RESEARCH CENTRE

**Nancy - Grand Est** 

IN PARTNERSHIP WITH: Université de Lorraine, CNRS

## 2021 ACTIVITY REPORT

# Project-Team MOCQUA

# Designing the Future of Computational Models

IN COLLABORATION WITH: Laboratoire lorrain de recherche en informatique et ses applications (LORIA)

## DOMAIN

Algorithmics, Programming, Software and Architecture

THEME Security and Confidentiality

## Contents

| 1      Team members, visitors, external collaborators      2        2      Overall objectives      3        3      Research program      3        3.1      Quantum computing      4        3.2      Higher-order computing      4        3.3      Dynamical systems      4        4      Application domains      5        4.1      Quantum computing      5        4.2      Higher-order computing      5        4.3      Simulation of dynamical systems by cellular automata      5        5      Highlights of the year      6        5.1      Awards      6        6      New software and platforms      6        6.1.2      ComplexityParser      7        6.1.2      ComplexityParser      7        7.1      Forcet point property for represented spaces      7        7.1.1      Fixed-point property for represented spaces      7        7.2.2      Optiagrams for symbolic dynamics      5        7.2.3      Diagrams for symbolic dynamics      5        7.2.4      Analysis of graphs in the field of economics      5        7.3      Implicit computational complexity      5<  | Pr | Project-Team MOCQUA   |  |  |
|--|----|---|--|--|
| 2 Overall objectives      5        3 Research program      5        3.1 Quantum computing      5        3.2 Higher-order computing      5        3.3 Dynamical systems      6        4 Application domains      5        4.1 Quantum computing      5        4.2 Higher-order computing      5        4.3 Simulation of dynamical systems by cellular automata      5        5 Highlights of the year      6        5.1 Awards      6        6 New software and platforms      6        6.1.1 Ven software      6        6.1.2 ComplexityParser      7        7.1 Computability over topological spaces      7        7.1.1 Fixed-point property for represented spaces      7        7.1.2 Apperiodic telesets      6        7.2.3 Diagrams for symbolic dynamics      5        7.3 Implicit computational complexity      5        7.4 Enumerative and probabilistic combinatorics of some discrete objects      5        7.3 Implicit computational complexity      5        7.4 Enumerative and probabilistic combinatorics of some discrete objects      5        7.3 Implicit computational complexity      5        7.4 Random cographs      7      7.5   | 1  | Team members, visitors, external collaborators  | 2  |  |
| 3      Research program      2        3.1      Quantum computing      2        3.2      Higher-order computing      2        3.3      Dynamical systems      4        4      Application domains      5        4.1      Quantum computing      5        4.2      Higher-order computing      5        4.3      Simulation of dynamical systems by cellular automata      5        5      Highlights of the year      6        6.1      New software and platforms      6        6.1.1      FiatLux      6        6.1.2      ComplexityParser      7        6.1.3      Quarea      7        7      New results      7        7.1.1      Fixed-point property for represented spaces      7        7.1.2      Approximation property for represented spaces      7        7.1.1      Fixed-point property for represented spaces      7        7.2.1      Probabilistic cellular automata for problem solving      7        7.2.3      Diagrams for symbolic dynamics      8        7.2.4      Analysis of graphs in the field of economics      5        7.3.4      Implicit computational complexity   | 2  | Overall objectives  | 3  |  |
| 4 Application domains      5        4.1 Quantum computing      5        4.2 Higher-order computing      5        4.3 Simulation of dynamical systems by cellular automata      5        5 Highlights of the year      6        5.1 Awards      6        6 New software and platforms      6        6.1.1 FiatLux      6        6.1.2 ComplexityParser      7        6.1.3 Qimaera      7        7      New results      7        7.1 Computability over topological spaces      7        7.1.2 Algorithmic property for represented spaces      7        7.1.2 Norbalilistic cellular automata for problem solving      8        7.2.1 Probabilistic cellular automata for problem solving      8        7.2.3 Diagrams for symbolic dynamics      9        7.4 Enumerative and probabilistic combinatorics of some discrete objects      9        7.4 Enumerative and probabilistic combinatorics of some discrete objects      9        7.4.3 Interval posets of permutations      10        7.5.4 Quantum, probabilistic and substructural programming languages      10        7.5.2 Computational quantum programming in idris      11        7.5.3 Variational quantum programming in idris      12        8 Bilateral contracts   | 3  | Research program3.1Quantum computing  | <b>3</b><br>3<br>4<br>4  |  |
| 5      Highlights of the year      6        5.1      Awards      6        6      New software and platforms      6        6.1      New software      6        6.1.1      FiatLux      6        6.1.2      ComplexityParser      7        6.1.3      Qimaera      7        7      New results      7        7.1      Computability over topological spaces      7        7.1.1      Fixed-point property for represented spaces      7        7.1.2      Algorithmic properties of sets      7        7.2      Dynamical systems      8        7.2.1      Probabilistic cellular automata for problem solving      8        7.2.3      Diagrams for symbolic dynamics      9        7.2.4      Analysis of graphs in the field of economics      9        7.4      Enumerative and probabilistic combinatorics of some discrete objects      9        7.4.1      Random cographs      9        7.4.2      Baxter Tree-like tableaux      10        7.4.3      Interval posets of permutations      10        7.5.4      Commutative monads for probabilistic programming languages      10        7.5.5      <  | 4  | Application domains4.1Quantum computing   | <b>5</b><br>5<br>5<br>5  |  |
| 6      New software and platforms      6        6.1      New software      6        6.1.1      FiatLux      6        6.1.2      ComplexityParser      7        6.1.3      Qimaera      7        7      New results      7        7.1      Computability over topological spaces      7        7.1.1      Fixed-point property for represented spaces      7        7.2      Dynamical systems      8        7.2.1      Probabilistic cellular automata for problem solving      7        7.2.2      Aperiodic tilesets      8        7.2.3      Diagrams for symbolic dynamics      9        7.3.4      Enumerative and probabilistic combinatorics of some discrete objects      9        7.4.1      Random cographs      9      9        7.4.2      Baxter Tree-like tableaux      10      10        7.4.3      Interval posets of permutations      10      10        7.5.4      Commutative monads for probabilistic programming languages      11      11        7.5.3      Variational quantum programming in idris      11      12.5.4      Semantics for variational quantum programming      12        8      Bilateral   | 5  | Highlights of the year        5.1 Awards  | <b>6</b><br>6  |  |
| 7 New results      7        7.1 Computability over topological spaces      7        7.1.1 Fixed-point property for represented spaces      7        7.1.2 Algorithmic properties of sets      7        7.2 Dynamical systems      8        7.2.1 Probabilistic cellular automata for problem solving      8        7.2.2 Aperiodic tilesets      8        7.2.3 Diagrams for symbolic dynamics      9        7.2.4 Analysis of graphs in the field of economics      9        7.3 Implicit computational complexity      9        7.4 Enumerative and probabilistic combinatorics of some discrete objects      9        7.4.2 Baxter Tree-like tableaux      10        7.4.3 Interval posets of permutations      10        7.5.4 Quantum, probabilistic and substructural programming languages      11        7.5.2 Commutative monads for probabilistic programming languages      11        7.5.4 Semantics for variational quantum programming in idris      11        7.5.4 Semantics for variational quantum programming      12        8 Bilateral contracts and grants with industry      12        9 Partnerships and cooperations      12        9.1 International initiatives      12        9.1.2 STIC/MATH/CLIMAT AmSud project      13        9.2 European initiatives | 6  | New software and platforms        6.1      New software        6.1.1      FiatLux        6.1.2      ComplexityParser        6.1.3      Qimaera  | 6<br>6<br>7<br>7   |  |
| 8 Bilateral contracts and grants with industry      12        8.1 Bilateral contracts with industry      12        9 Partnerships and cooperations      12        9.1 International initiatives      12        9.1.1 Inria associate team not involved in an IIL or an international program      12        9.1.2 STIC/MATH/CLIMAT AmSud project      13        9.2 European initiatives      14        9.2.1 FP7 & H2020 projects      14        9.2.2 Other guranean programs (initiatives)      14  | 7  | New results7.1Computability over topological spaces7.1.1Fixed-point property for represented spaces7.1.2Algorithmic properties of sets7.2Dynamical systems7.2.1Probabilistic cellular automata for problem solving7.2.2Aperiodic tilesets7.2.3Diagrams for symbolic dynamics7.2.4Analysis of graphs in the field of economics7.3Implicit computational complexity7.4Enumerative and probabilistic combinatorics of some discrete objects7.4.1Random cographs7.4.2Baxter Tree-like tableaux7.4.3Interval posets of permutations7.5Quantum, probabilistic and substructural programming languages7.5.1Recursive types in substructural type systems7.5.2Commutative monads for probabilistic programming languages7.5.3Variational quantum programming in idris7.5.4Semantics for variational quantum programming | 7<br>8<br>8<br>8<br>8<br>9<br>9<br>9<br>9<br>9<br>9<br>9<br>9<br>9<br>9<br>9<br>9<br>9<br>10<br>10<br>10<br>10<br>11<br>11<br>12 |  |
| 9 Partnerships and cooperations      12        9.1 International initiatives      12        9.1.1 Inria associate team not involved in an IIL or an international program      12        9.1.2 STIC/MATH/CLIMAT AmSud project      13        9.2 European initiatives      14        9.2.1 FP7 & H2020 projects      14        9.2.2 Other guranean programs (initiatives)      14   | 8  | Bilateral contracts and grants with industry        8.1 Bilateral contracts with industry   | <b>12</b><br>12  |  |
|  | 9  | Partnerships and cooperations        9.1      International initiatives        9.1.1      Inria associate team not involved in an IIL or an international program        9.1.2      STIC/MATH/CLIMAT AmSud project        9.2      European initiatives        9.2.1      FP7 & H2020 projects        9.2.2      Other auropean programs (initiatives)  | 12<br>12<br>13<br>14<br>14   |  |

