



## Preface

Robert Brijder<sup>1</sup> · Lulu Qian<sup>2</sup>

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The International Conference on DNA Computing and Molecular Programming is the main forum for dissemination of research on biomolecular computing. The scientific program of the conference offers various workshops, contributed and peer-reviewed talks, poster presentations and invited talks of leading scientists. The conference attracts a wide-range of scientists from various backgrounds, including mathematics, computer science, physics, chemistry, biology, and nanotechnology.

This special issue is devoted to the 23rd International Conference on DNA Computing and Molecular Programming (DNA 23) held from September 24th to 28th of 2017 at the University of Texas at Austin under the auspices of the International Society for Nanoscale Science, Computation, and Engineering (ISNSCE). After a thorough reviewing process, separate from the DNA 23 reviewing process, a selection of five papers has been accepted for this issue: four were presented in a preliminary form at DNA 23 and are significantly extended with additional material, while one is based on an invited talk.

The paper *Computational Complexity of Atomic Chemical Reaction Networks* by David Doty and Shaopeng Zhu studies various classes of abstract chemical reaction networks that have behavior similar to physical chemical reaction networks in which the species are molecules that are composed of atoms as indivisible units of matter (or, even stronger, in which the species are atomic themselves). The complexities of determining whether an arbitrary abstract chemical reaction network belong to these classes are investigated.

DNA-templated synthesis is a promising technique to achieve higher effective molarity and one-pot synthesis. This techniques uses tags to identify which compounds are to be brought together. The paper *DNA-Templated Synthesis*

*Optimization* by Bjarke N. Hansen, Kim S. Larsen, Daniel Merkle, and Alexei Mihalchuk provides a computational approach to inferring DNA-templated programs that minimize the number of different tags or strands that are needed in various scenarios. Also, a general brute-force linear programming method is provided that is able compute complete solutions for small problem instances.

The paper *Automated analysis of tethered DNA nanostructures using constraint solving* by Matthew R. Lakin and Andrew Phillips presents a fully automated procedure for analyzing the molecular geometry of tethered strand displacement systems. In particular, the paper shows that a constraint problem can be associated to such a tethered system that is satisfiable precisely when a plausible physical representation of the system exists. Moreover, satisfiability can be verified using standard satisfaction modulo theory solvers.

Two papers of this special issue study molecular self-assembly from a theoretical point of view. First, the paper *A Stochastic Approach to Shortcut Bridging in Programmable Matter* by Marta Andrés Arroyo, Sarah Cannon, Joshua J. Daymude, Dana Randall, and Andréa W. Richa considers self-assembly systems where simple computational elements with limited memory and communication, called particles, self-organize to solve global problems. The paper presents a stochastic algorithm in which particles self-organize to construct “optimal” bridges. More specifically, the algorithm is shown, in a rigorous way and using Markov-chain techniques, to achieve a near-optimal balance between length and cost. Moreover, simulations of this algorithm are compared in a qualitative way with army ant bridging behavior.

Finally, there is a paper concerning the nubot self-assembly model. The main difference between the nubot self-assembly model and other self-assembly models is that the former is able to perform growth that is exponential in time. The paper *A Minimal Requirement for Self-Assembly of Lines in Polylogarithmic Time* by Yen-Ru Chin, Jui-Ting Tsai, and Ho-Lin Chen investigates the features of the nubot that are essential to be able to achieve exponential growth. In particular, one supplementary layer and one state change per

✉ Robert Brijder  
robert.brijder@uhasselt.be

Lulu Qian  
luluqian@caltech.edu

<sup>1</sup> Hasselt University, Diepenbeek, Belgium

<sup>2</sup> Caltech, Pasadena, USA

nubot cannot achieve exponential growth, while two supplementary layers and one state change per nubot can achieve exponential growth.

The editors would like to thank the authors for their contributions and the reviewers for their thorough and constructive work contributing to the quality of the papers.

We also thank Joost Kok, Grzegorz Rozenberg, and the staff of Natural Computing for their meticulous work on assembling this special issue. Finally, we would like to thank the organizers, contributing authors, and attendees of DNA 23 for a lively and scientifically stimulating meeting.