論 文 の 内 容 の 要 旨

論文題目　EVOLUTIONARY CONSTRUCTION FRAMEWORK OF REACTION NETWORKS FOR MOLECULAR PROGRAMMING
（分子プログラミングにおける反応ネットワークの進化的合成フレームワーク）

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The emerging field of Molecular Programming explores the possibility to encode information and processes in biological and organic molecules. Its potential includes the direct interaction with biological systems and the enormous information-density of DNA, which makes it applicable to a wide range of fields such as medicine and smart material engineering.

Over the years, our understanding of biochemistry and the tools available have advanced at an amazing pace. As a result, it leads to better understanding of underlying processes, higher availability of DNA oligos and tools (enzymes, sequencing, analysis, and protocols), and above all the possibility to design and manufacture of artificial nucleic acid structures. Taking these advantages from DNA nanotechnology, many demonstrations of DNA-based molecular programs have been shown *in vivo* or *in vitro*. However, due to the lack of a systematic construction method and the complexity of the underlying molecular medium, these demonstrations are normally done by applying trial-and-error procedures, which take years and hundreds of expensive experiments to complete.

The goal of this thesis is to address the issue above by introducing a construction framework based on Evolutionary Computation techniques. This framework enables the full or semi automated construction of molecular programs in the form of reaction networks, starting from a desired behavior to the actual wet implementation. In practice, it was conveniently used to find credible solutions for real world problems, through three main components: an efficient

evolutionary algorithm, an interactive graphical user interface, and the utility modules.

The first component is an evolutionary algorithm called ERNe (Evolving Reaction Network). It is a combination of most advanced evolutionary methods and biochemical rules to efficiently search for reaction networks in molecular programs. Our results show that ERNe is much more efficient than other approaches, and with it we could successfully find credible biochemical answers to challenging autonomous molecular problems: *in vitro* batch oscillatory networks that match specific oscillation shapes.

The second and third components are interactive graphical user interface and the utility modules, with which several manual operations can be done. Examples are the use of the pruning module to find the minimal design of a solution, the use of a local search to find optimal parameters for a design performing a target behavior, and the use of Interactive Evolutionary Computation to efficiently direct user preference and knowledge into the search.