| 9.3     | Vational initiatives                             | 15 |
|---------|--|----|
|         | .3.1 ANR   | 15 |
|         | .3.2 Other initiatives                           | 16 |
| 10 Dis  | mination   | 16 |
| 10.1    | Promoting scientific activities                  | 16 |
|         | 0.1.1 Scientific events: organisation            | 16 |
|         | 0.1.2 Journal                                    | 17 |
|         | 0.1.3 Invited talks                              | 17 |
|         | 0.1.4 Leadership within the scientific community | 18 |
|         | 0.1.5 Scientific expertise                       | 18 |
| 10.2    | eaching - Supervision - Juries                   | 18 |
|         | 0.2.1 Supervision                                | 19 |
|         | 0.2.2 Juries                                     | 20 |
| 10.3    | Popularization                                   | 20 |
|         | 0.3.1 Articles and contents                      | 20 |
|         | 0.3.2 Interventions                              | 20 |
| 11 Scie | tific production                                 | 20 |
| 11.1    | Major publications                               | 20 |
| 11.2    | Publications of the year                         | 21 |
| 11.3    | Dther  | 23 |
| 11.4    | Sited publications                               | 23 |

## **Project-Team MOCQUA**

Creation of the Project-Team: 2020 March 01

## Keywords

#### Computer sciences and digital sciences

- A2.3.2. Cyber-physical systems
- A2.4.1. Analysis
- A6.5. Mathematical modeling for physical sciences
- A7.1.4. Quantum algorithms
- A7.2. Logic in Computer Science
- A7.3. Calculability and computability
- A8.1. Discrete mathematics, combinatorics
- A8.3. Geometry, Topology
- A8.6. Information theory

#### Other research topics and application domains

B9.5.1. – Computer science B9.5.2. – Mathematics B9.5.3. – Physics

## 1 Team members, visitors, external collaborators

#### **Research Scientists**

- Simon Perdrix [Team leader, Inria, Senior Researcher, receives team leadership in 2022, HDR]
- Mathilde Bouvel [CNRS, Researcher]
- Nazim Fatès [Inria, Researcher]
- Isabelle Gnaedig-Antoine [Inria, Researcher]
- Mathieu Hoyrup [Inria, Researcher]
- Christophe Vuillot [Inria, Researcher]
- Vladimir Zamdzhiev [Inria, Starting Faculty Position]

#### **Faculty Members**

- Emmanuel Jeandel [Team leader, Univ de Lorraine, Professor, transfers team leadership in 2022, HDR]
- Guilhem Gamard [Univ de Lorraine, Associate Professor, from Sep 2021]
- Emmanuel Hainry [Univ de Lorraine, Associate Professor]
- Romain Péchoux [Univ de Lorraine, Associate Professor, HDR]

#### **Post-Doctoral Fellows**

- Marc De Visme [CNRS, until Sep 2021]
- Timothée Goubault De Brugière [CNRS, from Mar 2021]

#### **PhD Students**

- Djamel Eddine Amir [Univ de Lorraine]
- Robert Booth [CNRS, from Oct 2018]
- Agustin Borgna [CNRS]
- Titouan Carette [Univ de Lorraine, until Nov 2021]
- Alexandre Clément [Univ de Lorraine]
- Alexandre Guernut [Inria, from Oct 2021]
- Mario Alberto Machado Da Silva [Univ de Lorraine, from Oct 2021]
- Vivien Vandaele [CNRS, CIFRE, from Sep 2021]
- Margarita Veshchezerova [EDF, CIFRE]

#### **Interns and Apprentices**

- Liliane Joy Dandy [Inria, from Mar 2021 until Jul 2021]
- Alexandre Guernut [CNRS, from Mar 2021 until Aug 2021]
- Benjamin Izart [Univ de Lorraine, from Jun 2021 until Sep 2021]
- Julia Krot [Inria, from Mar 2021 until Jul 2021]
- Julien Lamiroy [CNRS, from Sep 2021]
- Émile Larroque [Univ de Lorraine, from Feb 2021 until Jul 2021]
- Yosyp Mykhailiv [Univ de Lorraine, from Mar 2021 until Jul 2021]
- Arthur Rousseau [École Normale Supérieure de Paris, from Jun 2021 until Jul 2021]
- Hervé Sabrié [Univ de Lorraine, from May 2021 until Jul 2021]
- Marie Vela Mena [Inria, from Nov 2021]
- Nishigandha Nandkuma Yadav [Univ de Lorraine, from Mar 2021 until Jul 2021]

#### Administrative Assistants

- Sophie Drouot [Inria]
- Sylvie Hilbert [CNRS]

#### **Visiting Scientist**

• Lapo Cioni [Université de Florence, from Sep 2021 until Oct 2021]

## 2 Overall objectives

The goal of the Mocqua team is to tackle challenges coming from the emergence of new or future computational models. The landscape of computational models has indeed changed drastically in the last few years: the complexity of digital systems is continually growing, which leads to the introduction of new paradigms, while new problems arise due to this larger scale (tolerance to faulty behaviors, asynchronicity) and constraints of the present world (energy limitations). In parallel, new models based on physical considerations have appeared. There is thus a real need to accompany these changes, and we intend to investigate these new models and try to solve their intrinsic problems by computational and algorithmic methods.

