

2019-01284 - Visualisation of biochemical reaction networks using static analyzers

Level of qualifications required : Bachelor's degree or equivalent
Fonction : Internship Research

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 IdF (<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

The chemical reaction network formalism (CRN) is used to model biological processes at the cellular level. They explain the complex phenotypes as resulting from elementary molecular interactions. A CRN has a hypergraph structure (that is, a bipartite species / reaction graph labeled by a rate function) and can be interpreted at different levels of abstraction with different dynamics: differential, stochastic, discrete Petri net or Boolean.

Visualization of the structure of CRNs is not a well-solved problem today, and the automatic drawing tools are far from being able to compete with the manual drawings that modelers make in publications, and which show much better "logic" of the network.

Before performing simulations, however, many static analyzers can provide information on network inputs and outputs, dependency graphs, and influences, as well as on dynamic properties, such as algebraic or place-invariant invariants of the network. Petri net (set of molecular species whose sum of concentrations is constant), transition-invariants (set of reactions forming a circuit), etc.

The aim of the internship is to try to use this static information (calculated by BIOCHAM) on the network structure so as to define drawing strategies and to set up the visualization tools of the interaction graph (Graphviz) so that he produces automatic drawings close to the manual drawings found in the publications.

Main activities

Our previous work on some BIOCHAM static analyzers is described in

Sylvain Soliman. *Invariants and Other Structural Properties of Biochemical Models as a Constraint Satisfaction Problem*. Algorithms for Molecular Biology, 7 (15), 2012.

The work will involve using this information to design and experiment with different species placement strategies and reactions in the GraphViz visualization tool. The evaluation can be done on the BioModels model warehouse by comparing the results with the drawings of the corresponding publications.

Results may be published in the Systems Biology Graphical Notation (SBGN) community

General Information

- **Theme/Domain** : Interaction and visualization
Software Experimental platforms (BAP E)
- **Town/city** : PALAISEAU
- **Inria Center** : CRI Saclay - Île-de-France
- **Starting date** : 2019-04-01
- **Duration of contract** : 6 months
- **Deadline to apply** : 2019-09-30

Contacts

- **Inria Team** : LIFEWARE
- **Recruiter** :
Fages François / francois.fages@inria.fr

About Inria

Inria, the French national research institute for the digital sciences, promotes scientific excellence and technology transfer to maximise its impact. It employs 2,400 people. Its 200 agile project teams, generally with academic partners, involve more than 3,000 scientists in meeting the challenges of computer science and mathematics, often at the interface of other disciplines. Inria works with many companies and has assisted in the creation of over 160 startups. It strives to meet the challenges of the digital transformation of science, society and the economy.

The keys to success

We are seeking a highly talented and motivated candidate not afraid by crossing disciplinary frontiers.

Instruction to apply

Send an e-mail with CV + cover letter to Mr François Fages : francois.fages@inria.fr

Defence Security :

This position is likely to be situated in a restricted area (ZRR), as defined in Decree No. 2011-1425 relating to the protection of national scientific and technical potential (PPST). Authorisation to enter an area is granted by the director of the unit, following a favourable Ministerial decision, as defined in the decree of 3 July 2012 relating to the PPST. An unfavourable Ministerial decision in respect of a position situated in a ZRR would result in the cancellation of the appointment.

Recruitment Policy :

As part of its diversity policy, all Inria positions are accessible to people with disabilities.

Warning : you must enter your e-mail address in order to save your application to Inria. Applications must be submitted online on the Inria website. Processing of applications sent from other channels is not guaranteed.

Skills

This subject requires common and basic knowledge in algorithmics, programming, graphs and graphics.

Specific knowledge of the the Prolog programming language or of Computational 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