Turning Machines - DNA implementation of simple molecular robotics

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Abstract

Molecular robotics considers the problem of designing molecular-scale structures that sense, move and carry out a variety of tasks with nanoscale precision. The three main challenges are (i) theory - defining a model, characterizing its abilities, setting goal tasks, (ii) implementing the model - designing the robot structure - placing specific molecular components where you want them to create the desired structure, and (iii) actuation of the molecular-scale robot to perform desired tasks. In recent years there have been many advances in molecular self-assembly using DNA nanotechnology, in particular we can reliably form nanoscale structures using a technique called DNA Origami. The type of molecular robots we have seen emerge in the field thus far include DNA Walkers, which exploit DNA complementarity to walk along a track or random walk along a flat 2D DNA Origami surface via so-called DNA strand displacement reactions, and reconfigurable DNA structures that can change their structure when detecting a chemical input signal (e.g. changes in salt concentration, or the addition of a triggering DNA strand). However, both of these examples are limited in their computational ability. Walkers rely on specifically designed tracks, which limits the contexts in which they can perform computation (e.g. sorting molecular cargo on a surface), while reconfigurable DNA structures are capable of functioning in solution in isolation but are typically limited to a small set of states (e.g. binary switches) or lack of reversibility (e.g. reconfiguration of DNA molecular arrays [Jie Song et al, Science 2017]).

Our goal is to propose and implement a novel model for molecular robotics called the Turning Machine model. An input to the model is a line of simple robots each connected to its one or two neighbours via unit length arms: initially, each robot encodes a whole number specifying the number of 60o rotations to perform in order to eventually compute, or fold the entire line into, a final target shape. These individual arm rotations occur asynchronously and uniformly at random until the target shape has been reached. Simplicity was the key design principle in mind when developing the model in order for it to be feasible to implement using DNA. Our current design is both modular and scalable, exploits the geometry of double-layered DNA origami to achieve the desired turns, and is capable of reconfiguring between two target shapes. Our ultimate goal is to provide a DNA-based Turning Machine design that folds a wide variety of shapes, and can fold any one of these shapes into any other.