Francesc Font Tim Myers *Eds*.

Multidisciplinary Mathematical Modelling

Applications of Mathematics to the Real World





SEMA SIMAI Springer Series

ICIAM 2019 SEMA SIMAI Springer Series

Volume 11

Editor-in-Chief

Amadeu Delshams, Departament de Matemàtiques and Laboratory of Geometry and Dynamical Systems, Universitat Politècnica de Catalunya, Barcelona, Spain

Series Editors

Francesc Arandiga Llaudes, Departamento de Matemàtica Aplicada, Universitat de València, Valencia, Spain

Macarena Gómez Mármol, Departamento de Ecuaciones Diferenciales y Análisis Numérico, Universidad de Sevilla, Sevilla, Spain

Francisco M. Guillén-González, Departamento de Ecuaciones Diferenciales y Análisis Numérico, Universidad de Sevilla, Sevilla, Spain

Francisco Ortegón Gallego, Departamento de Matemáticas, Facultad de Ciencias del Mar y Ambientales, Universidad de Cádiz, Puerto Real, Spain

Carlos Parés Madroñal, Departamento Análisis Matemático, Estadística e I.O., Matemática Aplicada, Universidad de Málaga, Málaga, Spain

Peregrina Quintela, Department of Applied Mathematics, Faculty of Mathematics, Universidade de Santiago de Compostela, Santiago de Compostela, Spain

Carlos Vázquez-Cendón, Department of Mathematics, Faculty of Informatics, Universidade da Coruña, A Coruña, Spain

Sebastià Xambó-Descamps, Departament de Matemàtiques, Universitat Politècnica de Catalunya, Barcelona, Spain

This sub-series of the SEMA SIMAI Springer Series aims to publish some of the most relevant results presented at the ICIAM 2019 conference held in Valencia in July 2019.

The sub-series is managed by an independent Editorial Board, and will include peer-reviewed content only, including the Invited Speakers volume as well as books resulting from mini-symposia and collateral workshops.

The series is aimed at providing useful reference material to academic and researchers at an international level.

More information about this subseries at http://www.springer.com/series/16499

Francesc Font • Tim G. Myers Editors

Multidisciplinary Mathematical Modelling

Applications of Mathematics to the Real World



Editors
Francesc Font
Centre de Recerca Matemàtica
Bellaterra
Barcelona, Spain

Tim G. Myers Centre de Recerca Matemàtica Bellaterra Barcelona, Spain

ISSN 2199-3041 ISSN 2199-305X (electronic)
SEMA SIMAI Springer Series
ISSN 2662-7183 ISSN 2662-7191 (electronic)
ICIAM 2019 SEMA SIMAI Springer Series
ISBN 978-3-030-64271-6 ISBN 978-3-030-64272-3 (eBook)
https://doi.org/10.1007/978-3-030-64272-3

@ The Editor(s) (if applicable) and The Author(s), under exclusive license to Springer Nature Switzerland AG 2021

This work is subject to copyright. All rights are solely and exclusively licensed by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG. The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Preface

Since 2014, the Centre de Recerca Matemática (CRM) received PhD and post-doctoral funding from the La Caixa Foundation and the CERCA Programme of the Generalitat de Catalunya to carry out "interdisciplinary and collaborative research". These projects have been supervised by members of the CRM and also university researchers from biology, physics, nanoscience as well as local research centres. This has led to a broad range of research lines where, due to the influence of the non-mathematical partners, the focus has been firmly on practical problems.

In this book, we present work from a selection of talks resulting from this research and presented at the "International Congress on Industrial and Applied Mathematics", held in Valencia, 2019. The various chapters describe a wide variety of topics: cancer modelling, carbon capture by adsorption, nanoscale diffusion and complex systems to predict earthquakes. These mathematical studies were specifically aided via collaborations with biomedical engineers, physicists and chemists.

The wide range of topics described in this book reflects not only the multidisciplinary nature of the La Caixa programme but also the true versatility of mathematics.

Barcelona, Spain August 2020 Francesc Font Tim G. Myers

Contents

Spatiotemporal Dynamics of Cancer Phenotypic Quasispecies	
Under Targeted Therapy	1
Celia Penella, Tomás Alarcón, and Josep Sardanyés	
Guyer-Krumhansl Heat Conduction in Thermoreflectance	
Experiments	21
Matthew G. Hennessy and Tim G. Myers	
A Mathematical Model of Carbon Capture by Adsorption	35
Francesc Font, Tim G. Myers, and Matthew G. Hennessy	
Diffusion Processes at Nanoscale	49
Claudia Fanelli	
Maximum Likelihood Estimation of Power-Law Exponents for	
Testing Universality in Complex Systems	65
Víctor Navas-Portella, Álvaro González, Isabel Serra, Eduard Vives,	
and Álvaro Corral	

Editors and Contributors

About the Editors

Francesc Font received his PhD in Applied Mathematics from the Universitat Politècnica de Catalunya in 2014, and he is currently a Juan de la Cierva research fellow at the Centre de Recerca Matemàtica. He specialises in the mathematical modelling of transport phenomena and has worked on topics such as nanoscale heat transfer, Li-ion batteries or cell motility. Part of his research is in collaboration with industry, and he has been involved in industrial mathematics workshops throughout Europe.

