Lecture Notes in Computer Science

Commenced Publication in 1973 Founding and Former Series Editors: Gerhard Goos, Juris Hartmanis, and Jan van Leeuwen

Editorial Board

David Hutchison Lancaster University, UK Takeo Kanade Carnegie Mellon University, Pittsburgh, PA, USA Josef Kittler University of Surrey, Guildford, UK Jon M. Kleinberg Cornell University, Ithaca, NY, USA Friedemann Mattern ETH Zurich. Switzerland John C. Mitchell Stanford University, CA, USA Moni Naor Weizmann Institute of Science, Rehovot, Israel Oscar Nierstrasz University of Bern, Switzerland C. Pandu Rangan Indian Institute of Technology, Madras, India Bernhard Steffen University of Dortmund, Germany Madhu Sudan Massachusetts Institute of Technology, MA, USA Demetri Terzopoulos University of California, Los Angeles, CA, USA Doug Tygar University of California, Berkeley, CA, USA Moshe Y. Vardi Rice University, Houston, TX, USA Gerhard Weikum Max-Planck Institute of Computer Science, Saarbruecken, Germany Hirokazu Anai Katsuhisa Horimoto Temur Kutsia (Eds.)

Algebraic Biology

Second International Conference, AB 2007 Castle of Hagenberg, Austria, July 2-4, 2007 Proceedings



Volume Editors

Hirokazu Anai CREST, Japan Science and Technology Agency Honcho, Kawaguchi 332-0012, Japan E-mail: anai@jp.fujitsu.com

Katsuhisa Horimoto National Institute of Advanced Industrial Science and Technology (AIST) Computational Biology Research Center (CBRC) Tokyo, 135-0064, Japan E-mail: k.horimoto@aist.go.jp

Temur Kutsia Johannes Kepler University Research Institute for Symbolic Computation 4040 Linz, Austria E-mail: Temur.Kutsia@risc.uni-linz.ac.at

Library of Congress Control Number: 2007929551

CR Subject Classification (1998): F.3.1, F.4, D.2.4, I.1, J.3

LNCS Sublibrary: SL 1 - Theoretical Computer Science and General Issues

ISSN	0302-9743
ISBN-10	3-540-73432-5 Springer Berlin Heidelberg New York
ISBN-13	978-3-540-73432-1 Springer Berlin Heidelberg New York

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, re-use of illustrations, recitation, broadcasting, reproduction on microfilms or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer. Violations are liable to prosecution under the German Copyright Law.

Springer is a part of Springer Science+Business Media

springer.com

© Springer-Verlag Berlin Heidelberg 2007 Printed in Germany

Typesetting: Camera-ready by author, data conversion by Scientific Publishing Services, Chennai, IndiaPrinted on acid-free paperSPIN: 1208636806/31805 4 3 2 1 0

Preface

This volume contains the proceedings of the 2nd International Conference on Algebraic Biology (AB2007). It was held during July 2–4, 2007 in the Castle of Hagenberg, Austria, and was organized by the Research Institute for Symbolic Computation (RISC) of the Johannes Kepler University, Linz.

Algebraic biology is the interdisciplinary forum for the presentation of research on all aspects of applications of symbolic computation (computer algebra, computational logic, and related methods) in biology. The first conference on algebraic biology (AB 2005) was held during November 28–30, 2005 in Tokyo, Japan.

The initiation of the series of algebraic biology conferences was motivated by the recent trends in symbolic computation and biology: In symbolic computation, the recent advances in computer performance and algorithmic methods have accelerated the extension of the scientific fields to which symbolic computation can be applied. In biology, the determination of complete genomic sequences and the subsequent improvements of experimental techniques have yielded large amounts of information about the biological molecules underlying various biological phenomena. Under these circumstances, the marriage of symbolic computation and biology is expected to generate new algebraic models for biological phenomena and new symbolic techniques for biological data analysis.

This remains the intended profile of the series of algebraic biology conferences, and it figured in the manuscripts published in AB 2007. The papers in the present volume are evidence of the healthy growth in the field of algebraic biology.

We received 40 submissions from 22 countries (Armenia, Australia, Bulgaria, Canada, Chile, France, Germany, Greece, Hungary, India, Italy, Japan, Portugal, Romania, Russia, Spain, South Africa, Switzerland, Taiwan, The Netherlands, UK, and USA), and 19 papers were accepted for publication. Each submission was assigned to at least three Program Committee members, who carefully reviewed the papers, in many cases with the help of external referees. The merits of the submissions were discussed by the Program Committee over one week through the Internet, by means of the EasyChair conference management system.

