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Poster presentation

Designing a chemical program using chemical organization theory

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Background

Behaviours of biological organisms are results of complex but orchestrated biochemical reactions. The complexity of the reaction network is a source of robustness and adaptability of biological systems. Chemical programming as a potential novel computational paradigm has been investigated (cf. [1]). When exploiting biochemical reaction systems for computation, however, their complexity hinders users to control and program the systems as desired. A small modification to the reactions may cause the system to enter unknown behavioural regions. A major modification may exhibit little change in the global level. In order to harness the complexity, the gap between micro level (e.g., reaction rules) and macro level (e.g., chemotaxis behaviour) has to be bridged. As a method to link these two levels, we would like to introduce chemical organization theory. [2]. The utility of the theory is exemplified with a chemical program to solve the maximal independent set problem on an undirected graph.

Results

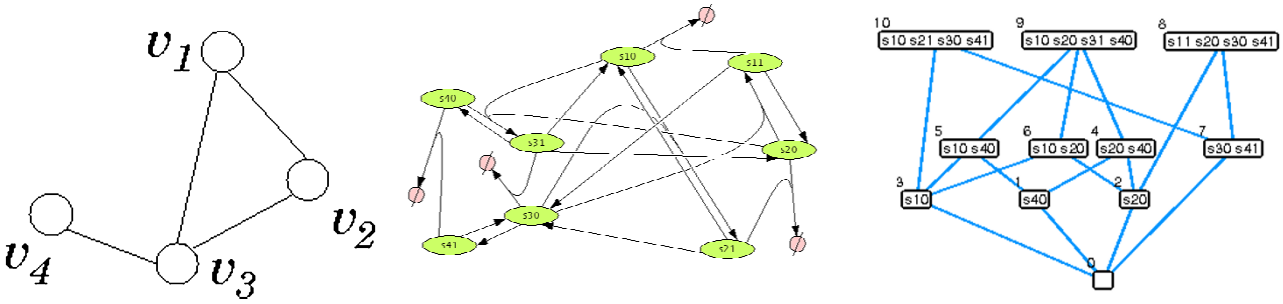
Given an undirected graph with N vertexes and M edges, a chemical program is designed as a chemical reaction network with $2N$ molecular species and $2(M + N)$ reactions as described in [3]. There are $2N$ species because two species are employed for each vertex to represent inclusion in or exclusion from the maximal independent set, respectively. Applying chemical organization theory, the reaction network is decomposed into overlapping sub-networks called **organizations**, sets of molecular species that are closed and self-maintaining. The organizational structure embedded in the network can be visualized as a Hasse diagram. Focusing on the organizations constituted of N species, the configuration of the species in any of these organizations corresponds to a maximal independent set.

Case study

In this section, we show through a concrete example how chemical organization theory benefits chemical programming. The problem instance is to find maximal independent sets on an undirected graph with four nodes and four edges as shown in the leftmost part of figure 1. A chemical reaction network (shown in the middle part) is designed as described in [3]. The organizational structure of the reaction network is shown on the right. Here, the largest organisations (8, 9, 10) correspond to the maximal independent sets {2, 4}, {3}, and {1, 4}. The correspondence between maximal independent sets and the largest organisations in the reaction network can be mathematically proven.

Conclusion

A chemical organization in a reaction network is defined as a set of molecular species that is closed and self-maintaining, induced only by the stoichiometry. In accordance with this notion, the reaction network is probed for the organizations and decomposed into overlapping sub-networks. The hierarchy of organizations provides a repertoire of dynamical behaviour patterns of the reaction system in terms of molecular species present (qualitative state). This rather high level of abstraction is useful, espe-



Undirected graph with four vertexes and four edges.

Reaction network to find maximal independent sets in given graph.

Organizational decomposition of the reaction network programmed.

Figure 1
Left: Undirected graph with four vertexes and four edges. Middle: Reaction network to find maximal independent sets in given graph. Right: Organizational decomposition of the reaction network programmed.

cially, for designing reaction systems with desired behaviour. The analysis is suitable for biological applications because of its independence of the reaction kinetics. Furthermore, the organization may be attributed to a complicated reaction process, and thus the complexity of biological systems is embraced in it. The organization-oriented design of chemical programs facilitates the exploitation of this complexity. A software tool for the organization analysis is currently developed in the Systems Biology Workbench framework and supports Systems Biology Markup Language.

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