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Alessandro Abate · Tatjana Petrov ·
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Computational Methods in Systems Biology

18th International Conference, CMSB 2020
Konstanz, Germany, September 23–25, 2020
Proceedings

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ISSN 0302-9743

ISSN 1611-3349 (electronic)

Lecture Notes in Bioinformatics

ISBN 978-3-030-60326-7

ISBN 978-3-030-60327-4 (eBook)

<https://doi.org/10.1007/978-3-030-60327-4>

LNCS Sublibrary: SL8 – Bioinformatics

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Preface

The 18th conference on Computational Methods in Systems Biology (CMSB 2020) was held during September 23–25, 2020. The conference was originally planned to be hosted by the University of Konstanz, but due to the COVID-19 pandemic, CMSB 2020 took place fully online. Recent editions of the CMSB conference series were organized by the University of Trieste (Italy), Masaryk University in Brno (Czech Republic), and TU Darmstad (Germany).

The scope of CMSB covers the analysis of biological systems, networks, data, and corresponding application domains. The conference brings together computer scientists, biologists, mathematicians, engineers, and physicists interested in a system-level understanding of biological processes. CMSB 2020 has retained the emphasis on system-level understanding of biological processes – by no means restricted to a narrow class of mathematical models – and has in particular stressed the importance of integrating the techniques developed separately in different areas. CMSB 2020 especially encouraged the presentation of new work concerning integration of machine learning techniques into modeling and analysis frameworks.

Topics featured in the workshop included formalisms for modeling biological processes, models and their biological applications, frameworks for model verification, validation, analysis, and simulation of biological systems, methods for synthetic biology and biomolecular computing, multi-scale modeling and analysis methods, collective behavior, high-performance computational systems biology, parallel implementations, and a new emphasis on machine learning for systems biology, model inference from experimental data, and model integration from biological databases.

CMSB 2020 was a three-day event, featuring three invited talks, two tutorials, single-track regular sessions, as well as an interactive session with tool presentations. The 30-minute presentations of regular papers and 20-minute presentations of tool papers were of high quality and the participation was lively, interactive, and stimulating.

45 Program Committee members helped to provide at least three reviews for each of the 30 submitted contributions, out of which 17 high-quality articles were accepted to be presented during the single-track sessions. Moreover, five tool paper submissions, each receiving three reviews for paper presentations, and two reviews from the Tool Evaluation Committee, were selected for presentation. All accepted contributions appear (a few after further feedback from a shepherding process by the Program Committee) as full papers in these proceedings. The articles were bundled into four thematic sessions, which is reflected in the organization of these proceedings: modeling and analysis; Boolean networks; identification and inference; and tools. We also hosted a session on tool papers, with five interactive tool demonstrations.

A highlight of CMSB 2020 was the presence of three high-profile invited speakers whom we also selected in view of the breadth of the event, covering formal and control theory methods, theoretical work and laboratory experiments, and modeling for

systems biology, and for collective animal behavior. Iain Couzin, Director of the Max Planck Institute of Animal Behavior, Department of Collective Behaviour and the Chair of Biodiversity and Collective Behaviour at the University of Konstanz, Germany, gave a seminar titled “Employing Immersive Virtual Reality to Reveal Common Geometric Principles of Individual and Collective Decision-Making.” Grégory Batt, a research scientist at Inria and at Institut Pasteur, France, gave a seminar titled “Methods and Tools for the Quantitative Characterization of Engineered Biomolecular Systems,” and Domitilla Del Vecchio, Professor of Mechanical Engineering at MIT, USA, gave a talk titled “Context dependence of biological circuits: Predictive models and engineering solutions.”

Further details on CMSB 2020 are featured on the website: <https://cmsb2020.uni-saarland.de>.

