

Biological Design Doctoral Defense

Software tools for design, simulation and characterization
of DNA and RNA nanostructures

School for Engineering of Matter, Transport and Energy

Erik Poppleton

Advisor: Petr Šulc

Abstract

Nucleic acid nanotechnology is a field of nanoscale engineering where the sequences of DNA and RNA molecules are carefully designed to create self-assembled nanostructures which higher spatial resolution than is available to top-down fabrication methods. In the 40 year history of the field, the structures created have scaled from small tile-like structures constructed from a few hundred individual nucleotides to micron-scale structures assembled from millions of nucleotides using the technique of "DNA origami". One of the key drivers of advancement in any modern engineering field is the parallel development of software which facilitates the design of components and performs *in silico* simulation of the target structure to determine its structural properties, dynamic behavior, and identify defects. For nucleic acid nanotechnology, the design software CaDNAno and simulation software oxDNA are the most popular choices for design and simulation, respectively. In this dissertation I will present my work on the oxDNA software ecosystem, including an analysis toolkit, a web-based graphical interface, and a new molecular visualization tool which doubles as a free-form design editor that covers some of the weaknesses of CaDNAno's lattice-based design paradigm. Finally, as a demonstration of the utility of these new tools I show oxDNA simulation and subsequent analysis of a nanoscale leaf-spring engine capable of converting chemical energy into dynamic motion. OxDNA simulations were used to investigate the effects of design choices on the behavior of the system and rationalize experimental results.



June 27, 2022; 9 AM; Biodesign Institute Bldg B, room B105

Zoom Link: Biodesign Institute Bldg B, room B105