LIPIcs – Leibniz International Proceedings in Informatics

LIPIcs is a series of high-quality conference proceedings across all fields in informatics. LIPIcs volumes are published according to the principle of Open Access, i.e., they are available online and free of charge.

Editorial Board

- Luca Aceto (*Chair*, Reykjavik University, IS and Gran Sasso Science Institute, IT)
- Christel Baier (TU Dresden, DE)
- Mikolaj Bojanczyk (University of Warsaw, PL)
- Roberto Di Cosmo (Inria and Université de Paris, FR)
- Faith Ellen (University of Toronto, CA)
- Javier Esparza (TU München, DE)
- Daniel Král’ (Masaryk University - Brno, CZ)
- Meena Mahajan (Institute of Mathematical Sciences, Chennai, IN)
- Anca Muscholl (University of Bordeaux, FR)
- Chih-Hao Luke Ong (University of Oxford, GB)
- Phillip Rogaway (University of California, Davis, US)
- Eva Rotenberg (Technical University of Denmark, Lyngby, DK)
- Raimund Seidel (Universität des Saarlandes, Saarbrücken, DE and Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Wadern, DE)

ISSN 1868-8969

https://www.dagstuhl.de/lipics
Contents

Preface
 Matthew R. Lakin and Petr Šulc ................................................. 0:vii

Organization

Steering Committee .......................................................... 0:ix
Program Committee .......................................................... 0:x
Additional Reviewers for Tracks A and B ................................ 0:xi
Organizing Committee for DNA 27 ......................................... 0:xii
Sponsors ........................................................................ 0:xiii

Regular Papers

Robust Digital Molecular Design of Binarized Neural Networks
 Johannes Linder, Yuan-Jyue Chen, David Wong, Georg Seelig, Luis Ceze, and Karin Strauss ................................................................. 1:1–1:20

Computing Properties of Thermodynamic Binding Networks: An Integer Programming Approach
 David Haley and David Doty .................................................. 2:1–2:16

Self-Replication via Tile Self-Assembly (Extended Abstract)
 Andrew Alseth, Daniel Hader, and Matthew J. Patitz .................. 3:1–3:22

Improved Lower and Upper Bounds on the Tile Complexity of Uniquely Self-Assembling a Thin Rectangle Non-Cooperatively in 3D
 David Furcy, Scott M. Summers, and Logan Withers ................. 4:1–4:18

ENSnano: A 3D Modeling Software for DNA Nanostructures
 Nicolas Levy and Nicolas Schabanel ......................................... 5:1–5:23

Directed Non-Cooperative Tile Assembly Is Decidable
 Pierre-Étienne Meunier and Damien Regnault .......................... 6:1–6:21

Molecular Machines from Topological Linkages
 Keenan Breik, Austin Luchsinger, and David Soloveichik ............ 7:1–7:20

Small Tile Sets That Compute While Solving Mazes
 Matthew Cook, Tristan Stérin, and Damien Woods ................... 8:1–8:20
Contents

Predicting Minimum Free Energy Structures of Multi-Stranded Nucleic Acid Complexes Is APX-Hard
   Anne Condon, Monir Hajiaghayi, and Chris Thachuk ........................................ 9:1–9:21

Reactamole: Functional Reactive Molecular Programming

Parallel Pairwise Operations on Data Stored in DNA: Sorting, Shifting, and Searching
   Tonglin Chen, Arnav Solanki, and Marc Riedel .............................................. 11:1–11:21
Preface

This volume contains the papers presented at DNA 27: the 27th International Conference on DNA Computing and Molecular Programming. The conference was originally scheduled to be held at the University of Oxford, but due to the ongoing COVID-19 pandemic it was changed to an online format. The virtual conference was held during September 13–16, 2021, and was organized under the auspices of the International Society for Nanoscale Science, Computation, and Engineering (ISNSCE). The DNA conference series aims to draw together researchers from the fields of mathematics, computer science, physics, chemistry, biology, and nanotechnology to address the analysis, design, and synthesis of information-based molecular systems.

Papers and presentations were sought in all areas that relate to biomolecular computing, including, but not restricted to: algorithms and models for computation on biomolecular systems; computational processes in vitro and in vivo; molecular switches, gates, devices, and circuits; molecular folding and self-assembly of nanostructures; analysis and theoretical models of laboratory techniques; molecular motors and molecular robotics; information storage; studies of fault-tolerance and error correction; software tools for analysis, simulation; and design; synthetic biology and in vitro evolution; and applications in engineering, physics, chemistry, biology, and medicine.

Authors who wished to orally present their work were asked to select one of two submission tracks: Track A (full paper) or Track B (one-page abstract with supplementary document). Track B is primarily for authors submitting experimental or theoretical results who plan to submit to a journal rather than publish in the conference proceedings. We received 33 submissions for oral presentations: 17 submissions to Track A and 16 submissions to Track B. Each submission was reviewed by at least three reviewers, with most reviewed by four or more reviewers. The Program Committee accepted 11 papers for Track A (65%) and 11 papers for Track B (69%). We also received 29 submissions for Track C (poster), of which five were selected as additional oral presentations by the Program Committee. This volume contains the papers accepted for Track A.

