The 5th chapter, by Klamt, Hädicke, and von Kamp, is dedicated to the "Stoichiometric and Constraint-Based Analysis of Biochemical Reaction Networks". Although the methods presented therein rely solely on the stoichiometry of metabolic networks, they provide essential information on key functional properties and deliver various testable predictions. The chapter presents the relevant mathematical foundations of different approaches of this kind and discusses various applications in biology and biotechnology.

The contribution of Blätke, Rohr, Heiner, and Marwan in Chap. 6 is focused on "A Petri Net Based Framework for Biomodel Engineering". Petri nets provide a versatile framework for the computation of biochemical reaction networks and gene regulatory networks, particularly useful in the context of systems biology. Starting with basic definitions, the authors provide an introduction to different classes of Petri nets, static and dynamic modeling applications, database-assisted automatic composition and modification of Petri nets as well as automatic reconstruction of networks based on time series data sets.

In Chap. 7, "Hybrid Modeling for Systems Biology", von Stosch, Carinhas and Oliveira deal with the theoretical fundamentals of hybrid semi-parametric modeling to integrate extensive experimental data sets obtained by "omics" technologies developed over recent years into global quantitative models. Their approach combines available knowledge about mechanisms in the form of parametric mathematical models (bottom-up) with nonparametric models that are determined from experimental data (top-down). Examples are given for small metabolic networks of insect cells (*Spodoptera frugiperda*, Sf9) used for production of baculoviruses, dynamic models of metabolism of animal cells (baby hamster kidney, BHK) in fed-batch cultures with unknown reaction kinetics, and a signal transduction network involving transcription factor A (TFA) with intrinsic time delays.

Finally, we would like to express our gratitude to all authors of the chapters in this book for their dedicated effort to provide useful tutorials, a task often much more time consuming than writing about latest research results to an informed community. Numerous experts in network theory and applications served as reviewers for the chapters. We are very grateful for their help in improving readability and tutorial value of the individual manuscripts. Last but not least, our thanks go to Barbara Hellriegel and Katherina Steinmetz from Springer Basel AG for their never ending endurance in waiting for the final manuscript as well as their support throughout the development of this project.

Magdeburg
June 23, 2014

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