While the bit remains undeniably the building block of computer architecture and software, it is fundamental for the development of new paradigms to investigate computations and programs working with inputs that cannot be reduced to finite strings of 0's and 1's. Our team will focus on a few instances of this phenomenon: programs working with qubits (quantum computing), programs working with functions as inputs (higher-order computation) and programs working in infinite precision (real numbers, infinite sequences, streams, coinductive data, ...).

## 3 Research program

#### 3.1 Quantum computing

While it can be argued that the quantum revolution has already happened in cryptography [41] or in optics [40], quantum computers are far from becoming a common commodity. This is despite the fact that many teams worldwide, both academic and industrial, are nowadays focusing much of their efforts

on building quantum computers. Indeed the challenges ahead to reach practical, sizable and accurate quantum computers remain tremendous.

Today's quantum devices are small in scale and still very noisy and are therefore called NISQ devices (for Noisy Intermediate Scale Quantum). They all differ fundamentally on the hardware substrate, and it is quite hard to predict which solution will finally be adopted. While some effort is underway to understand and utilize the potential of these NISQ devices, scaling up and implementing fault-tolerant and quantum error correction schemes will eventually become crucial for the potential of quantum computing to be reached.

As these devices are developed and scale up, the importance of software to operate them and programming languages to program them will grow. The practical applications in sight will require tighter interactions within the quantum stack, which extends from hardware to algorithms. Given its recent emergence, the landscape of quantum programming languages is constantly evolving. Comparably to compiler design, the foundation of quantum software therefore relies on an intermediate representation that is suitable for manipulation, easy to produce from software and easily encodable into hardware. A graphical language now firmly established as the choice for this is the ZX-calculus.

Many research questions are now to be addressed. For instance, what are the correct formalism and approaches for quantum programming languages? How to develop practical, and useful algorithms? What role can graphical intermediate representations such as ZX-calculus play in interaction between compilers and hardware with different characteristics, like lattice surgery fault-tolerance or quantum optics? Which quantum error correcting codes and fault-tolerant schemes can make large scale quantum computing reachable?

#### 3.2 Higher-order computing

While programs often operate on natural numbers or finite structures such as graphs or finite strings, they can also take functions as inputs. In that case, the program is said to perform higher-order computations, or to compute a higher-order functional. Functional programming or object-oriented programming are important paradigms allowing higher-order computations.

While the theory of computation is well developed for first-order programs, difficulties arise when dealing with higher-order programs. There are many non-equivalent ways of presenting inputs to such programs: an input function can be presented as a black-box, encoded in an infinite binary sequence, or sometimes by a finite description. Comparing those representations is an important problem. A particularly useful application of higher-order computations is to compute with infinite objects that can be represented by functions or symbolic sequences. The theory works well in many cases (to be precise, when these objects live in a topological space with a countable basis [55]), but is not well understood in other interesting cases. For instance, when the inputs are the second-order functionals (of type  $(\mathbb{N} \to \mathbb{N}) \to (\mathbb{N} \to \mathbb{N})$ ), the classical theory does not apply and many problems are still open.

#### 3.3 Dynamical systems

The most natural example of a computation with infinite precision is the simulation of a dynamical system. The underlying space might be  $\mathbb{R}^n$  in the case of the simulation of physical systems, or the Cantor space  $\{0, 1\}^{\mathbb{Z}}$  in the case of discrete dynamical systems.

From the point of view of computation, the main point of interest is the link between the long-term behavior of a system and its initial configuration. There are two questions here: (a) predict the behavior, (b) design dynamical systems with some prescribed behavior. The first will be mainly examined through the angle of reachability and more generally control theory for hybrid systems.

The model of cellular automata will be of particular interest. This computational model is relevant for simulating complex global phenomena which emerge from simple interactions between simple components. It is widely used in various natural sciences (physics, biology, etc.) and in computer science, as it is an appropriate model to reason about errors that occur in systems with a great number of components.

The simulation of a physical dynamical system on a computer is made difficult by various aspects. First, the parameters of the dynamical systems are seldom exactly known. Secondly, the simulation is usually not exact: real numbers are usually represented by floating-point numbers, and simulations of cellular automata only simulate the behavior of finite or periodic configurations. For some chaotic systems, this means that the simulation can be completely irrelevant.

## 4 Application domains

#### 4.1 Quantum computing

Quantum Computing is currently the most promising technology to extend Moore's law, whose end is expected to be reached soon with engraving technologies struggling to reduce transistor size. Thanks to promising algorithmic and complexity theoretic results on its computational power, quantum computing will represent a decisive competitive advantage for those who will control it.

Quantum Computing is also a major security issue, since it allows us to break today's asymmetric cryptography. Hence, mastering quantum computing is also of the highest importance for national security concerns. Small-scale quantum computers already exist and recent scientific and technical advances suggest that the construction of the first *practical* quantum computers will be possible in the coming years.

As a result, the major US players in the IT industry have embarked on a dramatic race, mobilizing huge resources: IBM, Microsoft, Google and Intel have each invested huge sums of money, and are devoting significant budgets to attract and hire the best scientists on the planet. Some states have launched ambitious national programs, including the United Kingdom, the Netherlands, Canada, China, Australia, Singapore, and very recently Europe, with the 10-year FET Flagship program in Quantum Engineering. The French government also recently announced its Plan Quantique – a 1.8 billion euro initiative to develop quantum technologies.

An important pillar of the Plan Quantique concerns the development of Large Scale Quantum computers. This will come with progress all across the quantum stack.

The Mocqua team contributes to the computer science approach to quantum computing, with expertise ranging all across the quantum stack from quantum software to fault-tolerance and quantum error-correction. We aim at a better understanding of the power and limitations of the quantum computer, and therefore of its impact on society. We also contribute to ease the development of the quantum computer by filling gaps across the quantum stack from programming languages to compilation and intermediate representations for fault-tolerant implementations on hardware.

#### 4.2 Higher-order computing

The idea of considering functions as first-class citizens and allowing programs to take functions as inputs has emerged since the very beginning of theoretical computer science through Church's  $\lambda$ -calculus and is nowadays at the core of functional programming, a paradigm that is used in modern software and by digital companies (Google, Facebook, ...). In the meantime higher-order computing has been explored in many ways in the fields of logic and semantics of programming languages.

One of the central problems is to design programming languages that capture most of, if not all, the possible ways of computing with functions as inputs. There is no Church thesis in higher-order computing and many ways of taking a function as input can be considered: allowing parallel or only sequential computations, querying the input as a black-box or via an interactive dialog, and so on.

The Kleene-Kreisel computable functionals are arguably the broadest class of higher-order continuous functionals that could be computed by a machine. However their complexity is such that no current programming language can capture all of them. Better understanding this class of functions is therefore fundamental in order to identify the features that a programming language should implement to make the full power of higher-order computation expressible in such a language.

#### 4.3 Simulation of dynamical systems by cellular automata

We aim at developing various tools to simulate and analyse the dynamics of spatially-extended discrete dynamical systems such as cellular automata. The emphasis of our approach is on the evaluation of the robustness of the models under study, that is, their capacity to resist various perturbations.

In the framework of pure computational questions, various examples of such systems have already been proposed for solving complex problems with a simple bio-inspired approach (e.g. the decentralized gathering problem [43]). We are now working on their transposition to various real-world situations. For example when one needs to understand the behaviour of large-scale networks of connected components such as wireless sensor networks. In this direction of research, a first work has been presented on how to achieve a decentralized diagnosis of networks made of simple interacting components and the results are rather encouraging [45]. Nevertheless, there are various points that remain to be studied in order to complete this model for its integration in a real network.

We have also tackled the evaluation of the robustness of a swarming model proposed by A. Deutsch to mimic the self-organization process observed in various natural systems (birds, fishes, bacteria, etc.) [2]. We now wish to develop our simulation tools to apply them to various biological phenomena where many agents are involved.

