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Corrado Priami (Ed.)

# Computational Methods in Systems Biology

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## Preface

Molecular biology has until now mainly focussed on individual molecules, on their properties as isolated entities or as complexes in very simple model systems. However, biological molecules in living systems participate in very complex networks, including regulatory networks for gene expression, intracellular metabolic networks and both intra- and intercellular communication networks. Such networks are involved in the maintenance (homeostasis) as well as the differentiation of cellular systems of which we have a very incomplete understanding.

Nevertheless, the progress in molecular biology has made possible the detailed description of the components that constitute living systems, notably genes and proteins. Large-scale genome sequencing means that we can (at least in principle) delineate all macromolecular components of a given cellular system, and microarray experiments as well as large-scale proteomics will soon give us large amounts of experimental data on gene regulation, molecular interactions and cellular networks. The challenge of the 21st century will be to understand how these individual components integrate into complex systems and the function and evolution of these systems, thus scaling up from molecular biology to systems biology. By combining experimental data with advanced formal theories from computer science, "the formal language for biological systems" to specify dynamic models of interacting molecular entities would be essential for: (i) understanding the normal behaviour of cellular processes, and how changes may affect the processes and cause disease – it may be possible to correlate genetic properties and symptoms in new and more efficient ways, based on an actual understanding of how various processes interact; (ii) providing predictability and flexibility to academic, pharmaceutical, biotechnology and medical researchers studying gene or protein functions. In particular, it may save time by reducing the number of experiments needed, if inadequate hypotheses can be excluded by computer simulation.

In response to the call for papers 39 were submitted to CMSB 2003. All the submitted papers were reviewed and the programme committee (listed below) selected 11 high-quality papers for publication in this volume. The care of the reviewers and of the programme committee members in reviewing the papers was surely valuable. A further 11 papers were selected only for presentation at the workshop in order to stimulate discussions (an abstract is included).

At the workshop Ehud Shapiro and Michael Stern gave two invited talks whose topics are described in papers included in this volume. The programme committee decided to accept for publication in this volume also some position papers that highlight the research trends in this new field of computational methods in systems biology. The reason is that because this is the first edition of a workshop in this fast-growing field a large view of potential topics of research was considered extremely important.

Rovereto, December 2002

Corrado Priami

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## Table of Contents

---

### I Invited Papers

---

Cells as Computation .....	1
<i>Amitai Regev and Ehud Shapiro</i>	
Formal Modeling of <i>C. elegans</i> Development: A Scenario-Based Approach ...	4
<i>Na'aman Kam, David Harel, Hillel Kugler, Rami Marely, Amir Pnueli, E. Jane Albert Hubbard, and Michael J. Stern</i>	

---

### II Regular Papers

---

Causal $\pi$ -Calculus for Biochemical Modelling .....	21
<i>Michele Curti, Pierpaolo Degano, and Cosima Tatiana Baldari</i>	
Graphs for Core Molecular Biology .....	34
<i>Vincent Danos and Cosimo Laneve</i>	
Contribution of Computational Tree Logic to Biological Regulatory Networks: Example from <i>Pseudomonas Aeruginosa</i> .....	47
<i>Sabine Peres and Jean-Paul Comet</i>	
Modeling Cellular Behavior with Hybrid Automata: Bisimulation and Collapsing .....	57
<i>Marco Antoniotti, Bhubaneswar Mishra, Carla Piazza, Alberto Policriti, and Marta Simeoni</i>	
Multiscale Modeling of Alternative Splicing Regulation .....	75
<i>Damien Eveillard, Delphine Ropers, Hidde de Jong, Christiane Branlant, and Alexander Bockmayr</i>	
A Method for Estimating Metabolic Fluxes from Incomplete Isotopomer Information .....	88
<i>Juho Rousu, Ari Rantanen, Hannu Maaheimo, Esa Pitkänen, Katja Saarela, and Esko Ukkonen</i>	
Dynamic Bayesian Network and Nonparametric Regression for Nonlinear Modeling of Gene Networks from Time Series Gene Expression Data .....	104
<i>SunYong Kim, Seiya Imoto, and Satoru Miyano</i>	

