

27th International Conference on DNA Computing and Molecular Programming

DNA 27, September 13–16, 2021, Oxford, UK
(Virtual Conference)

Edited by

Matthew R. Lakin

Petr Šulc



Editors

Matthew R. Lakin

Department of Computer Science, Department of Chemical & Biological Engineering,
Center for Biomedical Engineering, University of New Mexico, Albuquerque, NM, USA
mlakin@cs.unm.edu

Petr Šulc

School of Molecular Sciences, Arizona State University, Tempe, AZ, USA
psulc@asu.edu

ACM Classification 2012

Theory of computation → Models of computation; Applied computing → Molecular structural biology;
Applied computing → Biological networks; Information systems → Information storage systems

ISBN 978-3-95977-205-1

Published online and open access by

Schloss Dagstuhl – Leibniz-Zentrum für Informatik GmbH, Dagstuhl Publishing, Saarbrücken/Wadern,
Germany. Online available at <https://www.dagstuhl.de/dagpub/978-3-95977-205-1>.

Publication date

September, 2021

Bibliographic information published by the Deutsche Nationalbibliothek

The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed
bibliographic data are available in the Internet at <https://portal.dnb.de>.

License

This work is licensed under a Creative Commons Attribution 4.0 International license (CC-BY 4.0):
<https://creativecommons.org/licenses/by/4.0/legalcode>.



In brief, this license authorizes each and everybody to share (to copy, distribute and transmit) the work
under the following conditions, without impairing or restricting the authors' moral rights:

- Attribution: The work must be attributed to its authors.

The copyright is retained by the corresponding authors.

Digital Object Identifier: 10.4230/LIPIcs.DNA.27.0

ISBN 978-3-95977-205-1

ISSN 1868-8969

<https://www.dagstuhl.de/lipics>

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	
<i>Matthew R. Lakin and Petr Šulc</i>	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 <i>Johannes Linder, Yuan-Jyue Chen, David Wong, Georg Seelig, Luis Ceze, and Karin Strauss</i>	1:1–1:20
Computing Properties of Thermodynamic Binding Networks: An Integer Programming Approach <i>David Haley and David Doty</i>	2:1–2:16
Self-Replication via Tile Self-Assembly (Extended Abstract) <i>Andrew Alseth, Daniel Hader, and Matthew J. Patitz</i>	3:1–3:22
Improved Lower and Upper Bounds on the Tile Complexity of Uniquely Self-Assembling a Thin Rectangle Non-Cooperatively in 3D <i>David Furcy, Scott M. Summers, and Logan Withers</i>	4:1–4:18
ENSnano: A 3D Modeling Software for DNA Nanostructures <i>Nicolas Levy and Nicolas Schabanel</i>	5:1–5:23
Directed Non-Cooperative Tile Assembly Is Decidable <i>Pierre-Étienne Meunier and Damien Regnault</i>	6:1–6:21
Molecular Machines from Topological Linkages <i>Keenan Breik, Austin Luchsinger, and David Soloveichik</i>	7:1–7:20
Small Tile Sets That Compute While Solving Mazes <i>Matthew Cook, Tristan Stérin, and Damien Woods</i>	8:1–8:20

27th International Conference on DNA Computing and Molecular Programming (DNA 27).

Editors: Matthew R. Lakin and Petr Šulc



Leibniz International Proceedings in Informatics
Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

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
Titus H. Kluge, James I. Lathrop, Peter-Michael Osera, and Allison Rogers 10:1–10:20

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 Schwill, 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
Petr 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 Gopalkrishnan	Indian Institute of Technology, Bombay, India
Elton Graunard	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 Shih	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

Andrew Alseth
David Caballero
Christian Cuba Samaniego
Timothy Gomez
Leopold Green

Daniel Hader
Jacob Hendricks
Trent Rogers
Scott Summers
Xun Tang

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