We are also currently extending the range of applications of these techniques to the field of economy. We have started a collaboration with Massimo Amato, a professor in economy at the Bocconi University in Milan. Our aim is to propose a decentralized view of a business-to-business market and totally decentralized, agent-oriented models of such markets. Various banks and large businesses have already expressed their interest in such modelling approaches.

## 5 Highlights of the year

#### 5.1 Awards

- Renaud Vilmart, former PhD Student of the team, was awarded at the beginning of 2021 an accessit to the Gilles Kahn prize for best PhD.
- Liliane Joy Dandy got an award from Ecole Polytechnique for her internship (March 2021 to July 2021) with Vladimir Zamdzhiev and Emmanuel Jeandel. Related to this internship are the following preprint under review [31] and the new software Qimaera, see section 6.1.3.

## 6 New software and platforms

The already existing software FiatLux and ComplexityParser have continued to be developed. In addition, the development of a new set of libraries for the Idris 2 programming language was initiated under the name Qimaera.

#### 6.1 New software

#### 6.1.1 FiatLux

Keywords: Cellular automaton, Multi-agent, Distributed systems

- Scientific Description: FiatLux is a discrete dynamical systems simulator that allows the user to experiment with various models and to perturb them. It includes 1D and 2D cellular automata, moving agents, interacting particle systems, etc. Its main feature is to allow users to change the type of updating, for example from a deterministic parallel updating to an asynchronous random updating. FiatLux has a Graphical User Interface and can also be launched in a batch mode for the experiments that require statistics.
- **Functional Description:** FiatLux is a cellular automata simulator in Java specially designed for the study of the robustness of the models. Its main distinctive features are to allow users to perturb the updating of the system (synchrony rate) and the topology of the grid.
- **News of the Year:** The latest version of the software incorporates improvements that were implemented by Océane Chazé, a second-year student at Télécom Nancy. She improved the User Interface by simplifying the interactions with the grid of cells. She also improved the software by introducing new features which allow users to encode initial conditions and transitions rules in a more elaborate

way. This allows users to import some well-known models from external websites, e.g. Langton's self-reproducing rule or "classical" patterns in the Game of Life.

URL: https://project.inria.fr/fiatlux/

**Contact:** Nazim Fates

Participants: Nazim Fates, Olivier Boure

Partners: ENS Lyon, Université de Lorraine

#### 6.1.2 ComplexityParser

Name: ComplexityParser

Keywords: Static analysis, Complexity, Static typing

**Functional Description:** ComplexityParser is a static complexity analyzer for Java programs using a tier-based typing discipline. If a program is typable, this guarantees its runtime to be polynomial on the condition that it halts. The type inference is automatic, its complexity is linear in the size of the input program in practice.

URL: https://gitlab.inria.fr/complexityparser/complexityparser

Contact: Romain Péchoux

#### 6.1.3 Qimaera

Name: Qimaera

Keyword: Quantum programming

**Functional Description:** Variational Quantum Algorithms are hybrid classical-quantum algorithms where classical and quantum computation work in tandem to solve computational problems. These algorithms create interesting challenges for the design of suitable programming languages. We introduce Qimaera, which is a set of libraries for the Idris 2 programming language that enable the programmer to implement (variational) quantum algorithms where the full power of the elegant Idris language works in synchrony with quantum programming primitives that we introduce. The two key ingredients of Idris that make this possible are (1) dependent types which allow us to implement unitary (i.e. reversible and controllable) quantum operations, and (2) linearity which allows us to enforce fine-grained control over the execution of quantum operations that ensures compliance with the laws of quantum mechanics. We demonstrate that Qimaera is suitable for variational quantum programming by providing implementations of the two most prominent variational quantum algorithms – QAOA and VQE. To the best of our knowledge, this is the first implementation of these algorithms that has been achieved in a type-safe framework.

URL: https://github.com/zamdzhiev/Qimaera

Publication: hal-03519238

Contact: Vladimir Zamdzhiev

Participants: Liliane-Joy Dandy, Emmanuel Jeandel, Vladimir Zamdzhiev

#### 7 New results

#### 7.1 Computability over topological spaces

Participants: Djamel Eddine Amir, Mathieu Hoyrup.

#### 7.1.1 Fixed-point property for represented spaces

A space with a structure has the fixed-point property if every structure-preserving function from the space to itself has a fixed-point. We investigate which spaces have the fixed-point property for computable multivalued functions. We prove in particular that among the countably-based topological spaces, they are exactly the omega-continuous domains, an important class coming from semantics of programming languages. We apply our results to identify the complexity of indexing a basis of a topological space. Our article has been accepted in the Annals of Pure and Applied Logic [35].

#### 7.1.2 Algorithmic properties of sets

We investigated the relationship between the computability of sets and their topological properties. More precisely, we are studying which sets have "computable type", which is the property that any algorithm that semidecides the set can be converted into an algorithm that fully decides the set. We have obtained a topological characterization of this property for a large class of sets, namely the finite simplicial complexes. Our results give an easy way of determining whether a given set has computable type. In particular we have settled the question for famous sets from topology: the dunce hat, and Bing's house. An article is currently submitted.

We have also obtained a partial characterization of this property using homology theory. Essentially, this property is related to the fact that every point belongs to a cycle, a notion provided by homology, extending the notion of cycle in a graph. An article is in preparation.

#### 7.2 Dynamical systems

Participants: Nazim Fatès, Emmanuel Jeandel.

#### 7.2.1 Probabilistic cellular automata for problem solving

Directly related to the theme exposed in Sec. 4.3, we continued to explore the problem of self-stabilisation, as introduced by Dijkstra in the 1970's, in the context of cellular automata [44]. More precisely, we extended the scope of our results from k-colourings to shifts of finite type. We also presented various constructions and theorems that allow us to consolidate the framework of this problem. The last details for the presentation of our work have been worked out and our article has been accepted for a publication in *Fundamenta informaticae* [33].

Our work on a bio-inspired mechanism for data clustering has also been revised and is scheduled for a publication in 2022 [53]. Our method uses amoebae which evolve according to cellular automata rules: they contain the data to be processed and emit reaction-diffusion waves at random times. The waves transmit the information across the lattice and cause other amoebae to react, by being attracted or repulsed. The local reactions produce small homogeneous groups which progressively merge and realize the clustering at a larger scale.

We continued our work with Régine Marchand (IECL, Université de Lorraine) and Irène Marcovici on the problem of detecting failures in a distributed network [46]. The question that drives our research is to find out how we can detect that the failure rate has exceeded a given threshold without any central authority when some components progressively break down.

#### 7.2.2 Aperiodic tilesets

Our paper [12] with Michael Rao which proved the existence of an aperiodic set of 11 Wang tiles, along with the proof that this number is minimal, was published this year in Advances in Combinatorics. This work was done a few years ago and already available in public repositories (arXiv, HAL-Inria). It closed 50 years of research on this problem.

#### 7.2.3 Diagrams for symbolic dynamics

One of the main open question in the field of symbolic dynamics is to decide whether the conjugacy problem is computable. This is a problem on shifts of finite type, that can be reformulated in terms of matrices. Two matrices M and N with nonnegative integer coefficients are said to be strong-shift-equivalent in one step if M = RS and N = SR for nonnecessarily square matrices R and S with nonnegative integer coefficients. Strong shift equivalence is the reflexive and transitive closure of this relation.

In [36] we show how to use results from category theory, in particular the concept of PROPs as used for instance in the ZX-calculus, to provide a purely categorical version of this question. Rather than just a technical exercise, we show in the same paper that we can recover many invariants of strong shift equivalence rather surprisingly by considering preexisting categories with bialgebras that are well known in mathematics. Whether the approach could lead to the computability of strong shift equivalence remains to be seen.

