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Preface

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The International Conference on DNA Computing and Molecular Programming is the premier forum for research on biomolecular computing; a place where researchers come together to present recent theoretical and experimental results. The conference attracts scientists from diverse backgrounds, including mathematics, computer science, physics, chemistry, biology, and nanotechnology. Reflecting this diversity, presented work covers a wide spectrum of scientific styles from proving theorems on molecular models of computation and giving designs for molecular systems, all the way to results and analyses from wet-lab implementation using biomolecules such as DNA, RNA and protein.

This special issue contains a selection of eleven papers originally presented in preliminary form at DNA 22: the 22nd International Conference on DNA Computing and Molecular Programming, held in September 2016 at Ludwig-Maximilians-Universität (LMU) in Munich, Germany. All papers herein were reviewed independently of the conference referee process and contain extensive additional material.

The paper entitled *The importance of thermodynamics for molecular systems, and the importance of molecular systems for thermodynamics* by Ouldridge gives a pedagogical review and perspective on the thermodynamics of molecular systems, a core theory underlying much experimental and theoretical work in the field.

In their paper *Resiliency to Multiple Nucleation in Temperature-1 Self-Assembly*, Patitz, Schweller, Rogers, Summers and Winslow show theoretical results on hierarchical models of self-assembly where square tiles with coloured sides stick to each other to form large assemblies if they match colours on at least one tile-side, and where those assemblies may in turn stick to each other (these are called temperature 1, or noncooperative, 2HAM models). Naïve intuition would suggest that self-assembly growth might be difficult or impossible to control in such noncooperative models (that permit mismatching colours on adjacent tile-sides), however through the use of clever algorithmic techniques they show that growth can indeed be controlled in order to yield computational results (simulation of Turing machines, counting in binary, building aperiodic structures).

In *Hierarchical Self-Assembly of Fractals with Signal-Passing Tiles*, Hendricks, Olsen, Patitz, Rogers and Thomas show results on another hierarchical model of self-assembly where tiles, after binding to each other to form some 2D structure, make use of use-once 'chemical wires' to send signals along one surface of the assembled structure. They show that wide classes of fractals, including the famous Sierpinski triangle can be self-assembled (holes and all!) in this powerful signal-passing model.

Nondeterministic seedless oritatami systems and hardness of testing their equivalence by Han, Kim, Ota and Seki shows that in their nondeterministic 'oritatami' model of RNA co-transcriptional folding it is algorithmically difficult to decide if a given system will place a molecule at a given position (specifically, NP hard) and if two systems assemble the same set of final structures (co-NP hard).

The paper *On the Runtime of Universal Coating for Programmable Matter* by Daymude, Derakhshandeh, Gmyr, Porter, Richa, Scheideler and Strothmann, analyses the running time of a distributed algorithm in the 'ameobot' model where a collection of simple agents undergo state changes and move relative to each other to autonomously coat, or paint, the surface of 2D shapes.

Moving to the theory of well-mixed chemical systems (i.e. without geometry), in their paper *Democratic, Existential, and Consensus-Based Output Conventions in Stable Computation by Chemical Reaction Networks*, Brijder, Doty and Soloveichik look at the theory of stochastic chemical reaction networks and show that computational power in the error-free model remains the same under a variety of output conventions.

In *Chemical Reaction Network Designs for Asynchronous Logic Circuits*, Cardelli, Kwiatkowska and Whitby provide chemical reaction network designs for the

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construction of asynchronous logic circuits, including control flow elements and an adder, via implementation of the Muller C-element for asynchronous logic.

In their paper *Programming Discrete Distributions with Chemical Reaction Networks*, Cardelli, Kwiatkowska and Laurenti consider computation with stochastic chemical reaction networks where the goal is to have the distribution of the network's output states (here, a state is a vector of counts of a finite set of molecular species) be some target finite-support distribution.

Moving on to modelling and molecular design for DNA-based systems, in *Design Methods for 3D Wireframe DNA Nanostructures*, Orponen surveys design principles for building wireframe polyhedral nanostructures out of DNA, beginning with foundational ideas from the beginnings of the field in the early 1990's through to modern DNA origami structures composed of hundreds of DNA strands.

There have been a variety of designs for DNA robot walkers that move around on 2D patterned molecular surfaces; *Petri-net-based 2D Design of DNA Walker Circuits* by Gilbert, Heiner and Rohr analyses unintended behaviour (called leak) in DNA walker systems using a coloured stochastic Petri net approach.

DNA nanotubes are a simple class of nanostructures that have found myriad uses in the field, yet much remains to be understood about their properties. In their paper *A Coarse-Grained Model Captures the Temporal Evolution of DNA Nanotube Length Distributions*, Mardanlou, Yaghoubi, Green, Subramanian, Hariadi, Kim and Franco define and analyse a coarse-grained model of DNA nanotube growth from DNA tile monomers.

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