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# Preface

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In this special issue of Natural Computing the papers cover a diverse set of abstract, mathematical models of molecular systems that are able to self-assemble into designed structures and to perform prescribed computations. While some of the models are abstractions based on physical systems that have been experimentally realized via systems of synthetic DNA molecules, others represent novel directions for potential implementations of related molecular systems. However, the unifying theme for all of them is that they seek to explore the mathematical powers and limitations of molecular systems to build precise and complex structures and to perform distributed computations in chemical environments, as well as the abilities of researchers to efficiently and effectively design and analyze such systems. These results, and others like them, help to guide experimental directions and to provide a road map for future explorations that may lead to even greater control over matter at molecular levels, and diverse applications that today are out of reach.

The International Conference on DNA Computing and Molecular Programming is the premier venue for research related to the modeling, design, implementation, and analysis of programmed behavior in molecular systems. It is held under the auspices of the International Society for Nanoscale Science, Computation, and Engineering (ISNSCE) and brings together a large diversity of interdisciplinary scientists and engineers, including mathematicians, computer scientists, chemists, and physicists, among others, to present and discuss the latest achievements in the field. The conference features invited talks by leaders in the area, as well as peer-reviewed contributed talks, and poster presentations.

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This special issue is dedicated to the 26th International Conference on DNA Computing and Molecular Programming (DNA 26), held September 14-17, 2020, and intended to be at the University of Oxford, UK, but instead held online due to the COVID-19 pandemic. It contains four papers that were presented, in preliminary forms, at the conference but which were all subsequently expanded upon and subjected to a second, independent review process for inclusion in this issue.

In the paper "Population-Induced Phase Transitions and the Verification of Chemical Reaction Networks," authors James I. Lathrop, Jack H. Lutz, Robyn R. Lutz, Hugh D. Potter, and Matthew R. Riley examine the behaviors of molecular systems known as chemical reaction networks (CRNs). They investigate phase transitions in CRNs and show that, although several other methods fail to verify these CRN behaviors, formal theorem provers can succeed.

In "ALCH: An Imperative Language for Chemical Reaction Network-Controlled Tile Assembly," authors Titus H Klinge, James Lathrop, Sonia Moreno, Hugh D. Potter, Narun K. Raman, and Matthew R. Riley introduce a programming language used to design systems in the CRN-TAM, a recently introduced model of tile-based self-assembly that combines the local interactions of tiles in the abstract Tile Assembly Model (aTAM) with global signaling and control by CRNs. They demonstrate powerful primitives in the language and provide accompanying example systems.

In "Verification and Computation in Restricted Tile Automata," authors David Caballero, Timothy Gomez, Robert Schweller, and Tim Wylie work with Tile Automata, a tile-based model of self-assembly that is a further abstraction of the 2-Handed Assembly Model (2HAM), combining it with aspects of cellular automata. Tile Automata are able to combine via glues like 2HAM tiles, but the behaviors of those glues can be dynamically activated and deactivated. They present a variety of results that include simulating Turing machines "efficiently", working within a "freezing" version of the model in which a tile can be in each state a maximum of one time, and exploring the complexities of verifying various properties of systems.

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In the final paper of the issue, "Turning Machines: a simple algorithmic model for molecular robotics," authors Irina Kostitsyna, Cai Wood, and Damien Woods present a novel model of self-assembling "robots," called Turning Machines. These Turning Machines start in a chain and are able to fold, and each robot can be programmed to fold a given number of times. As the folding asynchronously occurs, the robots turn with respect to their neighbors, causing the line to bend into designed shapes. They present primitives in the model, useful for building some classes of shapes, and also prove that other shapes are impossible to form without potential for errors.

Since this is a special issue of Natural Computing consisting of select papers from DNA 26, we would first like to again thank everyone who helped to make DNA 26 a success despite the hardships of COVID-19 that forced it to become a virtual conference. This includes the members of the Program Committee, the members of the Steering Committee, especially Steering Committee Chair Anne Condon, and most importantly the members of the Organizing Committee - Andrew Phillips and Andrew Turberfield (co-chairs) and Claire Garland and staff from the Institute of Physics. Without help from all of them the conference could not have been successful, and the success of the conference is what led to this special issue. We'd also like to thank the authors for accepting the invitation and providing greatly enhanced versions of their conference papers for this issue, and the anonymous reviewers who carefully reviewed the papers, making suggestions that led to many improvements. Finally, we thank the editors of Natural Computing who have given us direction and provided the resources necessary to put this issue together.