#### 7.2.4 Analysis of graphs in the field of economics

In collaboration with colleagues form Bocconi University and University of Trento, we developed some economic and operational foundations of a new method of financing companies' financial obligations [32]. In this new banking business model, a network funder sets an optimal combination of netting and financing. Given a network of companies and their respective invoices, and under the condition of a full settlement of the invoices, we applied a multilateral netting algorithm to the network, conceived as an oriented multi-graph. Our problem, which is NP-complete, was to find a set of invoices which maximises the amount of debt reduced given a quantity of loanable funds. We designed a policy which finds a trade-off and tested our methods on an empirical dataset from an electronic invoicing operator consisting of more than 60,000 companies. The first results show that this method is economically significant and feasible.

#### 7.3 Implicit computational complexity

Participants: Emmanuel Hainry, Emmanuel Jeandel, Romain Péchoux.

We have developped COMPLEXITYPARSER, a static complexity analyzer for Java programs implementing a tier-based type discipline. If a program is typable, its runtime is guaranteed to be polynomial on the condition that it halts. The type inference is automatic; its complexity is linear in the size of the input program in practice.

COMPLEXITYPARSER is implemented in Java (5,000 lines of code) and it uses the ANTLR framework to generate a parser. The code is under the Apache 2.0 License.

A tool paper presenting the operation and main features of the software was accepted and presented at the ICTAC 2021 conference [16].

#### 7.4 Enumerative and probabilistic combinatorics of some discrete objects

Participants: Mathilde Bouvel.

#### 7.4.1 Random cographs

Cographs form one of the simplest hereditary graph classes. They can be defined as the graphs not containing the path with 4 vertices as an induced subgraph. A characterization of cographs which is essential for us is the following: cographs are the graphs which can be encoded by trees in a specific family, called *cotrees*.

We are interested in the asymptotic properties of uniform random cographs when the number of vertices tends to infinity.

In a first paper [11], we prove convergence towards a Brownian limiting object in the space of graphons, which we call the *Brownian cographon*. We then show that the degree of a uniform random vertex in a uniform cograph with *n* vertices is of order *n*, and converges after normalization to the Lebesgue measure on [0, 1]. We finally analyze the vertex connectivity (i.e. the minimal number of vertices whose removal disconnects the graph) of random connected cographs, and show that this statistics converges in distribution without renormalization. Our proofs use the encoding of cographs via cotrees, combined with the symbolic method and singularity analysis.

In a second paper [34], we focus on independent sets (or equivalently, cliques) in uniform random cographs. First, we prove that, with high probability as *n* gets large, the largest independent set in a uniform random cograph with *n* vertices has size o(n), answering a question of Kang, McDiarmid, Reed and Scott. The proof relies on the convergence to the Brownian cographon, and on the self-similarity properties of this object. Second, and unexpectedly given the above results, we show that for  $\beta > 0$  sufficiently small, the expected number of independent sets of size  $\beta n$  in a uniform random cograph with *n* vertices grows exponentially fast with *n*. This time the proof relies on singularity analysis of the associated bivariate generating functions.

In [34], we also prove permutation analogues of all the results mentioned above.

#### 7.4.2 Baxter Tree-like tableaux

The article [22] is the result of a collaboration started at LaBRI in 2012 (when M. Bouvel was there). We took the opportunity of the "work from home" situation to complete this work.

Tree-like tableaux are objects in bijection with alternative or permutation tableaux, which are classical objects in combinatorics. Our work defines and studies a new subclass of tree-like tableaux enumerated by the famous Baxter numbers. We exhibit simple bijective links between these objects and three other combinatorial classes: (packed or mosaic) floorplans, twisted Baxter permutations and triples of non-intersecting lattice paths. From several (and unrelated) works, these last objects are already known to be enumerated by Baxter numbers, and our main contribution is to provide a unifying approach to bijections between Baxter objects, where Baxter tree-like tableaux play the key role.

#### 7.4.3 Interval posets of permutations

The paper [26] results from the research internship of B. Izart in our team (June-September 2021), and from the visit of L. Cioni to Loria (September-October 2021).

The goal of this research project was to investigate the links between interval posets of permutations and substitution decomposition trees. The interval poset of a permutation is the set of intervals of a permutation, ordered with respect to inclusion. It has been introduced and studied recently in [54]. Substitution decomposition trees, on the other hand, are a rather classical tool in the study of permutation classes, which was not used in [54].

We first describe a procedure to obtain the interval poset of a permutation from its substitution decomposition tree. We then give alternative proofs of some of the results in [54], and we solve the open problems that it posed (and some other enumerative problems) using techniques from symbolic and analytic combinatorics. Finally, we compute the Möbius function on interval posets.

#### 7.5 Quantum, probabilistic and substructural programming languages

Participants: Emmanuel Jeandel, Vladimir Zamdzhiev.

#### 7.5.1 Recursive types in substructural type systems

Recursive datatypes [39] in programming languages generalise inductive datatypes by allowing the programmer to construct more expressive types (e.g. streams) without imposing any restrictions on the admissible logical polarities of the underlying type expressions. As part of a larger program, we wish to understand how this can be achieved in quantum computation. However, before this question may be

answered, it is useful to understand how such types behave in the setting of Substructural Type Systems, which quantum programming is a part of.

In this work, we describe a substructural type system with mixed linear and non-linear recursive types called LNL-FPC (the linear/non-linear fixpoint calculus). Just as in FPC, we show that LNL-FPC supports type-level recursion which in turn induces term-level recursion. We also provide sound and computationally adequate categorical models for LNL-FPC which describe the categorical structure of the substructural operations of Intuitionistic Linear Logic at all non-linear types, including the recursive ones. In order to do so, we describe a new technique for solving recursive domain equations. We also show that the requirements of our abstract model are reasonable by constructing a large class of concrete models that have found applications in classical programming, but also in emerging programming paradigms such as quantum programming and circuit description programming languages.

These results are published in the journal Logical Methods in Computer Science [13]. The final revisions for the journal article were completed in 2021, but most of the work was done in 2020. This work is also an extended version of our paper that was published in ICFP'19 [50].

#### 7.5.2 Commutative monads for probabilistic programming languages

*Domain theory* [47], a mathematical theory that is a staple of denotational semantics, provides an elegant order-theoretic view of computation. However, domain theory has struggled to keep up with advances in probabilistic computation, because adding probabilistic choice to the domain-theoretic approach to semantics has been a challenge. The canonical model of (sub)probability measures in domain theory is the family of valuations - certain maps from the lattice of open subsets of a dcpo (directed-complete partial order) to the unit interval. These valuations form a *strong* monad  $\mathcal{V}$  on **DCPO** (the category of dcpo's and Scott-continuous functions) [48]. However, whether this monad  $\mathcal{V}$  is *commutative* (a very desirable property for the semantics) has been an open problem since 1989.

As part of this research project, we present three commutative submonads of  $\mathcal{V}$  and a general topological method for finding even more. Our results ameliorate, to a large extent, the above 33 year old open problem. We show how to use our monads to provide a sound and adequate denotational semantics for the Probabilistic FixPoint Calculus (PFPC) – a call-by-value simply-typed lambda calculus with mixedvariance recursive types, term recursion and probabilistic choice. We also show that in the special case where we consider continuous dcpo's, then all three monads coincide with the valuations monad  $\mathcal{V}$  and we fully characterise the induced Eilenberg-Moore categories by showing that they are all isomorphic to the category of continuous Kegelspitzen of Keimel and Plotkin [49]. These results are published in LICS'21 [10].

