About the research centre or Inria department

Located at the heart of the main national research and higher education cluster, member of the Université Paris Saclay, a major actor in the French Investments for the Future Programme (Idex, LabEx, IRT, Equipex) and partner of the main establishments present on the plateau, the centre is particularly active in three major areas: data and knowledge; safety, security and reliability; modelling, simulation and optimisation (with priority given to energy).

The 450 researchers and engineers from Inria and its partners who work in the research centre’s 31 teams, the 100 research support staff members, the high-level equipment at their disposal (image walls, high-performance computing clusters, sensor networks), and the privileged relationships with prestigious industrial partners, all make Inria Saclay Île-de-France a key research centre in the local landscape and one that is oriented towards Europe and the world.

Context

This research internship is offered at Inria Saclay ÎdF (https://www.inria.fr/en/centre/saclay) in the LIFEWARE project team (http://lifeware.inria.fr). This team works in computational systems biology and develops the Biochemical Abstract Machine (BIOCHAM http://lifeware.inria.fr/biocham4) software for modeling, analyzing and now synthesizing biochemical reaction networks (CRNs) using methods from fundamental computer science and mathematics. The software developments are expected to be integrated in BIOCHAM.

The internship will be supervised by François Fages and Sylvain Soliman.

Assignment

Graph matching problems concern the detection of similarities between two graphs G and H. The exact graph matching problem is the problem of existence of a graph isomorphism between G and H. The subgraph isomorphism problem (SISO), i.e. the existence of a graph isomorphism between a subgraph of G and H, is an NP-complete problem. SISO provide a standard notion of graph motif and are widely used in pattern recognition in various domains. In the context of systems biology, the question of detecting model reduction relationships between biochemical reaction networks (CRN bipartite directed graphs) in large model repositories, led us to the notion of subgraph epimorphism (SEPI), i.e. subgraph morphism surjective on vertices and edges. The existence of a SEPI from G to H is indeed equivalent to the existence of a sequence of deletions or mergings of vertices in G that lead to a graph isomorphic to H, which, in the context of CRNs, are basic operations for simplifying a model by neglecting or merging some species or reactions. We have shown that the SEPI problem is NP-complete but that its encoding as a constraint satisfaction problem, and the use of constraint programming or SAT solvers, provide a sufficiently efficient solution in practice with few exceptions.

The goal of this research internship is to develop this approach in mainly two directions:

- investigate the theory of a refinement of SEPIs in which only adjacent vertices can be merged (at distance two in the bipartite graph of a CRN), and differences with graph minors,
- investigate the theory of minimal SEPI upper bounds, and maximal SEPI lower bounds, with the restrictions above.
To this end, an implementation will be made by refining the existing implementation using a SAT solver, and integrated in BIOCHAM for evaluation on large scale in BioModels.

**Main activities**

Our previous work on this subject is described in


The theoretical work will consist in investigating similar properties for the notion of restricted SEPs.

The implementation work using SAT solvers will be expected to be integrated in BIOCHAM and evaluated on the repository of models BioModels as initially done in


**Skills**

This subject requires a pronounced taste for graph theory, and common and basic knowledge in algorithmics and programming.

Specific knowledge about SAT solvers, constraint programming, Prolog, or systems biology will be a plus.

**Benefits package**

- Subsidised catering service
- Partially-reimbursed public transport
- Social security
- Paid leave
- Flexible working hours
- Sports facilities

**Remuneration**

500 euros/month + living compensation for foreigners