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Dissertation press release 5.11.2018

Folding biomolecules to complex nanoscale shapes

Title of the dissertation	Algorithmic Design of Biomolecular Nanostructures
Contents of the dissertation	Nanotechnology, a field where matter is controlled and manipulated at the scale of a billionth of a meter, is emerging as a breakthrough technology with broad implications for science, technology and society at large. In the nature-inspired bottom-up approaches to nanotechnology, biomolecules such as DNA and RNA are programmed to autonomously self-assemble to custom shapes and patterns. In this dissertation, we introduce a novel algorithmic approach for automatically generating DNA sequences from user-defined shapes so that the DNA strands fold to nanoscale realizations of the target shapes. For this purpose, we develop and implement algorithms for unknotted weaving of long DNA strands on the target structures. We demonstrate the generality of our approach by folding, among other things, a molecular version of a computer-graphics benchmark model known as the Stanford bunny, and a nanoscale sketch of the Fennoscandic map. The nanoscale bunny we synthesized is approximately one-thousandth the width of a human hair in its diameter. Our approach not only significantly expands the possibilities for designing self-assembled nanostructures, but also offers concrete advantages for applications in areas such as biomedicine. In addition, the high degree of automation provided by our implementation enables researchers to quickly design and test a variety of nanostructures for their desired applications.
Field of the dissertation	Computer Science
Doctoral candidate	Abdulmelik Mohammed, M.Sc.(Tech.)
Time of the defence	16.11.2018 at 12 noon
Place of the defence	Aalto University School of Science, lecture hall T2, Konemiehentie 2, Espoo
Opponent	Professor Nataša Jonoska, University of South Florida, US
Custos	Professor Pekka Orponen, Aalto University School of Science, Department of Computer Science
Electronic dissertation	http://urn.fi/URN:ISBN:978-952-60-8282-0
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