The above results show that the three submonads we identified are suitable for modeling *discrete* probabilistic choice. Whether they can be used to model *continuous* probabilistic choice is unclear, because we do not know if they contain enough valuations. In order to tackle this question, we present a fourth commutative submonad of  $\mathcal{V}$ , called the *central valuations monad*, denoted  $\mathcal{Z}$ . Unlike the previous three monads, which are constructed via topological methods, here we use algebraic ideas in order to define  $\mathcal{Z}$ . This monad is larger than our previous three monads and it might be the largest commutative one possible. In fact,  $\mathcal{V} = \mathcal{Z}$  iff  $\mathcal{V}$  is commutative (open problem for 33 years). We also present some evidence that this monad is large enough to model continuous probabilistic choice, but a definitive answer to this question is left for future work. These results are published in CALCO'21 [19].

#### 7.5.3 Variational quantum programming in idris

Variational Quantum Algorithms [52, 51, 42] are hybrid classical-quantum algorithms where classical and quantum computation work in tandem to solve computational problems. These algorithms create interesting challenges for the design of suitable programming languages, because they have to be able to accommodate both classical and quantum programming primitives simultaneously.

As part of this research project, we develop a set of libraries for the Idris 2 programming language that enable the programmer to implement (variational) quantum algorithms where the full power of the elegant Idris language works in synchrony with quantum programming primitives that we introduce. The two key ingredients of Idris that make this possible are (1) dependent types which allow us to implement unitary (i.e. reversible and controllable) quantum operations; and (2) linearity which allows us to enforce

fine-grained control over the execution of quantum operations that ensures compliance with the laws of quantum mechanics. We demonstrate that our libraries, named Qimaera, are suitable for variational quantum programming by providing implementations of the two most prominent variational quantum algorithms – QAOA [42] and VQE [52]. To the best of our knowledge, this is the first implementation of these algorithms that has been achieved in a type-safe framework.

The results of this work are described in a preprint, currently under peer-review [31]. The software is open-source, available under the MIT license here. These results were obtained during the (bachelor) internship of Liliane-Joy Dandy in our team and she was awarded the **"Research Internship Prize"** at École Polytechnique for her work.

#### 7.5.4 Semantics for variational quantum programming

The results in the previous research project show how we may approach variational quantum programming within an existing programming language. As part of this research project, we adopt a more theoretical and formal viewpoint and we consider a type system for variational quantum programming and we show how to design a suitable mathematical semantics for it.

In particular, we consider a programming language that can manipulate both classical and quantum information. Our language is type-safe and designed for variational quantum programming. The classical subsystem of the language is the Probabilistic FixPoint Calculus (PFPC), which is a lambda calculus with mixed-variance recursive types, term recursion and probabilistic choice. The quantum subsystem is a first-order linear type system that can manipulate quantum information. The two subsystems are related by mixed classical/quantum terms that specify how classical probabilistic effects are induced by quantum measurements, and conversely, how classical (probabilistic) programs can influence the quantum dynamics. We also describe a sound and computationally adequate denotational semantics for the language. Classical probabilistic effects are interpreted using a recently-described commutative probabilistic monad on **DCPO** (see Subsection 7.5.2). Quantum effects and resources are interpreted in a category of von Neumann algebras that we show is enriched over (continuous) domains. This strong sense of enrichment allows us to develop novel semantic methods that we use to interpret the relationship between the quantum and classical probabilistic effects. By doing so we provide the first denotational analysis that relates models of classical probabilistic programming to models of quantum programming.

The results of this project are published in POPL'22 [17] and most of the work was done in the year 2021.

### 8 Bilateral contracts and grants with industry

#### 8.1 Bilateral contracts with industry

The team is supervising two CIFRE PhDs in collaboration with industry partners.

One is a partnership with EDF: Margarita Veshchezerova is working on "Quantum Computing for Combinatorial Optimisation" under the supervision of Emmanuel Jeandel and Simon Perdrix from the team, and Marc Porcheron at EDF.

One is with ATOS: Vivien Vandaele is working on "Optimisation du calcul quantique tolérant aux fautes par le ZX-Calculus" under the supervision of Simon Perdrix and Christophe Vuillot from the team, and Simon Martiel at ATOS.

## 9 Partnerships and cooperations

#### 9.1 International initiatives

#### 9.1.1 Inria associate team not involved in an IIL or an international program

#### TCPRO3

Title: Termination and Complexity Properties of Probabilistic Programs

Duration: June 2020 -> June 2023

#### Coordinator: Georg Moser (georg.moser@uibk.ac.at)

#### **Partners:**

• University of Innsbruck

#### Inria contact: Romain Péchoux

**Summary:** The major goal of the associate team TC(Pro)<sup>3</sup> is to develop methods for reasoning on quantitative properties of probabilistic programs and models. Such tools have applications in quantum computing as quantum programs can be considered as particular cases of probabilistic transition systems where measurement plays the role of probabilistic choice.

In 2021, the team has worked on the adaptation of expectation transformers, a semantic method for dealing with program expectations such as expected costs or expected values, to a quantum programming language with classical data. As a result, the team has defined a generic notion of "quantum expectation transformer". This notion uses the algebraic structure of Kegelspitzen used to study the denotational semantics of probabilistic programming languages. By specifying several distinct Kegelspitze, we obtain an expected cost analysis, an expected value analysis, and a denotational semantics our quantum programs. Moreover, this new technique strictly generalizes predicate transformers and expectation transformers.

#### 9.1.2 STIC/MATH/CLIMAT AmSud project

#### 21STIC10 Qapla

Participants:Simon Perdrix, Vladimir Zamdzhiev, Agustín Borgna, Titouan Carette,<br/>Alexandre Clément, Margarita Veshchezerova.

Title: Quantum Aspects of Programming Languages

#### **Partner Institution(s):** • <u>ICC</u>, Argentina

- UNQ, Argentina
- UFSM, Brazil
- UChile, Chile
- AMU, France
- CNRS, France
- Inria, France
- CentraleSupélec, France
- Université Paris-Saclay, France
- ENS Paris-Saclay, France
- Université de Lorraine, France
- UdelaR, Uruguay

#### Date: 2021

**Summary:** The design of quantum programming languages is a rich framework that allows studying intrinsic properties of the computation we are modelling, such as parallelism, entanglement, superposition, etc; also, it is a way to study new logics (quantum logics with a computational ground), as well as to study classical logics from a new perspective. Finally, studying the foundational bases of programming languages gives a path towards developing proper implementations. This project proposes to study several aspects of quantum programming languages, with different approaches (quantum control/classical data, quantum control and data, categorical techniques, semantical techniques, realizability). The final aim is to merge different approaches in order to study quantum programming languages from logics to implementations.

#### 9.2 European initiatives

#### 9.2.1 FP7 & H2020 projects

#### NEASQC

Participants: Emmanuel Jeandel, Simon Perdrix, Romain Péchoux.

Title: NExt ApplicationS of Quantum Computing

Partner Institution(s): • ATOS-Bull

- Université de Lorraine
- AstraZeneca
- Cesga
- EDF
- HQS
- HSBC
- ICHEC
- Tilde
- Total
- University of Leiden
- Universidade da Coruna

Duration: 01/09/2020-31/08/2024

**Summary:** The project brings together academic experts and industrial end-users to investigate and develop a new breed of Quantum-enabled applications that can take advantage of NISQ (Noise Intermediate-Scale Quantum) systems in the near future. NEASQC is use-case driven. Along with EDF we are investigating smart energy management in this context.

## 9.2.2 Other european programs/initiatives

#### **HPCQS**

Participants: Simon Perdrix, Emmanuel Jeandel, Romain Péchoux, Christophe Vuillot, Vladimir Zamdzhiev.

