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主 論 文 の 要 旨

論文題目　**Swarm Intelligence-Based DNA Computation**
(群知能に基づいた DNA コンピューティング)

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論 文 内 容 の 要 旨

This thesis is a summary of four independent but related manuscripts on computational design of synthetic bio-molecular systems based on DNA strand displacement reaction.
In the first part, we report the design of the DNA-based circuit in well-mixed chemical systems. One of the biggest obstacles in the molecular programming is that there is still no direct method to compile arbitrary mathematical models into biochemical reactions in order to solve given computational problems. In this part, the application of the DNA strand displacement system based on the nature-inspired computation is observed. By using the Immune Network Theory and Chemical Reaction Networks, a compilation of DNA-based operations and the formulation of its mathematical model are derived. Furthermore, the application of this system is compared with the conventional implementation by silicon-based programming. From results obtained, we can see a positive correlation between the two. One of the possible applications of this DNA-based model is for a decision-making scheme of intelligent computers and molecular robots.
In the second part, we report the design of the spatially localized DNA architecture based on computation with molecular walkers. The main challenge in developing of evolvable, autonomous, and programmable bio-molecular machines is to introduce the ability to cope with external changes. In this part, we use DNA strand displacement as the main mechanism for modeling a complex-computation capable DNA circuit. Particularly, we focus on a system that can be reinforced to make intelligent decisions.

The goal is to design a reactive synthetic bio-molecular system that is also adaptive to external stimulus. An instance of nature-inspired computational algorithms, namely the ant food-foraging system, has inspired the design in this work. It also incorporates the usage of DNA-based geometrical components or nanostructures, termed DNA origami. We verified the correctness of our algorithm in-silico through quantitative measurement of reaction kinetics. From the obtained results, it is indicated that the circuit can respond correspondingly regardless of the initial conditions, with some limited thresholds. This is in contrast to the currently available DNA strand displacement systems that are dependent to their initial conditions and can only be used for once. The potential applications include decision-making capable machines, and reusable DNA circuits.

In the third part, we discuss the model-based coordination strategy for DNA-based agents. Coordination is one important feature in delivering distributed systems. A typical approach in developing silicon-based agents, such as mechanical robotics, is by designing individual-level behavior that emerges into global functionality. Meanwhile, as DNA-based agents are based on chemical reactions, programming of every individual behavior still remains a big challenge. Once all reactants have been mixed into a solution the reactions occur immediately. This introduces nontrivial challenges in logical control. In this part, a strategy for coordinated and event-driven DNA-based systems by using a Petri Nets model is reported. First, we introduce computational primitives based on DNA strand displacement reactions. Second, we abstract their molecular implementation by Petri Nets for higher-level design. Third, we propose a model of interacting multi-agent systems based on DNA-only reactions as the main contribution of this work. The design is verified via in-silico simulation. Furthermore, we show the results from initial experiments of Petri Nets operators. From the obtained results, we believe that our design strategy is suitable for coordinating interaction of distributed DNA-based systems.

In the last part, the in-vitro implementation of the DNA-based Finite State Machine is reported. Furthermore, a design of probabilistic DNA gate is proposed, to simulate stochastic-like computation based on bio-molecular reactions.