Besides the contributed papers, this volume also includes three invited papers, by Reinhard Laubenbacher (Discrete Models of Biochemical Networks: The Toric Variety of Nested Canalyzing Functions), Bud Mishra (Algebraic Systems Biology: Theses and Hypotheses), and Gheorghe Paun (Membrane Computing as a Framework for Bio-Modeling).

The tutorial session of the conference provided an opportunity for scientists in symbolic computation and biology to come together and learn about each others' research problems and problem-solving techniques. The session consisted of five symbolic computation and five biology tutorials. Four tutorial speakers submitted their papers to the proceedings. These papers are included in this volume.

We are pleased to start our collaboration with Springer, who agreed to publish the conference proceedings in the *Lecture Notes in Computer Science* series.

We, the AB Steering Committee, and the organizers of the conference, are grateful to the following sponsors for their financial contributions towards its operation and success: Austrian Grid, Linzer Hochschulfonds, MapleSoft, the National Institute of Advanced Industrial Science and Technology, Raiffeisen Landesbank Oberösterreich, RISC Software GmbH, Special Research Program SFB F013 of the Austrian Science Fund (FWF), and the Upper Austrian Government.

Our thanks are also due to the members of the Program Committee and the additional referees, and to those who ensured the effective running of the conference.

July 2007

Hirokazu Anai Bruno Buchberger Hoon Hong Katsuhisa Horimoto Temur Kutsia

Conference Organization

Conference Chairs

Hirokazu Anai	Fujitsu Laboratories Ltd., Japan
Bruno Buchberger	Johannes Kepler University of Linz, Austria
Hoon Hong	North Carolina State University, USA
Katsuhisa Horimoto	National Institute of Advanced Industrial Science
	and Technology, Japan

Program Chairs

Hirokazu Anai	Fujitsu Laboratories Ltd., Japan
Katsuhisa Horimoto	National Institute of Advanced Industrial Science
	and Technology, Japan
Temur Kutsia	Johannes Kepler University of Linz, Austria

Program Committee

Tatsuya Akutsu	Kyoto University, Japan
Armin Biere	Johannes Kepler University of Linz, Austria
Bruno Buchberger	Johannes Kepler University of Linz, Austria
Vincenzo Capasso	Università degli studi di Milano, Italy
Luca Cardelli	Microsoft Research, Cambridge, UK
Gautam Dasgupta	Columbia University, USA
François Fages	INRIA Rocquencourt, France
Shinji Hara	University of Tokyo, Japan
Sepp Hochreiter	Johannes Kepler University of Linz, Austria
Hoon Hong	North Carolina State University, USA
Hans Irschik	Johannes Kepler University of Linz, Austria
Erich Kaltofen	North Carolina State University, USA
Veikko Keränen	Rovaniemi University of Applied Sciences, Finland
James F. Lynch	Clarkson University, USA
Manfred Minimair	Seton Hall University, USA
Enno Ohlebusch	University of Ulm, Germany
Stanly Steinberg	University of New Mexico, USA
Bernd Sturmfels	University of California at Berkeley, USA
Carolyn L. Talcott	SRI International, USA
Ashish Tiwari	SRI International, USA

Jens Volkert	Johannes Kepler University of Linz, Austria
Dongming Wang	Beihang University, China and UPMC-CNRS, France
Kazuhiro Yokoyama	Rikkyo University, Japan
Ruriko Yoshida	Duke University, USA

Invited Speakers

Reinhard Laubenbacher	Virginia Bioinformatics Institute, USA
Bud Mishra	New York University, USA
Gheorghe Păun	Institute of Mathematics, Romanian Academy,
	Romania

Tutorial Speakers

Sachiyo Aburatani	National Institute of Advanced Industrial Science and Technology, Japan
Nobuhiro Go	Japan Atomic Energy Agency
John Harrison	Intel Corporation
Hoon Hong	North Carolina State University, USA
Hans Irschik	Johannes Kepler University of Linz, Austria
Veikko Keränen	Rovaniemi University of Applied Sciences, Finland
Francis Thackeray	Transvaal Museum, Northern Flagship Institution,
	South Africa
Hiroyuki Toh	Kyushu University, Japan
Bridget S. Wilson	University of New Mexico, USA
Limsoon Wong	National University of Singapore

Local Organization

Betina Curtis	Johannes Kepler University of Linz, Austria
Temur Kutsia	Johannes Kepler University of Linz, Austria

External Reviewers

Andreas Deutsch	Irina Kogan
Kord Eickmeyer	Sung Koh
Martin Giese	Richard Mayr
Tomohisa Hayakawa	Andrew Millar
Steffen Heber	Stefan Müller
Monika Heiner	Jose Carlos Nacher
Meng Jin	Wei Niu
Manuel Kauers	Dirk Nowotka

