# Design and Simulation of Autonomous DNA Devices

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## 1 Introduction

The creation of nanomechanical devices built upon DNA nanostructures of relatively large size has spawned a variety of theoretical designs for sophisticated DNA autonoma. There is a wide variety of applications that programmable, bottom-up nanorobotics entail in nanorobotics and nanocomputing. Of special interest are autonomous DNA devices capable of universal computation and universal translational motion, which we investigate, model and simulate.

To have programmable DNA nanostructures and nanorobots capable of complex motion has obvious applications: imagine a series of walkers on a nanostructure with a programmable delivery object. Having such information carriers has applications in nanorobotics and fabrication, with obvious extensions into medical uses.

In order to make this fully realizable, it is useful to create universal Turing machines. Universal Turing machines are useful because they can be theoretically used to simulate any other Turing machine, and ultimately is a measure of computability itself. We define universal translational motion by that determined by the head of a universal Turing machine.

Of course, this means that implementing such a device in DNA is crucial (due to its generalization capability) and a considerable number of attempts

have been tried. For instance, Rothemund designed a universal Turing machine based in DNA, and Shapiro et al has an autonomous 2-state 2-color finite state automata (though, not a Turing machine). The reactions for Rothemund's DNA, however, require manual reaction transitions in order to carry out the enzymic operations.

However, the two key factors are autonomy *and* universality: it is preferable for such devices to not require manual temperature and chemical input in order move the computation forward, and it is preferable to have complex motion instead of simpler, unidirectional motion. So far, neither have been found together.

## 2 Summary

In order to validate the approach of a universal (computational, i.e. Turing-complete, and translational) DNA automata, we simulate the proposed designs and investigate solutions to potential problems in the implementation.

There has been a significant body of work on subsets of the above. Precursors to autonomous motion include Turberfield's free running DNA machine [10], Mao's autonomous DNA motor using DNA enzymes[6], and a wide variety of walkers powered by DNA fuels or ATP[23, 40, 42]. In fact, one of the unidirectional DNA walkers have been experimentally verified in our wet lab[a unidirectional DNA walker moving autonomously along a track].

There is also been effort in developing automata and universal Turing machines in a variety of molecular computing schemes. Of note is Rothemund's Turing machine design[4], which features a universal Turing machine with transition table encoded in a circular DNA. Another is Shapiro's automata[8], which does not constitute a full Turing machine and destroys data but still has innovations including using a DNA sticky end to encode state and symbol for the automata.

In this paper, we present a design for a universal Turing machine (specifically,

2-state 5-color) implemented with DNA enzymes to provide the state changes. At a high level, the structure has a series of molecules (only one of which is active at a given point in time) representing the head of a Turing machine; each state transition has the head-molecule attaching to a symbol-molecule (representing the data tape), and the resulting structure becoming cleaved into a new head-molecule and symbol-molecule. The two new molecules become ligated to floating rule-molecules and these structures encode the information to generate a new active head-molecule and state.

Given this design, we also aim to simulate an inductive step of this procedure: that is, using the software Visual GEC, we construct the system described above and simulate a full cycle using the correct enzymes (both ligation and cleavage). Some difficulties include the use of unnatural DNA bases denoted as $E$ and $F$– this is required in order to minimize futile reactions which decrease the efficiency of the structure.

With the validation that a computational simulation of this structure provides, we gain confidence in the ability of this Turing machine to compute with a reasonable amount of error tolerance, and therefore validate the approach of a promising new design in DNA automata.

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