Computation of the Kinetics of Chemical Reaction Networks

General information

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Motivations

A *chemical reaction* is a transformation between two sets of chemical species, called *chemical complexes*. An example of chemical reaction is the combustion of hydrogen:

$$2H_2 + O_2 \longrightarrow 2H_2O$$

The species of this example are H_2, O_2, and H_2O and the complexes are $2H_2 + O_2$ and $2H_2O$. A set of chemical reaction networks is called *chemical reaction network (CRN)*. Mathematically, a chemical reaction network is a finite directed graph with vertices labelled by distinct chemical complexes. Each chemical complex is a nonnegative linear combination of chemical species. Often chemical reaction networks are regarded as dynamical systems: the concentrations of the chemical species are described by partial differential equations (PDEs) containing them and their derivatives with respect to space and time variables. Therefore properties of CRNs can be detected and described via computations on their mathematical modes, e.g., graphs and polynomials.

Internship subject

In this project we will describe and compute some specific properties of CRNs in terms of polynomials and graphs. The project includes the following steps.

1. Learning the background
2. Understanding the problem
3. Programming & Computations

The required background includes some main definitions on CRN, general knowledge of graph theory and elementary polynomial algebra. An excellent introduction to CRN can be learnt via Feinberg's standard book [1]. As the required knowledge on graphs and polynomial algebra for this project is quite introductory, this can be taught during the discussions and meetings with the student directly.

The main topic of the investigations is binomiaity and toricity of CRNs, which has recently been addressed by the author and his collaborators in [2]. The binomiality and toricity problems can be modeled as a graph of CRNs or via polynomial algebra. Understanding this problem is the key point of the project.

We propose two problems on binomiality of CRNs, one of which (or both) can be chosen by the student. The first problem is a certain preprocessing in the graph of a CRN so that the binomiality can be detected efficiently. The student is required to program the preprocessing and the binomiality test on the graphs. Optionally, complexity of the method can be investigated. The second problem is assigning a certain polynomial algebra model to a reversible CRN. This model has a nice form which enables us to transform the problem into a first order logic problem which is equivalent to doing linear algebra over integer numbers. Programming this model and solving the linear algebra problem efficiently is the main task for this problem.

Work environment

The internship will take place in Nancy within the VeriDis team of Inria Nancy – Grand Est, a stimulating international research group that is common to Inria, CNRS, University of Lorraine, and the Max-Planck Institute for Informatics in Saarbrücken, and is located at LORIA on the science campus of Nancy. The city of Nancy is a lively university town of intermediate size (about 300,000 inhabitants) in the North-East of France. It offers affordable housing and is home to a rich cultural life and historic treasures, in particular from the 18th and the early 20th century.

References

[1] Martin Feinberg. *Foundations of Chemical Reaction Network Theory*, volume 202 of *Applied Mathematical Sciences*. Springer, 2019.

[2] D. Grigoriev, A. Iosif, H. Rahkooy, T. Sturm, A. Weber. *Efficiently and Effectively Recognizing Toricity of Steady State Varieties*, arXiv preprint *arXiv:1910.04100*