Finally, we would like to thank the local organizing team: Jacob Davidson, Matej Hajnal, Huy Phung, Stefano Tognazzi (University of Konstanz) for their supportive, can-do attitude. We thank to Stefano Tognazzi, for the technical and logistic solutions regarding streaming the conference online, as well as for organising the virtual tour of the city of Konstanz. We further thank to Jennifer Durai and Aamir Rizwani, for their engagement towards a smooth virtual experience for all presenters and participants. Thanks to Springer for continuing to host the CMSB proceedings in its Lecture Notes series. Thanks to the generous support of the Centre for the Advanced Study of Collective Behaviour (CASCb), it was possible to offer a free registration for the digital edition of CMSB 2020. Thanks to Ezio Bartocci, François Fages, and Jérôme Feret from the Steering Committee of CMSB for support and encouragement, to all the Program Committee members and additional reviewers for their great work in ensuring the quality of the contributions to CMSB 2020, as well as to all the participants for contributing to this memorable event. Thanks to Saarland University for hosting the web-domain of CMSB 2020 and to Whova Virtual Conference Platform for their services.

September 2020

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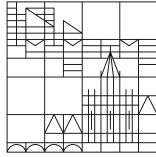
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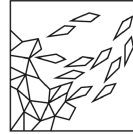
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Invited Talks

Context Dependence of Biological Circuits: Predictive Models and Engineering Solutions

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Abstract. Engineering biology has tremendous potential to impact applications, from energy, to environment, to health. As the sophistication of engineered biological circuits increases, the ability to predict system behavior becomes more limited. In fact, while a system's component may be well characterized in isolation, its salient properties often change in surprising ways once it interacts with other systems in the cell. This context-dependence of biological circuits makes it difficult to perform rational design and leads to lengthy, combinatorial, design procedures where each component is re-designed ad hoc when other parts are added to a system. In this talk, I will overview some causes of context-dependence. I will then focus on problems of resource loading and describe a design-oriented mathematical model that accounts for it. I will introduce a general engineering framework, grounded on control theoretic concepts, that can serve as a basis for creating devices that are "insulated" from context. Example devices will be introduced for both bacterial and mammalian genetic circuits. These solutions support rational and modular design of sophisticated genetic circuits and can serve for engineering biological circuits that are more reliable and predictable.

Methods and Tools for the Quantitative Characterization of Engineered Biomolecular Systems

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Abstract. Despite many years of research, no standard approach has emerged to rationally design novel genetic circuits implementing non-trivial functions. Synthetic biology still largely relies on tinkering. This comes notably from our limited capacities to quantitatively predict the behavior of biological systems in different cellular contexts. Iterative approaches, employing design-built-test-and-learn (DBTL) strategies, have the potential to circumvent this problem.

In this presentation, I will describe some of our efforts to develop an integrated framework supporting DBTL approaches. Firstly, I will present experimental platforms that we have developed to run experiments in an automated manner. Automation increases throughput, and also, more importantly in fact, improves standardization and reproducibility. Secondly, I will present recent results we obtained on the characterization and modeling of several natural and engineered microbial systems, together with applications to real-time control and treatment optimization. Finally, I will conclude with recent results on the optimal design of parallel experiments.

Keywords: Bioreactor and cytometry automation • Microfluidics and microscopy automation • Plate reader automation • Optogenetics • Deterministic and stochastic modeling • Model predictive control • Process and treatment optimization • Optimal experimental design • Cybergenetics • Antimicrobial resistance • protein bioproduction in yeast

Acknowledgements. This work has been done in collaboration with all the members of the InBio group at Inria and Institut Pasteur.

Employing Immersive Virtual Reality to Reveal Common Geometric Principles of Individual and Collective Decision-Making

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Abstract. Understanding how social influence shapes biological processes is a central challenge in contemporary science, essential for achieving progress in a variety of fields ranging from the organization and evolution of coordinated collective action among cells, or animals, to the dynamics of information exchange in human societies. Using an integrated experimental and theoretical approach, involving automated tracking, immersive virtual reality (VR), and computational visual field reconstruction, I will discuss the discovery of universal geometric principles of perceptual decision-making across vast scales of biological organization, from neural collectives within the brains of individual invertebrates and vertebrates, to the collective movement decisions made by fish schools and primate societies.

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