## Lecture Notes in Computer Science

*Commenced Publication in 1973* Founding and Former Series Editors: Gerhard Goos, Juris Hartmanis, and Jan van Leeuwen

#### Editorial Board

David Hutchison Lancaster University, UK Takeo Kanade Carnegie Mellon University, Pittsburgh, PA, USA Josef Kittler University of Surrey, Guildford, UK Jon M. Kleinberg Cornell University, Ithaca, NY, USA Alfred Kobsa University of California, Irvine, CA, USA Friedemann Mattern ETH Zurich, Switzerland John C. Mitchell Stanford University, CA, USA Moni Naor Weizmann Institute of Science, Rehovot, Israel Oscar Nierstrasz University of Bern, Switzerland C. Pandu Rangan Indian Institute of Technology, Madras, India Bernhard Steffen TU Dortmund University, Germany Madhu Sudan Microsoft Research, Cambridge, MA, USA Demetri Terzopoulos University of California, Los Angeles, CA, USA Doug Tygar University of California, Berkeley, CA, USA Gerhard Weikum Max Planck Institute for Informatics, Saarbruecken, Germany

# DNA Computing and Molecular Programming

18th International Conference, DNA 18 Aarhus, Denmark, August 14-17, 2012 Proceedings



Volume Editors

Darko Stefanovic University of New Mexico Department of Computer Science MSC01 1130, 1 University of New Mexico 87131 Albuquerque, NM, USA E-mail: darko@cs.unm.edu

Andrew Turberfield University of Oxford Department of Physics, Clarendon Laboratory Parks Road, Oxford OX 1 3PU, UK E-mail: a.turberfield@physics.ox.ac.uk

ISSN 0302-9743 e-ISSN 1611-3349 ISBN 978-3-642-32207-5 e-ISBN 978-3-642-32208-2 DOI 10.1007/978-3-642-32208-2 Springer Heidelberg Dordrecht London New York

Library of Congress Control Number: 2012942854

CR Subject Classification (1998): F.1, F.2.2, J.3, E.1, I.2, G.2, F.4

LNCS Sublibrary: SL 1 - Theoretical Computer Science and General Issues

© Springer-Verlag Berlin Heidelberg 2012

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Typesetting: Camera-ready by author, data conversion by Scientific Publishing Services, Chennai, India

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, re-use of illustrations, recitation, broadcasting, reproduction on microfilms or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer. Violations are liable to prosecution under the German Copyright Law.

### Preface

This volume contains the papers presented at DNA 18: the 18th International Conference on DNA Computing and Molecular Programming, held August 14–17, 2012 at Aarhus University, Aarhus, Denmark.

Research in DNA computing and molecular programming draws together mathematics, computer science, physics, chemistry, biology, and nanotechnology to address the analysis, design, and synthesis of information-based molecular systems. This annual meeting is the premier forum where scientists of diverse backgrounds come together with the common purpose of advancing the engineering and science of biology and chemistry from the point of view of computer science, physics, and mathematics. Continuing this tradition, under the auspices of the International Society for Nanoscale Science, Computation, and Engineering (ISNSCE), DNA18 focused on the most recent experimental and theoretical results that promise the greatest impact.

The DNA 18 Program Committee received 37 paper submissions, of which 11 were selected for oral presentation and inclusion in the proceedings, and another 11 for oral presentation. Others were selected for poster presentations. Additional poster presentations came from a poster-only submission track.

The conference program included two tutorials—Milan Stojanovic, Columbia University: "Aptamers in Sensing and Molecular Computing"; and Damien Woods, California Institute of Technology: "A Crash Course in the Theory of Computing."

The conference program also included a plenary Turing Lecture by Grzegorz Rozenberg, University of Leiden: "Processes Inspired by Interactions of Chemical Reactions in Living Cells", and invited talks by Drew Berry, Walter and Eliza Hall Institute of Medical Research: "Visualizations of the Molecular Machines That Create Flesh and Blood"; Jeremy Gunawardena, Harvard Medical School: "Protein Computing"; Radhika Nagpal, Harvard University: "The TERMES Project: An Expedition in Large-Scale Self-assembly"; and Peng Yin, Harvard University: "Modular Self-Assembly of Molecular Shapes."

On the day before the conference, dnatec2012, a one-day workshop on structural DNA nanotechnology, was held, with contributions from Ned Seeman, New York University: "Using DNA's Inherent Chemical Information to Control Structure"; Andy Ellington, University of Texas: "DNA Nanotechnology: Too Small and Too Costly"; William Shih, Harvard Medical School: "Self-Assembled DNA-Nanostructure Tools for Molecular Biophysics"; Hao Yan, Arizona State University: "Designer DNA Architectures for Programmable Self-Assembly"; Andrew Turberfield, Oxford University: "Molecular Machinery from DNA"; Itamar Willner, Hebrew University of Jerusalem: "Nanobiotechnology with DNA"; Chengde Mao, Purdue University: "Self-Assembled DNA Nanocages"; Masayuki Endo, Kyoto University: "Direct Observation of Single Enzymatic and Chemical Reactions in the Designed DNA Nanostructures"; Friedrich Simmel, Technische Universität München: "DNA Devices and Circuits as Components for Cell-Like Microcompartments"; Thom H. LaBean, North Carolina State University: "Building Agency into Molecular Materials"; and Luc Jaeger, University of California Santa Barbara: "Is RNA Self-assembly the Same as DNA Self-assembly?".