## VIII Table of Contents

Discrete Event Simulation for a Better Understanding of Metabolite Channeling – A System Theoretic Approach .....	114
<i>Daniela Degenring, Mathias Röhl, and Adelinde M. Uhrmacher</i>	
Mathematical Modeling of the Influence of RKIP on the ERK Signaling Pathway .....	127
<i>Kwang-Hyun Cho, Sung-Young Shin, Hyun-Woo Kim, Olaf Wolkenhauer, Brian McFerran, and Walter Kolch</i>	
A Method to Identify Essential Enzymes in the Metabolism: Application to <i>Escherichia Coli</i> .....	142
<i>Ney Lemke, Fabiana Herédia, Cláudia K. Barcellos, and José C. M. Mombach</i>	
Symbolic Model Checking of Biochemical Networks .....	149
<i>Nathalie Chabrier and François Fages</i>	

---

## III Presentation Abstracts

---

Coupled Oscillator Models for a Set of Communicating Cells .....	163
<i>Will Casey</i>	
Representing and Simulating Protein Functional Domains in Signal Transduction Using Maude .....	164
<i>Steven Eker, Keith Laderoute, Patrick Lincoln, M.G. Sriram, and Carolyn Talcott</i>	
A Core Modeling Language for the Working Molecular Biologist .....	166
<i>Marc Chiaverini and Vincent Danos</i>	
Integrating Simulation Packages via Systems Biology Mark-Up Language .....	167
<i>Manuel Corpas</i>	
Recreating Biopathway Databases towards Simulation .....	168
<i>Masao Nagasaki, Atsushi Doi, Hiroshi Matsuno, and Satoru Miyano</i>	
How to Synthesize an Optimized Genetic $\lambda$ -Switching System? A System-Theoretic Approach Based on SQP .....	170
<i>Kwang-Hyun Cho, Jong-Ho Cha, and Olaf Wolkenhauer</i>	
Simulation Study of the TNF $\alpha$ Mediated NF- $\kappa$ B Signaling Pathway .....	171
<i>Kwang-Hyun Cho, Sung-Young Shin, Hyeon-Woo Lee, and Olaf Wolkenhauer</i>	
Detection and Analysis of Unexpected State Components in Biological Systems .....	172
<i>Anastasia Pagnoni and Andrea Visconti</i>	

Model Validation of Biological Pathways Using Petri Nets – Demonstrated for Apoptosis .....	173
<i>Monika Heiner, Ina Koch, and Jürgen Will</i>	

An Overview of Data Models for the Analysis of Biochemical Pathways ...	174
<i>Yves Deville, David Gilbert, Jacques van Helden, and Shoshana Wodak</i>	

Discrete Event Systems and Client-Server Model for Signaling Mechanisms .....	175
<i>Gabriel Ciobanu and Dorin Huzum</i>	

---

#### **IV Position Papers**

Enhanced Operational Semantics in Systems Biology .....	178
<i>Pierpaolo Degano and Corrado Priami</i>	

Issues in Computational Methods for Functional Genomics and Systems Biology .....	182
<i>Magali Roux-Rouquié, Leroy Hood, Sandrine Imbeaud, and Charles Auffray</i>	

Integrating Biological Process Modelling with Gene Expression Data and Ontologies for Functional Genomics (Position Paper) .....	187
<i>Liviu Badea and Doina Tilicea</i>	

Computer Simulation of Protocells .....	194
<i>Doron Lancet</i>	

How to Solve Semantic Puzzles of Systems Biology .....	198
<i>Olaf Langmack</i>	

Evolution as Design Engineer .....	202
<i>David L. Dill and Patrick Lincoln</i>	

Inference, Modeling and Simulation of Gene Networks .....	207
<i>Satoru Miyano</i>	

<b>Author Index .....</b>	213
---------------------------	-----