Title: High Performance Computer and Quantum Simulator hybrid

#### Partner Institution(s): • Forschungszentrum Juelich GmbH, Germany

- JSC at Forschungszentrum Jülich, Germany
- GENCI/CEA, France
- Barcelona Supercomputing Center, Spain
- CINECA, Italy
- NUIG-ICHEC, Ireland
- Atos, France
- ParTec, Germany
- FlySight, Italy
- ParityQC, Austria

- CEA, France
- CNRS, France
- Inria, France
- CNR, Italy
- the University of Innsbruck, Austria
- Fraunhofer IAF, Germany
- Eurice, Germany

#### Duration: 01/12/2021-31/11/2025

**Summary:** HPCQS aims to develop, deploy and coordinate a European federated infrastructure, tightly integrating two quantum simulators each controlling about 100+ qubits (quantum bits) in the Tier-0 HPC systems Joliot Curie of GENCI, operated at CEA/TGCC, and the JUWELS modular supercomputer at JSC. The seamless integration of quantum hardware with classical computing resources, creating a hybrid system, is an essential step forward to utilize the power of quantum computers for handling first practical applications.

#### 9.3 National initiatives

## 9.3.1 ANR

#### ANR PRCE SoftQPro (ANR-17-CE25-0009)

**Participants:** Simon Perdrix, Emmanuel Jeandel, Emmanuel Hainry, Romain Péchoux.

Title: Solutions logicielles pour l'optimisation des programmes et ressources quantiques

#### Partner Institution(s): • LORIA, France

- ATOS-Bull, France
- LRI, France
- CEA-Saclay, France

#### Duration: Dec. 2017 - Dec. 2022

**Summary:** Quantum computers can theoretically solve problems out of reach of classical computers. We aim at easing the crucial back and forth interactions between the theoretical approach to quantum computing and the technological efforts made to implement the quantum computer. Our software-based quantum program and resource optimisation (SoftQPRO) project consists in developing high level techniques based on static analysis, certification, transformations of quantum graphical languages, and optimisation techniques to obtain a compilation suite for quantum programming languages. We will target various computational model back-ends (e.g. QRAM, measurement-based quantum computations) as well as classical simulation. Classical simulation is central in the development of the quantum computer, on both ends: as a way to test quantum programs but also as a way to test quantum computer prototypes. For this reason we aim at designing sophisticated simulation techniques on classical high-performance computers (HPC).

#### ANR PRCI VanQuTe (ANR-17-CE24-0035)

Participants: Simon Perdrix, Emmanuel Jeandel.

Title: Validation of near-future quantum technologies

#### Partner Institution(s): • LIP6, France

- LORIA, France
- NTU, Singapore
- SUTD, Singapore
- NUS, Singapore

#### Duration: Fev. 2018 - Jan. 2022

**Summary:** In the last few years we have seen unprecedented advances in quantum information technologies. Already quantum key distribution systems are available commercially. In the near future we will see waves of new quantum devices, offering unparalleled benefits for security, communication, computation and sensing. A key question to the success of this technology is their verification and validation.

Quantum technologies encounter an acute verification and validation problem. On the one hand, since classical computations cannot scale-up to the computational power of quantum mechanics, verifying the correctness of a quantum-mediated computation is challenging. On the other hand, the underlying quantum structure resists classical certification analysis. Members of our consortium have shown, as a proof-of-principle, that one can bootstrap a small quantum device to test a larger one. The aim of VanQuTe is to adapt our generic techniques to the specific applications and constraints of photonic systems being developed within our consortium. Our ultimate goal is to develop techniques to unambiguously verify the presence of a quantum advantage in near future quantum technologies.

## 9.3.2 Other initiatives PIA-GDN/Quantex

Participants: Simon Perdrix, Emmanuel Jeandel.

Title: Simulation/Emulation of Quantum Computation

#### Partner Institution(s): • ATOS-Bull, France

- LRI, France
- CEA-Grenoble, France
- LORIA, France

Duration: Feb. 2018 - Jan 2021

**Summary:** The lack of quantum computers leads to the development of a variety of software-based simulators to assist in the research and development of quantum algorithms. This proposal focuses on the development of a combined software-based and hardware-accelerated toolbox for quantum computation. A quantum computing stack including specification language, libraries and optimisation/execution tools will be built upon a well-defined mathematical framework mixing classical and quantum computation. Such an environment will be dedicated to supporting the expression of quantum algorithms for the purpose of investigation and verification.

## **10** Dissemination

#### 10.1 Promoting scientific activities

#### 10.1.1 Scientific events: organisation

• Mathieu Hoyrup co-organized a Dagstuhl seminar on Descriptive Set Theory and Computable Topology in November (link)

• Simon Perdrix co-organized a school on Quantum computing and Operational Research, in November at Montpellier (link)

#### Member of the conference program committees

- Mathilde Bouvel is a member of the steering committee of the series of conferences *Permutation Patterns*.
- Nazim Fatès was a member of the program committees of AUTOMATA 21 and ASCAT 2022.
- Simon Perdrix was a member of the program committee of QPL 21.
- Vladimir Zamdzhiev was a member of the program committees of ACT 21, QPL 21 and PlanQC 21.

#### Reviewer

- Mathilde Bouvel served as a reviewer for the conference ICALP 2021 (Track B).
- Vladimir Zamdzhiev was a reviewer for the conferences LICS 21, MFCS 21 and ESOP 2022.
- Christophe Vuillot served as a reviewer for the following conferences: ISIT 2021, ITCS 2022

#### 10.1.2 Journal

#### Member of the editorial boards

- Emmanuel Jeandel: Member of the editorial board of the journal RAIRO-ITA.
- Nazim Fatès: Member of the editorial board of the *Journal of cellular automata*. He also co-edited a special issue of *Physica D* on the theme "Discrete Models of Complex Systems: recent trends and analytical challenges".
- Mathilde Bouvel: Member of the editorial boaed of the journal Annals of combinatorics

#### **Reviewer - reviewing activities**

- Nazim Fatès served as reviewer for the following journals: *Theoretical Computer Science, Journal of cellular automata* and *Physica A*.
- Mathilde Bouvel served as a reviewer for the following journals: *Discrete Applied Mathematics, Journal of Symbolic Computation,* and *Discrete Mathematics.*
- Vladimir Zamdzhiev served as a reviewer for the journal ACM Transactions on Quantum Computing.
- Christophe Vuillot served as a reviewer for the following journals: *Nature, Physical Review X Quantum, Quantum, Physical Review Research, IEEE Transactions on Information Theory.*

#### 10.1.3 Invited talks

- Emmanuel Jeandel was invited to present his work in the French event "Journées SDA2" in Caen, November 2021.
- Nazim Fatès was invited to present his work on robust computing with cellular automata in a international online series of seminars on cellular automata. The talk is available on a YouTube recording. In November, this conference was given again for the researchers of the university of Sao Paolo, Brazil.
- Mathieu Hoyrup was invited to give a talk at the third Workshop on Digitalization and Computable Models WDCM in Novosibirsk (online), June 2021. He was also invited to give a talk at a minisymposium on at the Joint Annual Conference of the German Mathematical Society (DMV) and the Austrian Mathematical Society (ÖMG) 2021 (link) in Passau (online), September 2021.

- Simon Perdrix gave an invited seminar at Collège de France : "Langages graphiques pour programmer et raisonner en informatique quantique" (May 2021) (link).
- Vladimir Zamdzhiev gave an invited talk at the international event "Logic, Quantum Computing, and Artificial Intelligence" on 03.07.2021 titled "Semantics for Variational Quantum Programming".
- Christophe Vuillot gave an invited talk at the IRMA (Strasbourg, France) Physics and Mathematics Colloquim Quantum computing and Quantum information on 24.06.2021 titled 'The Challenge of Universal and Fault-Tolerant Quantum Computation''.

