

Computational Systems Biology in Cancer: Modeling Methods and Applications

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Abstract: In recent years it has become clear that carcinogenesis is a complex process, both at the molecular and cellular levels. Understanding the origins, growth and spread of cancer, therefore requires an integrated or system-wide approach. Computational systems biology is an emerging sub-discipline in systems biology that utilizes the wealth of data from genomic, proteomic and metabolomic studies to build computer simulations of intra and intercellular processes. Several useful descriptive and predictive models of the origin, growth and spread of cancers have been developed in an effort to better understand the disease and potential therapeutic approaches. In this review we describe and assess the practical and theoretical underpinnings of commonly-used modeling approaches, including ordinary and partial differential equations, petri nets, cellular automata, agent based models and hybrid systems. A number of computer-based formalisms have been implemented to improve the accessibility of the various approaches to researchers whose primary interest lies outside of model development. We discuss several of these and describe how they have led to novel insights into tumor genesis, growth, apoptosis, vascularization and therapy.

Keywords: cancer, computational systems biology, simulation, modeling, cellular automata

Background

Living organisms are complex systems. Nowhere is this complexity more evident than in the genesis and development of cancer. While cancer may originate from genetic and molecular changes that occur in a single cell, the subsequent proliferation, migration and interaction with other cells is crucial to its further development. In their landmark paper, Hanahan and Weinberg described six hallmarks they thought necessary for the transition from normal cells to invasive cancers (Hanahan and Weinberg, 2000). These included: 1) self-sufficiency in growth signals, 2) insensitivity to growth inhibitory signals, 3) evading apoptosis, 4) limitless replicative potential, 5) sustained angiogenesis, and 6) tissue invasion and metastasis. While genetic instability was not explicitly included in this list, it was included as an implicit enabling alteration that might start a normal cell down a mutagenic pathway leading to the acquisition of one or more of these essential characteristics.

The molecules that govern the cell growth and division cycle in response to external and internal signals are numerous and interact through complex, multiply-connected pathways over a wide range of temporal and spatial scales. Tumors reflect this complexity in that they are composed of several different cell types that interact to create malignant growth (Burkert et al. 2006). Despite the widespread acceptance of this complexity, the majority of biological and biomedical studies still utilize a strictly reductionist approach, focusing on the interactions of at most a few genes or proteins in each experiment. Systems biology, an integrative discipline that attempts to describe and understand biology as systems of interconnected components, has arisen partly as a response to these traditional reductionist approaches. Systems biology is a young field made possible by the explosion of data from genomic, transcriptomic, proteomic and metabolomic techniques developed within the last decade (Hollywood et al. 2006; Bugrim et al. 2004; Jares, 2006).

Computational systems biology, which is a sub-discipline of systems biology, has developed both as a tool supporting the processing of these massive amounts of data and as a modeling discipline, building upon this "omic" data in order to predict biological behavior (Ideker et al. 2001a; Alberghina et al. 2004). Not surprisingly, both experimental and computational systems biology approaches have provided fruitful insights into cancer.

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Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis

Brendan G. Carr



Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis:

Computational Systems Biology Stefan M. Kallenberger, Stefan Legewie, Roland Eils, 2013-11-26 Apoptosis is a form of cellular suicide central to various aspects in biology including tissue homeostasis and embryonic development It is typically dysregulated in cancer Understanding the apoptotic signal transduction network is thus a central goal of cancer research Quantitative modeling approaches provided valuable insights into determinants of cell fate decisions and promise to become a valuable tool to optimize therapeutic strategies In this chapter we summarize modeling approaches used in systems biology of apoptosis In addition we give an overview of apoptosis related research questions that can be addressed by modeling Moreover we review top down and bottom up modeling approaches applied to apoptosis and particularly focus on ordinary differential equation ODE modeling We describe bistability temporal switching crosstalk between death and survival and discuss approaches to model cell to cell variability Computational Systems Biology Andres Kriete, Roland Eils, 2013-11-26

