

Lecture Notes in Bioinformatics

3082

Edited by S. Istrail, P. Pevzner, and M. Waterman

Editorial Board: A. Apostolico S. Brunak M. Gelfand
T. Lengauer S. Miyano G. Myers M.-F. Sagot D. Sankoff
R. Shamir T. Speed M. Vingron W. Wong

Subseries of Lecture Notes in Computer Science

Vincent Danos Vincent Schachter (Eds.)

Computational Methods in Systems Biology

International Conference CMSB 2004
Paris, France, May 26 - 28, 2004
Revised Selected Papers



Springer

Series Editors

Sorin Istrail, Celera Genomics, Applied Biosystems, Rockville, MD, USA
Pavel Pevzner, University of California, San Diego, CA, USA
Michael Waterman, University of Southern California, Los Angeles, CA, USA

Volume Editors

Vincent Danos
Université Paris 7
Equipe PPS Case 7014
2 place Jussieu, 75251 Paris Cedex 05, France
E-mail: Vincent.Danos@pps.jussieu.fr

Vincent Schachter
CNRG Genoscope
2 rue Gaston Cremieux, 91000 Evry, France
E-mail: vs@genoscope.cns.fr

Library of Congress Control Number: 2005922242

CR Subject Classification (1998): I.6, D.2.4, J.3, H.2.8, F.1.1

ISSN 0302-9743
ISBN 3-540-25375-0 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
springeronline.com

© Springer-Verlag Berlin Heidelberg 2005
Printed in Germany

Typesetting: Camera-ready by author, data conversion by Scientific Publishing Services, Chennai, India
Printed on acid-free paper SPIN: 11409083 06/3142 5 4 3 2 1 0

Preface

The Computational Methods in Systems Biology (CMSB) workshop series was established in 2003 by Corrado Priami. The purpose of the workshop series is to help catalyze the convergence between computer scientists interested in language design, concurrency theory, software engineering or program verification, and physicists, mathematicians and biologists interested in the systems-level understanding of cellular processes. Systems biology was perceived as being increasingly in search of sophisticated modeling frameworks whether for representing and processing system-level dynamics or for model analysis, comparison and refinement. One has here a clear-cut case of a must-explore field of application for the formal methods developed in computer science in the last decade.

This proceedings consists of papers from the CMSB 2003 workshop. A good third of the 24 papers published here have a distinct formal methods origin; we take this as a confirmation that a synergy is building that will help solidify CMSB as a forum for cross-community exchange, thereby opening new theoretical avenues and making the field less of a potential application and more of a real one. Publication in Springer's new Lecture Notes in Bioinformatics (LNBI) offers particular visibility and impact, which we gratefully acknowledge.

Our keynote speakers, Alfonso Valencia and Trey Ideker, gave challenging and somewhat humbling lectures: they made it clear that strong applications to systems biology are still some way ahead. We thank them all the more for accepting the invitation to speak and for the clarity and excitement they brought to the conference. We also wish to thank René Thomas for his keynote lecture on recent mathematical advances in the qualitative analysis of genetic regulation networks. As one can tell from the proceedings, his work has inspired many recent applications of formal methods to the engineering of biological models.

We are glad to take here the opportunity to express our gratitude to the members of the program committee and to the referees for their effort in the paper selection process and for their willingness to participate in the open-minded debate needed given the interdisciplinary nature of the area of computational systems biology. We would also like to thank the authors for their interest in the workshop and for their high-quality submissions and communications.

Finally, we wish to extend our warmest thanks to Monique Meugnier, Catherine Sarlande and Serge Smidtas for their invaluable help in organizing the workshop, and to the participating institutions, Genoscope, Genopole, CNRS, University of Paris 7, and the BioPathways Consortium, which provided financial support.

