Nat Comput (2017) 16:259–260
DOI 10.1007/s11047-017-9618-1

Preface

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Published online: 22 March 2017

The International Conference on DNA Computing and Molecular Programming is the premier forum for biomolecular computing research, where scientists with diverse backgrounds come together to present recent experimental and theoretical results in the field. Continuing this tradition, the 21st International Conference on DNA Computing and Molecular Programming (DNA 21), organized under the auspices of the International Society for Nanoscale Science, Computation, and Engineering (ISNSCE), draws together research in mathematics, computer science, physics, chemistry, biology and nanotechnology to address the analysis, design and synthesis of information-based molecular systems.

This special issue contains a selection of three papers, two of which were presented in preliminary form at the 21st International Conference on DNA Computing and Molecular Programming, held from 17th to 21st August 2015, at the Wyss Institute for Biologically Inspired Engineering, Harvard University, Massachusetts, USA. All papers herein were reviewed independently of the conference paper review process and, for those presented at the conference, contain substantial additional material.

Design of nucleic acid strands with long low-barrier folding pathways, by Anne Condon, Bonnie Kirkpatrick and Ján Maňuch, presents designs for nucleic acid strands that have long folding pathways relative to strand length. The strands follow, with high probability, low-energy barrier folding pathways from a given initial structure to a given target, by visiting a large number of distinct intermediate structures that grows superlinearly with strand length. The strand designs make use of a lock and switch mechanism, and ensure that shorter alternative pathways have significantly higher energy barriers. The study provides a theoretical framework, based on a conceptually simple stacked pair energy model, as a first step towards understanding how nucleic acid strands can be programmed to support long and complex computations.

Dominance and Deficiency for Petri Nets and Chemical Reaction Networks, by Robert Brijder, studies the long-term behavior of discrete chemical reaction networks (CRNs), using techniques from both Petri net theory and CRN theory. The paper presents a sufficient condition for a CRN whose total number of molecules cannot grow unboundedly, to have the property that none of the non-terminal reactions can fire for any of its recurrent configurations. The sufficient condition depends only on the structure of the CRN, and can be checked for a broad range of CRNs in a computationally efficient way. Various non-trivial CRNs from the literature satisfy the condition, enabling predictions about their long-term behavior. This work could in future assist with engineering CRNs that perform deterministic computations, independently of reaction rates.

Reflections on Tiles (in Self-Assembly), by Jacob Hendricks, Matthew J. Patitz and Trent A. Rogers, defines the Reflexive Tile Assembly Model (RTAM), which is obtained from the extensively studied abstract Tile Assembly Model (aTAM) by allowing tiles to reflect across their horizontal and vertical axes. The authors show that RTAM is not computationally universal when a new tile can bind to a single tile in a growing assembly (temperature 1), but is computationally universal when a new tile must

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bind cooperatively to two tiles (temperature 2). They also show that when the temperature is 1 and the assembly starts from a single seed tile, N by N squares can be assembled using N tile types when N is odd, but that this is not possible when N is even. Finally, they show preliminary results toward the classification of which finite connected shapes in two-dimensional discrete space can be assembled by a singly seeded RTAM system. These results provide a framework for the study of self-assembling systems unable to enforce the reflection constraints of aTAM, including certain experimental implementations of DNA-based tiles.

The editors would like to thank the authors for their contributions, the reviewers for their diligent work, and the staff and editors of Natural Computing for assembling this special issue. We also thank the members of the organizing, steering, and program committees of DNA 21, together with the authors and attendees, for creating a scientifically rich and vibrant meeting.