

Kerian Thuillier

PhD in Computer Science

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🔗 <https://kthuillier.github.io/>

Github <https://github.com/kthuillier>

Research Profile

Keywords: optimization modulo theory (OMT) – machine learning – dynamic systems – formal methods – bioinformatics

My research lies at the intersection of **formal methods, hybrid optimization, and machine learning**. Specifically, I focus on solving **inverse problems in complex dynamic systems** inspired by biology, using SMT-based and machine learning frameworks. My work addresses the core challenges of **scalability, robustness, and explainability** within these domains. This foundation motivates future research on **hybrid approaches** that integrate formal guarantees with the predictive power of machine learning.

I am committed to **open science** and to ensuring the **reproducibility** of my results.

Current Position

Postdoctoral Researcher

Dec. 2024 – Nov. 2026

Université Paris-Saclay – PEPR IA SAIF / LMF (UMR 9021)

Advisors: Benedikt Bollig, Matthias Függer, Thomas Nowak

Research topic: Scalable and explainable machine-learning methods for parameter estimation in chemical reaction networks (CRN) modeling bacterial growth in bioreactors.

Education

PhD in Computer Science

Oct. 2021 – Sep. 2024

Université de Rennes – CNRS / IRISA (UMR 6074)

Thesis defended: 27 September 2024

Title: *Hybrid Satisfiability Methods for the Inference of Boolean Regulatory Rules Controlling Metabolic Networks* 

Supervisors: Anne Siegel (CNRS / IRISA - Rennes), Loïc Paulevé (CNRS / LaBRI - Bordeaux)

Jury: François Fages (Centre INRIA Saclay), Simon de Givry (INRAE Toulouse), Emmanuelle Becker (Univ. Rennes / IRISA - Rennes), Misbah Razzaq (INRAE Tours), Laurent Tournier (INRAE Jouy-en-Josas)

Research-Oriented Master's Degree in Computer Science

2018 – 2021

École Normale Supérieure de Rennes (ENS Rennes)

Master's Degree in Computer Science

2019 – 2021

Université de Rennes 1

Dissertation: *Inferring Boolean regulatory rules controlling hybrid biological models* 

Bachelor's Degree in Computer Science

2015 – 2019

Université de Rennes 1 (third year at ENS Rennes)

Qualifications

Qualification for Maître de Conférences, CNU Section 27

Valid 2025–2029

Publications

All scripts and datasets required to reproduce results are publicly available on GitHub.

Peer-Reviewed Journal Articles

- M. Függer, T. Nowak, and K. Thuillier (2025). *Distributed computing inspired by biology*. Seminars in Cell & Developmental Biology, 175.  
- K. Thuillier, C. Baroukh, A. Bockmayr, L. Cottret, L. Paulev , and A. Siegel (2022). *MERRIN: Metabolic Regulation Rule Inference from time series data*. Oxford Bioinformatics.  
Presented at European Conference on Systems Biology (ECCB)

Peer-Reviewed International Conferences

- K. Thuillier, A. Siegel, and L. Paulev  (2024). *CEGAR-Based Approach for Solving Combinatorial Optimization Modulo Quantified Linear Arithmetics Problems*. AAAI Conference on Artificial Intelligence.  
- K. Thuillier, C. Baroukh, A. Bockmayr, L. Cottret, L. Paulev , and A. Siegel (2021). *Learning Boolean Controls in Regulated Metabolic Networks: A Case-Study*. Computational Methods in Systems Biology (CMSB).  