The editors would like to thank the members of the Program Committee and the external reviewers for their hard work in reviewing the papers and providing comments to the authors. They also thank the members of the Organizing Committee and the Steering Committee, and particularly the Committee Chairs, Kurt Vesterager Gothelf and Natasha Jonoska, for their support and advice. Generous financial support by the conference sponsors—the Danish National Research Foundation, Aarhus University, and DNA Technology A/S (Risskov, Denmark)—is gratefully acknowledged.

June 2012

Darko Stefanovic Andrew Turberfield

## Organization

DNA 18 was organized by the Danish National Foundation Center for DNA Nanotechnology at Aarhus University in cooperation with the International Society for Nanoscale Science, Computation, and Engineering (ISNSCE).

#### **Steering Committee**

Natasha Jonoska (Chair)	University of South Florida, USA
Luca Cardelli	Microsoft Research, UK
Anne Condon	University of British Columbia, Canada
Masami Hagiya	University of Tokyo, Japan
Lila Kari	University of Western Ontario, Canada
Satoshi Kobayashi	University of Electro-Communication, Chofu,
	Japan
Chengde Mao	Purdue University, USA
Satoshi Murata	Tohoku University, Japan
John Reif	Duke University, USA
Grzegorz Rozenberg	University of Leiden, The Netherlands
Nadrian Seeman	New York University, USA
Friedrich Simmel	Technische Universität München, Germany
Andrew Turberfield	Oxford University, UK
Hao Yan	Arizona State University, USA
Erik Winfree	California Institute of Technology, USA

#### **Organizing Committee**

Kurt Vesterager Gothelf (Chair)	Aarhus University, Denmark
Ebbe Sloth Andersen	Aarhus University, Denmark
Stinne Høst	Aarhus University, Denmark
Sarah Helmig	Aarhus University, Denmark
Thom LaBean	North Carolina State University, USA

#### **Program Committee**

Darko Stefanovic (Co-chair)	University of New Mexico, USA
Andrew Turberfield (Co-chair)	Oxford University, UK
Luca Cardelli	Microsoft Research, UK
Eugen Czeizler	Aalto University, Finland
Erik Demaine	Massachusetts Institute of Technology, USA
David Doty	California Institute of Technology, USA

Andrew Ellington Kurt Gothelf Natasha Jonoska Lila Kari Yamuna Krishnan Chengde Mao Satoshi Murata Jennifer Padilla John Reif Rebecca Schulman Georg Seelig Friedrich Simmel David Soloveichik Erik Winfree Hao Yan Peng Yin

#### Referees

Andersen, Ebbe Chandran, Harish Chen, Xi Gao, Yuan Gopalkrishnan, Nikhil Karpenko, Daria Kopecki, Steffen Lakin, Matthew Marblestone, Adam Minnich, Amanda Patitz, Matthew Ran, Tom Schaus, Thomas Seki, Shinnosuke

Duke University, USA Johns Hopkins University, USA University of Washington, USA Technische Universität München, Germany University of California, San Francisco, USA California Institute of Technology, USA Arizona State University, USA Harvard University, USA

University of Texas at Austin, USA

University of Western Ontario, Canada

Tokyo Institute of Technology, Japan

National Centre for Biological Sciences, India

University of South Florida, USA

Aarhus University, Denmark

Purdue University, USA

New York University, USA

Simjour, Amir Song, Tianqi Sun, Wei Wei, Bryan Williams, Lance Zhang, David Zizza, Rosalba

#### **Sponsoring Institutions**

The Danish National Research Foundation Aarhus University DNA Technology A/S

# Table of Contents

Turing Universality of Step-Wise and Stage Assembly	1
at Temperature 1 Bahar Behsaz, Ján Maňuch, and Ladislav Stacho	1
A Type System for DNAQL Robert Brijder, Joris J.M. Gillis, and Jan Van den Bussche	12
Deterministic Function Computation with Chemical Reaction Networks	25
Reachability Bounds for Chemical Reaction Networks and Strand Displacement Systems Anne Condon, Bonnie Kirkpatrick, and Ján Maňuch	43
Synthesizing Minimal Tile Sets for Complex Patterns in the Framework of Patterned DNA Self-Assembly Eugen Czeizler and Alexandru Popa	58
A Geometric Approach to Gibbs Energy Landscapes and Optimal DNA Codeword Design Max H. Garzon and Kiran C. Bobba	73
A DNA Based Molecular Logic Gate Capable of a Variety of Logical Operations Anton Kan, Koh-ichiroh Shohda, and Akira Suyama	86
Deciding Whether a Regular Language Is Generated by a Splicing System Lila Kari and Steffen Kopecki	98
Probabilistic Reasoning with a Bayesian DNA Device Based on Strand Displacement	110

DNA Self-Assembly and Computation Studied with a Coarse-Grained	
Dynamic Bonded Model Carsten Svaneborg, Harold Fellermann, and Steen Rasmussen	123
Space and Energy Efficient Computation with DNA Strand Displacement Systems	135
Chris Thachuk and Anne Condon	100
Author Index	151