Conference web-site: <http://www.biopathways.org/CMSB04/>

Vincent Danos
Vincent Schachter

Table of Contents

Long Papers

An Explicit Upper Bound for the Approximation Ratio of the Maximum Gene Regulatory Network Problem <i>Sergio Pozzi, Gianluca Della Vedova, Giancarlo Mauri</i>	1
Autonomous Mobile Robot Control Based on White Blood Cell Chemotaxis <i>Matthew D. Onsum, Adam P. Arkin</i>	9
Beta Binders for Biological Interactions <i>Corrado Priami, Paola Quaglia</i>	20
Biomimetic in Silico Devices <i>C. Anthony Hunt, Glen E.P. Ropella, Michael S. Roberts, Li Yan</i>	34
Building and Analysing an Integrative Model of HIV-1 RNA Alternative Splicing <i>A. Bockmayr, A. Courtois, D. Eveillard, M. Vezain</i>	43
Graph-Based Modeling of Biological Regulatory Networks: Introduction of Singular States <i>Adrien Richard, Jean-Paul Comet, Gilles Bernot</i>	58
IMGT-Choreography: Processing of Complex Immunogenetics Knowledge <i>Denys Chaume, Véronique Giudicelli, Kora Combres, Chantal Ginestoux, Marie-Paule Lefranc</i>	73
Model Checking Biological Systems Described Using Ambient Calculus <i>Radu Mardare, Corrado Priami, Paola Quaglia, Oleksandr Vagin</i>	85
Modeling the Molecular Network Controlling Adhesion Between Human Endothelial Cells: Inference and Simulation Using Constraint Logic Programming <i>Eric Fanchon, Fabien Corblin, Laurent Trilling, Bastien Hermant, Danielle Gulino</i>	104
Modelling Metabolic Pathways Using Stochastic Logic Programs-Based Ensemble Methods <i>Huma Lodhi, Stephen Muggleton</i>	119

Projective Brane Calculus <i>Vincent Danos, Sylvain Pradalier</i>	134
Residual Bootstrapping and Median Filtering for Robust Estimation of Gene Networks from Microarray Data <i>Seiya Imoto, Tomoyuki Higuchi, SunYong Kim, Euna Jeong, Satoru Miyano</i>	149
Spatial Modeling and Simulation of Diffusion in Nuclei of Living Cells <i>Dietmar Volz, Martin Eigel, Chaitanya Athale, Peter Bastian, Harald Hermann, Constantin Kappel, Roland Eils</i>	161
The Biochemical Abstract Machine BIOCHAM <i>Nathalie Chabrier-Rivier, François Fages, Sylvain Soliman</i>	172
Towards Reusing Model Components in Systems Biology <i>Adeline M. Uhrmacher, Daniela Degenring, Jens Lemcke, Mario Kraehmer</i>	192
VICE: A Virtual Cell <i>D. Chiarugi, M. Curti, P. Degano, R. Marangoni</i>	207
Short Papers	
Biological Domain Identification Based in Codon Usage by Means of Rule and Tree Induction <i>Antonio Neme, Pedro Miramontes</i>	221
Black Box Checking for Biochemical Networks <i>Dragan Bošnački</i>	225
CMBSlib: A Library for Comparing Formalisms and Models of Biological Systems <i>Sylvain Soliman, François Fages</i>	231
Combining State-Based and Scenario-Based Approaches in Modeling Biological Systems <i>Jasmin Fisher, David Harel, E. Jane Albert Hubbard, Nir Piterman, Michael J. Stern, Naamah Swerdlin</i>	236
Developing SBML Beyond Level 2: Proposals for Development <i>Andrew Finney</i>	242

General Stochastic Hybrid Method for the Simulation of Chemical Reaction Processes in Cells <i>Martin Bentele, Roland Eils</i>	248
The Biodegradation Network, a New Scenario for Computational Systems Biology Research <i>Florencio Pazos, David Guijas, Manuel J. Gomez, Almudena Trigo, Victor de Lorenzo, Alfonso Valencia</i>	252
Invited Contributions	
Brane Calculi, Interactions of Biological Membranes <i>Luca Cardelli</i>	257
Author Index	279