Tim G. Myers is a Senior Researcher at the Centre de Recerca Matemàtica, Adjunct Professor at the Universitat Politecnica de Catalunya and Adjunct Professor of Industrial Mathematics at the University of Limerick. He has been involved in a wide variety of Industrial Mathematics initiatives and is currently the co-ordinator for all European Study Groups with Industry. He is a co-author of "Optics Near Surfaces and at the Nanometer Scale" and has written over 90 journal publications on a range of applied mathematics topics.

Contributors

Tomás Alarcón ICREA, Barcelona, Spain

Departament de Matemàtiques, Universitat Autònoma de Barcelona, Barcelona, Spain

Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain

Álvaro Corral Barcelona Graduate School of Mathematics, Barcelona, Spain Complexity Science Hub Vienna, Vienna, Austria

Departament de Matemàtiques, Universitat Autònoma de Barcelona, Barcelona, Spain

Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain

x Editors and Contributors

Claudia Fanelli Universitat Politècnica de Catalunya, Barcelona, Spain

Francesc Font Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain

Álvaro González Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain GFZ German Research Centre for Geosciences, Potsdam, Germany

Matthew G. Hennessy Mathematical Institute, University of Oxford, Oxford, UK

Tim G. Myers Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain

Víctor Navas-Portella Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain

Barcelona Graduate School of Mathematics, Barcelona, Spain Facultat de Matemàtiques i Informàtica, Universitat de Barcelona, Barcelona, Spain

Celia Penella Universitat Pompeu Fabra, Barcelona, Spain

Josep Sardanyés Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain

Isabel Serra Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain Barcelona Supercomputing Center, Barcelona, Spain

Eduard Vives Departament de Matèria Condensada, Facultad de Física, Universitat de Barcelona, Barcelona, Catalonia, Spain

Universitat de Barcelona Institute of Complex Systems (UBICS), Facultat de Física, Universitat de Barcelona, Barcelona, Catalonia, Spain

Spatiotemporal Dynamics of Cancer Phenotypic Quasispecies Under Targeted Therapy



1

Celia Penella, Tomás Alarcón, and Josep Sardanyés

Abstract Cancer cells have an enormous genetic and phenotypic heterogeneity. Despite modelling this heterogeneity is not trivial, several mathematical and computational models have used the so-called quasispecies theory. This theory, originally conceived to describe the evolution of information in prebiotic systems, has also been applied to investigate fast evolving replicons with large mutation rates, such as RNA viruses and cancer cells. Here, we investigate a quasispecies system composed of healthy and cancer cells with different phenotypic traits. The phenotypes of tumour cells are coded by binary strings including three different compartments with genes involved in cells' proliferation, in genomic stability, and the so-called housekeeping genes. Previous works have studied this system in well-mixed settings with autonomous ordinary differential equations and stochastic bit-string models. Here, we extend the stochastic bit-strings approach to a spatially explicit system using a cellular automaton (CA). In agreement with the prediction of the wellmixed systems, the spatial one also shows a transition towards tumour extinction at increasing tumour cells' mutation rates, displaying however different stationary distributions of cancer phenotypes. We also use the CA to simulate targeted cancer therapies against different tumour phenotypes. Our results indicate that a combination therapy targetting the fastest proliferative cancer cells with and without

C. Penella

Universitat Pompeu Fabra, Barcelona, Spain

T. Alarcón

ICREA, Barcelona, Spain

Departament de Matemàtiques, Universitat Autònoma de Barcelona, Cerdanyola del Vallès, Barcelona, Spain

Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain

e-mail: talarcon@crm.cat

J. Sardanyés (⊠)

Centre de Recerca Matemàtica, Bellaterra, Barcelona, Spain

e-mail: jsardanyes@crm.cat

© The Author(s), under exclusive license to Springer Nature Switzerland AG 2021 F. Font, T. G. Myers (eds.), *Multidisciplinary Mathematical Modelling*, SEMA SIMAI Springer Series 11, https://doi.org/10.1007/978-3-030-64272-3_1