#### 10.1.4 Leadership within the scientific community

- Nazim Fatès was appointed as the chair of the IFIP Working Group 1.5 on Cellular automata and discrete complex systems.
- Vladimir Zamdzhiev was invited to be a member of the IFIP TC1/TC2 Working Group on *Foundations of Quantum Computation*, which is currently under creation and is expected to be formed in early 2022.

#### 10.1.5 Scientific expertise

• Nazim Fatès was a member on a working group on the prospective of the use of artificial intelligence in the labour world. This national group, initiated by the INRS institute, is composed of about 20 persons and prepares a report and a national presentation on the effects of artificial intelligence on working conditions in a ten-year horizon, with a special emphasis on the security of persons.

#### 10.2 Teaching - Supervision - Juries

- Licence
  - Isabelle Gnaedig:
    - \* To the limits of the computable, 6 hours, Opening course-conference of the collegium "Lorraine INP", Université de Lorraine, Nancy, France.
  - Emmanuel Hainry:
    - \* Operating Systems, 30h, L1, IUT Nancy Brabois, Université de Lorraine, Nancy, France.
    - \* Algorithmics, 40h, L1, IUT Nancy Brabois.
    - \* Dynamic Web, 60h, L1, IUT Nancy Brabois.
    - \* Databases, 30h, L1, IUT Nancy Brabois.
    - \* Object Oriented Languages, 16h, L2, IUT Nancy Brabois.
    - \* Complexity, 30h, L2, IUT Nancy Brabois.
  - Emmanuel Jeandel:
    - \* Algorithmics and Programming 1, 60h, L1 Maths-Info, Université de Lorraine, Nancy, France.
    - \* Networking, 60h, L2 and L3 Informatique.
    - \* Formal Languages, 30h, L2 Informatique.
    - \* Functional Programming, 14h, L3 Informatique.
    - \* System Administration, 24h, Licence Pro Informatique Paysagère.
- Master
  - Nazim Fatès:
    - \* Systèmes distribués adaptatifs, 12h, Master 2, informatique, Université de Lorraine, Nancy, France.

- \* Agents intelligents et collectifs, 15h, Master 1, sciences cognitives, Université de Lorraine, Nancy, France.
- \* Models of computation, 12h, Master 2, informatique, Université de Lorraine, Nancy, France.
- \* IAE Nancy-School of Management, Marketing et Gestion Commerciale, Lecture on Artificial intelligence and Ethics, 3h, Université de Lorraine, Nancy, France.
- Formation pour les enseignants du secondaire, "Enseigner l'Informatique au Lycée" (Diplôme inter-universitaire), Histoire de l'informatique, 3h, Université de Lorraine, Nancy, France.
- Isabelle Gnaedig:
  - \* Rule-based Programming, 28 hours, M2, Telecom-Nancy, Université de Lorraine, Nancy, France.
- Emmanuel Jeandel:
  - \* Algorithmics and Complexity, 30h, M1 Informatique, Université de Lorraine, Nancy, France.
  - \* Networking, 24h, M1 Informatique, Université de Lorraine, Nancy, France.
- Simon Perdrix:
  - \* Informatique quantique, 12h, Master 1, informatique, Université de Lorraine, Nancy, France.
  - \* Algorithmes quantiques, 3h, L3, UTT.
- Christophe Vuillot:
  - \* Informatique quantique, 12h, Master 1, informatique, Université de Lorraine, Nancy, France.
  - \* Introduction à l'informatique quantique, 12h, M2, Telecom Paris
- Vladimir Zamdzhiev:
  - \* Models of computation, 6h CM + 6h TD, Master 2, informatique, Université de Lorraine, Nancy, France.
  - \* Programming in Haskell, 16h CM + 8h TD, Master 1, informatique, Université de Lorraine, Nancy, France.

#### 10.2.1 Supervision

- PhD: Titouan Carette, "Langage diagrammatique pour l'ordinateur quantique", Start: October 2018, Advisors: Emmanuel Jeandel and Simon Perdrix. Titouan defended in November 2021 [21].
- PhD in progress: Djamel Eddine Amir, "Computability of subsets of topological spaces", Start: October 2020, Advisors: Emmanuel Jeandel and Mathieu Hoyrup.
- PhD in progress: Alexandre Clément, "Graphical Languages for Quantum Control", Start: September 2019, Advisors: Emmanuel Jeandel and Simon Perdrix.
- PhD in progress: Robert Booth, "Formalismes pour la vérification de technologies quantiques", Start: November 2018, Advisors: Damian Markham and Simon Perdrix.
- PhD in progress: Agustin Borgna "Vers une formalisation d'une cha^ıne de compilation pour un ordinateur quantique", Start: October 2019, Advisors: Simon Perdrix and Benoit Valiron (LMF).
- PhD in progress: Alexandre Guernut, "Efficient Fault-Tolerant Quantum Computation with Quantum LDPC Codes", Start: October 2021, Advisors: Emmanuel Jeandel and Christophe Vuillot.
- PhD in progress: Vivien Vandaele, "Optimisation du calcul quantique tolérant aux fautes par le ZX-Calculus", Start: September 2021, Advisors: Simon Perdrix and Christophe Vuillot, joint supervision with Simon Martiel at ATOS (CIFRE).

• PhD in progress: Margarita Veshchezerova, "Quantum Computing for Combinatorial Optimisation", Start: October 2019, Advisors: Emmanuel Jeandel and Simon Perdrix, joint supervision with Marc Porcheron at EDF (CIFRE).

#### 10.2.2 Juries

- Emmanuel Jeandel participated in the PhD defense of Henri de Boutray (Université de Franche-Comté)
- Emmanuel Jeandel participated in the HdR defense of Irène Marcovici (Université de Lorraine) and Nathalie Aubrun (Université Paris-Saclay)
- Emmanuel Jeandel reviewed the PhD manuscript of Pacôme Perrotin (Aix-Marseille University)
- Simon Perdrix participated in the PhD defense of Clément Meignat (Sorbonne Université)
- · Simon Perdrix was external examiner in the PhD viva of Maria Stasinou (Oxford University)

#### **10.3** Popularization

#### 10.3.1 Articles and contents

Nazim Fatès published an article for the wide-audience online magazine *The conversation*. The article, « Le temps passe-t-il pour l'intelligence artificielle ?» presents some reflection on the question of temporality and artificial intelligence.

Nazim Fatès published a video on Alan Turing, « La machine de Turing, un modèle pour le calcul ? ». This video is available on YouTube; it was realised with the audiovisual services of the Université de Lorraine and released for the "Fête de la science".

Simon Perdrix has been interviewed by Olivier Ezratty and Fanny Bouton in "Decode Quantum" (link)

#### 10.3.2 Interventions

Nazim Fatès gave a series of lectures destined to a wide audience on the theme of artificial intelligence:

- « AI-calypse Now : comment l'intelligence artificielle a-t-elle muté pour devenir un enjeu planétaire ? », AI now conference, online presentation, June 3, 2021.
- « Visage(s) de l'intelligence artificielle », Troisième forum nancéien de l'IA en Santé, Centre Prouvé de Nancy, November 23, 2021.
- « Penser avec l'intelligence artificielle », Octobre 21, 2021, Association des émérites de l'université de Lorraine, Nancy.
- « AI-calypse now ! Quelques réflexions autour des limites de l'intelligence artificielle », Conference for the members of the laboratory Georessources, December 2021.

Nazim Fatès participated in a debate following a theatre play, *We are The robots*, ARTEM, Nancy, April 2, 2021.

## 11 Scientific production

#### **11.1 Major publications**

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#### 11.2 Publications of the year

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#### International peer-reviewed conferences

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