Andy Poggio Luis-Garcia Puente Sven Rahmann Georg Regensburger Adrien Richard Paul Ruet Peter Ruoff Eberhard Voit Andreas Weber Bican Xia Hitoshi Yanami

Sponsors

Austrian Grid Linzer Hochschulfonds MapleSoft National Institute of Advanced Industrial Science and Technology, Japan Raiffeisen Landesbank Oberösterreich RISC Software GmbH Special Research Program SFB F013 of the Austrian Science Fund (FWF) Upper Austrian Government

Table of Contents

Algebraic Systems Biology: Theses and Hypotheses (Invited Talk) Bud Mishra	1
Discrete Models of Biochemical Networks: The Toric Variety of Nested Canalyzing Functions (Invited Talk) Abdul S. Jarrah and Reinhard Laubenbacher	15
Membrane Computing as a Framework for Bio-modeling (An Informal Glimpse) (Invited Talk) Gheorghe Păun	23
Relating Attractors and Singular Steady States in the Logical Analysis of Bioregulatory Networks	36
Translating Time-Course Gene Expression Profiles into Semi-algebraic Hybrid Automata Via Dimensionality Reduction	51
On Proving the Absence of Oscillations in Models of Genetic Circuits François Boulier, Marc Lefranc, François Lemaire, Pierre-Emmanuel Morant, and Aslı Ürgüplü	66
Attenuation Regulation as a Term Rewriting System Eugene Asarin, Thierry Cachat, Alexander Seliverstov, Tayssir Touili, and Vassily Lyubetsky	81
Glucose-Insulin Control of Type1 Diabetic Patients in H_2/H_{∞} Space Via Computer Algebra	95
Exact Parameter Determination for Parkinson's Disease Diagnosis with PET Using an Algebraic Approach <i>Hiroshi Yoshida, Koji Nakagawa, Hirokazu Anai, and</i> <i>Katsuhisa Horimoto</i>	110
Efficient Haplotype Inference with Pseudo-boolean Optimization Ana Graça, João Marques-Silva, Inês Lynce, and Arlindo L. Oliveira	125
An Algebraic Algorithm for the Identification of Glass Networks with Periodic Orbits Along Cyclic Attractors Igor Zinovik, Daniel Kroening, and Yury Chebiryak	140

Analyzing Pathways Using SAT-Based Approaches Ashish Tiwari, Carolyn Talcott, Merrill Knapp, Patrick Lincoln, and Keith Laderoute	155
Algorithmic Algebraic Model Checking IV: Characterization of Metabolic Networks Venkatesh Mysore and Bud Mishra	170
Cascaded Games Jittisak Senachak, Mun'delanji Vestergaard, and René Vestergaard	185
On Differential Algebraic Decision Methods for the Estimation of Anaerobic Digestion Models Elena Chorukova, Sette Diop, and Ivan Simeonov	202
Protein Structure Prediction Using Residual Dipolar Couplings Ioannis Z. Emiris and Sotirios I. Pantos	217
A Stochastic Pi Calculus for Concurrent Objects Céline Kuttler, Cédric Lhoussaine, and Joachim Niehren	232
Modeling Static Biological Compartments with Beta-binders Maria Luisa Guerriero, Corrado Priami, and Alessandro Romanel	247
Deducing Interactions in Partially Unspecified Biological Systems Paolo Baldan, Andrea Bracciali, Linda Brodo, and Roberto Bruni	262
Reduction of Algebraic Parametric Systems by Rectification of Their Affine Expanded Lie Symmetries	277
Prefix Reversals on Binary and Ternary Strings Cor Hurkens, Leo van Iersel, Judith Keijsper, Steven Kelk, Leen Stougie, and John Tromp	292
Toric Ideals of Phylogenetic Invariants for the General Group-Based Model on Claw Trees $K_{1,n}$ Julia Chifman and Sonja Petrović	307
Inference of Protein-Protein Interactions by Using Co-evolutionary Information (Tutorial Talk) Tetsuya Sato, Yoshihiro Yamanishi, Katsuhisa Horimoto, Minoru Kanehisa, and Hiroyuki Toh	322
A Short Survey of Automated Reasoning (Tutorial Talk) John Harrison	334
Inference of Complex Regulatory Network for the Cell Cycle System in Saccharomyces Cerevisiae (Tutorial Talk) Sachiyo Aburatani	350

Manifestation and Exploitation of Invariants in Bioinformatics (Tutorial	
Talk)	365
Limsoon Wong	
Author Index	379