Invited Talks & Oral Presentations

Invited Talks

- *Aggrometabiont Days*, IRISA (UMR 6074), Rennes Dec. 2025
20min, Topic: Regulatory controls of bacteria metabolism
- Laboratoire M thodes Formelles (LMF, UMR 9021), Gif-sur-Yvette Dec. 2024
1h, Topic: talking about my PhD results
- Laboratoire d'Informatique et des Syst mes (LIS, UMR 7020), Marseille Dec. 2024
1h, Topic: talking about my PhD results
- *Knowledge Representation and Reasoning* team, University of Potsdam, Germany 2023
1h, *Weekly seminar*, Topic: Solving quantified linear constraints in ASP
- *ASP days*, LaBRI (UMR 5800), Bordeaux Nov. 2022
20min, Topic: Solving quantifier-free linear constraints in ASP

Oral Presentations on Extended Abstracts

- Workshop *Mod lisation du M tabolisme*, Toulouse 2024
Inf rence de r gles de r gulation m tabolique   partir de s ries temporelles
- Session *Operational Research in Bioinformatics*, ROADEF, Rennes 2023
Satisfaction of Hybrid Optimization Problems Applied to Bioinformatics
- *GT-BioSS* national days, Nantes 2022
MERRIN: MEtabolic Regulation Rule INference from time series data
- Session *Optimisation Combinatoire pour la Bioinformatique*, ROADEF, Montpellier 2020
A MILP Approach for Genome Haplotyping

- Session *Optimisation Combinatoire pour la Bioinformatique*, ROADEF, Montpellier 2020
A MILP Approach for the Metabolic Network Completion Problem

Softwares and Research Artifacts

All softwares and datasets are open-sources, maintained and available on GitHub.

- **merrinasp**  Software
ASP-based solver for combinatorial optimization modulo quantified linear arithmetic (OMT+qLRA)
- **merrin**  Software
Tool for the inference of regulatory rules controlling the metabolism
- **Benchmarks of OMT+qLRA problems** [Zenodo] Benchmark
First benchmark for this class of problems, inspired from Systems Biology
- **Regulated metabolic models of *E.coli***  Biological Models
Models reconstructed from litteratures, no previous computational models available

Preliminary Patent Application

- **B. Bollig, M. Függer, T. Nowak, and K. Thuillier** (2025). Under review
IPC: G06N 20/00 and C12Q 1/00
Title: *Parametrization of biochemical digital twins on timed data with deep neural networks*
Content: Computational method to decrease memory usage and computation times for training physics-informed neural networks (PINNs) in the context of parameter estimation of powerlaw ODE systems modeling bacterial growth dynamics. The core of the method relies on Taylor series approximations of ODES to simulate ODE dynamics.

Fundings

- 3 months mobility grant** May 2023
Research Visit at University of Potsdam and Freie Universität Berlin (Germany)
Funding Body: Doctoral School MathSTIC (Rennes, France)
Project: Technical development of ASP-based encodings (with Prof. T. Schaub, University of Potsdam) and multiscale modeling of *E. coli* (with Prof. A. Bockmayr, Freie Universität Berlin).
Grant awarded but relinquished due to personal health reasons

Outreach

- Participant and award recipient of *Sciences en Cour[t]s* 2022
5-minute short film: Patatogène
Awards: Audience Award, Best Screenplay Award, Science Outreach Award (tie)

Supervision

- Supervision of Master 1's internship** May – Jul. 2023
Master 1 student in Bioinformatics, Université de Rennes
Topic: Inference of metabolic regulatory rules using Answer Set Programming

Teaching Experience

Responsibilities included exam design, project supervision, and grading.

- Operations Research (M1 Computer Science), Université de Rennes 24h ETD
Designed all TP subjects and scripts
 - Graph Modeling and Algorithms (L3 Computer Science), Université de Rennes 20h ETD
Upgraded all TD subjects
 - Programming (L1 Computer Science), Université de Rennes 20h ETD
 - Logic (L3 Computer Science), Université de Rennes 12h ETD
 - Introduction to Algorithms (L3 Mathematics), ENS Rennes 20h ETD

Academic Service

- **Reviewer** CMSB 2024
 - **Session co-organizer and chairman** ROADEF 2023
Session: *Operational Research in Bioinformatics*
 - **Organizer of monthly seminars** 2021–2023
Data Knowledge Management department at IRISA, Rennes