Enumeration of Reachability Certificates in Chemical Reaction Networks

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Petri nets are both theoretically and practically interesting for many different fields. For chemistry, it can be used to model chemical reaction networks and transformation of matter in such networks. Through Petri nets we can thus model many different problems and answer many questions. Tools for such analysis already exists. An example is `LoLA` [5, 9], that can determine many properties about a given Petri net, such as existence of deadlocks, reversibility of the net, or quasiliveness of a given transition [9]. For the modelling of chemical systems it is of particular interest to formulate reachability queries, which helps explore the properties of pathways and characterize the landscape of potential pathways in a reaction network. In particular the notion of realisability of a pathway can be defined using Petri nets, which has a direct connection to the concept of *network (auto)catalysis*, and on a higher abstraction level also to *chemical hypercycles* [1, 6, 7].

Reachability analysis in existing Petri nets tools is typically dealt with as a decision question, with some tools, e.g., LoLA [5], being able to provide a certificate for positive answers. However, in analysis of chemical systems it is often interesting to investigate the concrete answer, and even more interesting to *enumerate* multiple alternative answers to questions, an ability that we have not found any traditional Petri net tools to have.

The initial focus of this project is to explore the question of enumeration of reachability certificates for Petri nets. Due to the combinatorial nature of the problem, the project will invariably include investigation of methods for state-space reduction, such as stubborn sets [8], and how they are applicable to the scenario of enumeration of solutions. The aim is to engineer a practical, reuseable implementation of a solution enumeration algorithm, which requires careful attention to design of algorithms and data structures.

The next steps of the project will be to investigate the "shape" of reachability certificates. Traditionally such a certificate consists of a sequence of events, which corresponds to a so-called *collective token interpretation* of Petri nets [2]. However, for modelling chemistry it is important to be able to keep track of individual molecules, e.g., for modelling isotope tracing experiments. Thus, an *individual token interpretation* [3] is needed, and the shape of a reachability certificate must then include the history of each token, e.g., in the form of a *causal net* [4]. The investigation is therefore into how practically efficient enumeration, up to isomorphism, can be performed in this interpretation.

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