We express our sincere appreciation to our invited speakers: Michael Brenner, Luca Cardelli, Chengde Mao, Petra Schwille, Friedrich Simmel, and Reidun Twarock. We thank all of the authors who contributed papers to these proceedings at a difficult time, and who presented papers and posters during the conference. Last, but by no means least, the editors are especially grateful to the members of the Program Committee and the additional invited reviewers for their hard work in reviewing the papers on a tight deadline and for providing insightful and constructive comments to the authors.

Matthew Lakin
Petr Šulc

September 2021
Organization

Steering Committee

Anne Condon (Chair) University of British Columbia, Canada
Luca Cardelli University of Oxford, UK
Masami Hagiya University of Tokyo, Japan
Natasha Jonoska University of South Florida, USA
Chengde Mao Purdue University, USA
Satoshi Murata Tohoku University, Japan
John H. Reif Duke University, USA
Grzegorz Rozenberg University of Leiden, The Netherlands
Rebecca Schulman Johns Hopkins University, USA
Nadrian C. Seeman New York University, USA
Friedrich Simmel Technical University Munich, Germany
David Soloveichik University of Texas at Austin, USA
Andrew J. Turberfield University of Oxford, UK
Erik Winfree California Institute of Technology, USA
Damien Woods Maynooth University, Ireland
Hao Yan Arizona State University, USA
Program Committee

Matthew Lakin (Co-chair) University of New Mexico, USA
Petří Šulc (Co-chair) Arizona State University, USA
Stefan Badelt University of Vienna, Austria
Jonathan Bath University of Oxford, UK
Luca Cardelli University of Oxford, UK
Ho-Lin Chen National Taiwan University, Taiwan (R.O.C.)
Yuan-Jyue Chen Microsoft Research, Redmond, USA
Anne Condon University of British Columbia, Canada
David Doty University of California, Davis, USA
Jonathan Doye University of Oxford, UK
Constantine Evans Evans Foundation and Maynooth University, Ireland
Elisa Franco University of California, Los Angeles, USA
Cody Geary Aarhus University, Denmark
Manoj Gopalakrishnan Indian Institute of Technology, Bombay, India
Elton Graugnard Boise State University, USA
Masami Hagiya University of Tokyo, Japan
Lila Kari University of Waterloo, Canada
Titus Klinge Drake University, USA
Satoshi Kobayashi University of Electro-Communications, Tokyo, Japan
James Lathrop Iowa State University, USA
Chenxiang Lin Yale University, USA
Satoshi Murata Tohoku University, Japan
Eyal Nir Ben Gurion University, Israel
Pekka Orponen Aalto University, Finland
Matthew Patitz University of Arkansas, USA
Lulu Qian California Institute of Technology, USA
John H. Reif Duke University, USA
Flavio Romano Ca Foscari University of Venice, Italy
Lorenzo Rovigatti Sapienza University of Rome, Italy
Dominic Scalise California Institute of Technology, USA
Nicolas Schabanel CNRS and École Normale Supérieure de Lyon, France
Joseph Schaeffer Google Health, USA
Robert Schweller University of Texas Rio Grande Valley, USA
Shalin Shah Bloomberg, USA
William Shuh Harvard University, USA
David Soloveichik University of Texas at Austin, USA
Darko Stefanovic University of New Mexico, USA
Jaimie Stewart California Institute of Technology, USA
Chris Thachuk University of Washington, USA
Grigory Tikhomirov University of California Berkeley, USA
Andrew Turberfield University of Oxford, UK
Shelley Wickham University of Sydney, Australia
Damien Woods Maynooth University, Ireland
Fei Zhang Rutgers University, USA
### Additional Reviewers for Tracks A and B

<table>
<thead>
<tr>
<th>Andrew Alseth</th>
<th>Daniel Hader</th>
</tr>
</thead>
<tbody>
<tr>
<td>David Caballero</td>
<td>Jacob Hendricks</td>
</tr>
<tr>
<td>Christian Cuba Samaniego</td>
<td>Trent Rogers</td>
</tr>
<tr>
<td>Timothy Gomez</td>
<td>Scott Summers</td>
</tr>
<tr>
<td>Leopold Green</td>
<td>Xun Tang</td>
</tr>
</tbody>
</table>
Organizing Committee for DNA 27

Andrew Phillips (Co-chair)  Microsoft Research, Cambridge, UK
Andrew Turberfield (Co-chair)  University of Oxford, UK
Claire Garland  Institute of Physics, UK
Sponsors

International Society for Nanoscale Science, Computation, and Engineering
Biological Physics Group, Institute of Physics
Department of Physics, University of Oxford
Microsoft Research