This comprehensively revised second edition of Computational Systems Biology discusses the experimental and theoretical foundations of the function of biological systems at the molecular cellular or organismal level over temporal and spatial scales as systems biology advances to provide clinical solutions to complex medical problems In particular the work focuses on the engineering of biological systems and network modeling Logical information flow aids understanding of basic building blocks of life through disease phenotypes Evolved principles gives insight into underlying organizational principles of biological organizations and systems processes governing functions such as adaptation or response patterns Coverage of technical tools and systems helps researchers to understand and resolve specific systems biology problems using advanced computation Multi scale modeling on disparate scales aids researchers understanding of dependencies and constraints of spatio temporal relationships fundamental to biological organization and function **Computational Systems Biology**

Roland Eils, Andres Kriete, 2013-11-26 *An Introduction to Computational Systems Biology* Karthik Raman, 2021-05-30 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 others Genome Research ,2007 **Index Medicus** ,2002 Vols for 1963 include as pt 2 of the Jan issue Medical

subject headings Numerical Methods and Advanced Simulation in Biomechanics and Biological Processes Miguel Cerrolaza, Sandra Shefelbine, Diego Garzón-Alvarado, 2017-12-28 Numerical Methods and Advanced Simulation in Biomechanics and Biological Processes covers new and exciting modeling methods to help bioengineers tackle problems for which the Finite Element Method is not appropriate The book covers a wide range of important subjects in the field of numerical methods applied to biomechanics including bone biomechanics tissue and cell mechanics 3D printing computer assisted surgery and fluid dynamics Modeling strategies technology and approaches are continuously evolving as the knowledge of biological processes increases Both theory and applications are covered making this an ideal book for researchers students and R D professionals Provides non conventional analysis methods for modeling Covers the Discrete Element Method DEM Particle Methods PM MessLess and MeshFree Methods MLMF Agent Based Methods ABM Lattice Boltzmann Methods LBM and Boundary Integral Methods BIM Includes contributions from several world renowned experts in their fields Compares pros and cons of each method to help you decide which method is most applicable to solving specific problems **American Book Publishing Record** ,2003 **Advanced Computing in Industrial Mathematics** Krassimir Georgiev, Michail Todorov, Ivan Georgiev, 2017-10-25 This book presents recent research on Advanced Computing in Industrial Mathematics which is one of the most prominent interdisciplinary areas bringing together mathematics computer science scientific computations engineering physics chemistry medicine etc Further the book presents the major tools used in Industrial Mathematics which are based on mathematical models and the corresponding computer codes which are used to perform virtual experiments to obtain new data or to better understand previous experimental findings The book gathers the peer reviewed papers presented at the 11th Annual Meeting of the Bulgarian Section of SIAM BGSIAM from December 20 to 22 2016 in Sofia Bulgaria *Cancer Research* ,2009-06

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Table of Contents Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis

1. Understanding the eBook Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - The Rise of Digital Reading Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Advantages of eBooks Over Traditional Books
2. Identifying Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform

- Popular eBook Platforms
 - Features to Look for in an Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - User-Friendly Interface
4. Exploring eBook Recommendations from Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Personalized Recommendations
 - Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis User Reviews and Ratings
 - Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis and Bestseller Lists
 5. Accessing Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis Free and Paid eBooks
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 6. Navigating Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis eBook Formats
 - ePub, PDF, MOBI, and More
 - Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis Compatibility with Devices
 - Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis Enhanced eBook Features
 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Highlighting and Note-Taking Computational Systems Biology Chapter 19 Applications In Cancer Research

Mathematical Models Of Apoptosis

- Interactive Elements Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
8. Staying Engaged with Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 9. Balancing eBooks and Physical Books Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
 11. Cultivating a Reading Routine Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Setting Reading Goals Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Carving Out Dedicated Reading Time
 12. Sourcing Reliable Information of Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Fact-Checking eBook Content of Computational Systems Biology Chapter 19 Applications In Cancer Research Mathematical Models Of Apoptosis
 - Distinguishing Credible Sources
 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development

- Exploring Educational eBooks

14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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