



RESEARCH CENTER  
Saclay - Île-de-France

FIELD

# Activity Report 2017

## Section New Results

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## COMETE Project-Team

## 6. New Results

### 6.1. Foundations of information hiding

Information hiding refers to the problem of protecting private information while performing certain tasks or interactions, and trying to avoid that an adversary can infer such information. This is one of the main areas of research in Comète; we are exploring several topics, described below.

#### 6.1.1. Information Leakage Games

In [19] we studied a game-theoretic setting to model the interplay between attacker and defender in the context of information flow, and to reason about their optimal strategies. In contrast with standard game theory, in our games the utility of a mixed strategy is a convex function of the distribution on the defender's pure actions, rather than the expected value of their utilities. Nevertheless, the important properties of game theory, notably the existence of a Nash equilibrium, still hold for our (zero-sum) leakage games, and we provided algorithms to compute the corresponding optimal strategies. As typical in (simultaneous) game theory, the optimal strategy is usually mixed, i.e., probabilistic, for both the attacker and the defender. From the point of view of information flow, this was to be expected in the case of the defender, since it is well known that randomization at the level of the system design may help to reduce information leaks. Regarding the attacker, however, this seems the first work (w.r.t. the literature in information flow) proving formally that in certain cases the optimal attack strategy is necessarily probabilistic.

#### 6.1.2. Efficient Utility Improvement for Location Privacy

The continuously increasing use of location-based services poses an important threat to the privacy of users. A natural defense is to employ an obfuscation mechanism, such as those providing geo-indistinguishability [24], a framework for obtaining formal privacy guarantees that has become popular in recent years. Ideally, one would like to employ an optimal obfuscation mechanism, providing the best utility among those satisfying the required privacy level. In theory optimal mechanisms can be constructed via linear programming. In practice, however, this is only feasible for a radically small number of locations. As a consequence, all known applications of geo-indistinguishability simply use noise drawn from a planar Laplace distribution.

In [12], we studied methods for substantially improving the utility of location obfuscation, while maintaining practical applicability as a main goal. We provided such solutions for both infinite (continuous or discrete) as well as large but finite domains of locations, using a Bayesian remapping procedure as a key ingredient. We evaluated our techniques in two real world complete datasets, without any restriction on the evaluation area, and showed important utility improvements with respect to the standard planar Laplace approach.

#### 6.1.3. Trading Optimality for Performance in Location Privacy

Location-Based Services (LBSs) provide invaluable aid in the everyday activities of many individuals, however they also pose serious threats to the user's privacy. There is, therefore, a growing interest in the development of mechanisms to protect location privacy during the use of LBSs. Nowadays, the most popular methods are probabilistic, and the so-called optimal method achieves an optimal trade-off between privacy and utility by using linear optimization techniques.

Unfortunately, due to the complexity of linear programming, the method is unfeasible for a large number  $N$  of locations, because the constraints are  $O(N^3)$ . In [20], we have proposed a technique to reduce the number of constraints to  $O(N^2)$ , at the price of renouncing to perfect optimality. We have showed however that on practical situations the utility loss is quite acceptable, while the gain in performance is significant.



#### **6.1.4. Methods for Location Privacy: A comparative overview**

The growing popularity of location-based services, allowing to collect huge amounts of information regarding users' location, has started raising serious privacy concerns. In [13] we analyzed the various kinds of privacy breaches that may arise in connection with the use of location-based services, and we surveyed and compared the metrics and the mechanisms that have been proposed in the literature.

#### **6.1.5. Quantifying Leakage in the Presence of Unreliable Sources of Information**

Belief and min-entropy leakage are two well-known approaches to quantify information flow in security systems. Both concepts stand as alternatives to the traditional approaches founded on Shannon entropy and mutual information, which were shown to provide inadequate security guarantees. In [16] we unified the two concepts in one model so as to cope with the frequent (potentially inaccurate, misleading or outdated) attackers' side information about individuals on social networks, online forums, blogs and other forms of online communication and information sharing. To this end we proposed a new metric based on min-entropy that takes into account the adversary's beliefs.

#### **6.1.6. Differential Inference Testing: A Practical Approach to Evaluate Anonymized Data**

In order to protect individuals' privacy, governments and institutions impose some obligations on data sharing and publishing. Mainly, they require the data to be "anonymized". In this paper, we have shortly discussed the criteria introduced by European General Data Protection Regulation to assess anonymized data. We have argued that the evaluation of anonymized data should be based on whether the data allows individual based inferences, instead of being centered around the concept of re-identification as the regulation has proposed.

Then, we have proposed an inference-based framework that can be used to evaluate the robustness of a given anonymized dataset against a specific inference model, e.g. a machine learning model.

Our approach evaluates the anonymized data itself, and deals with the related anonymization technique as a black-box. Thus, it can be used to assess datasets that are anonymized by organizations which may prefer not to provide access to their techniques. Finally, we have used our framework to evaluate two datasets after being anonymized using  $k$ -anonymity and  $l$ -diversity.

#### **6.1.7. Formal Analysis and Offline Monitoring of Electronic Exams**

More and more universities are moving toward electronic exams (in short e-exams). This migration exposes exams to additional threats, which may come from the use of the information and communication technology. In [17], we have identified and defined several security properties for e-exam systems. Then, we have showed how to use these properties in two complementary approaches: model-checking and monitoring.

We have illustrated the validity of our definitions by analyzing a real e-exam used at the pharmacy faculty of University Grenoble Alpes (UGA) to assess students. On the one hand, we have instantiated our properties as queries for ProVerif, a process calculus based automatic verifier for cryptographic protocols,

and we have used it to check our modeling of UGA exam specifications. ProVerif found some attacks. On the other hand, we have expressed our properties as Quantified Event Automata (QEAs), and we have synthesized them into monitors using MarQ, a Java tool designed to implement QEAs. Then, we have used these monitors to verify real exam executions conducted by UGA. Our monitors found fraudulent students and discrepancies between the specifications of UGA exam and its implementation.

#### **6.1.8. On the Compositionality of Quantitative Information Flow**

In the min-entropy approach to quantitative information flow, the leakage is defined in terms of a minimization problem, which, in the case of large systems, can be computationally rather heavy. The same happens for the recently proposed generalization called  $g$ -vulnerability. In [18] we studied the case in which the channel associated to the system can be decomposed into simpler channels, which typically happens when the observables consist of several components. Our main contribution is the derivation of bounds on the  $g$ -leakage of the whole system in terms of the  $g$ -leakages of its components. We also considered the particular cases of min-entropy leakage and of parallel channels, generalizing and systematizing results from the literature. We demonstrated the effectiveness of our method and evaluate the precision of our bounds using examples.

## 6.2. Foundations of Concurrency

Distributed systems have changed substantially in the recent past with the advent of phenomena like social networks and cloud computing. In the previous incarnation of distributed computing the emphasis was on consistency, fault tolerance, resource management and related topics; these were all characterized by *interaction between processes*. Research proceeded along two lines: the algorithmic side which dominated the Principles Of Distributed Computing conferences and the more process algebraic approach epitomized by CONCUR where the emphasis was on developing compositional reasoning principles. What marks the new era of distributed systems is an emphasis on managing access to information to a much greater degree than before.

### 6.2.1. Declarative Framework for Semantical Interpretations of Structured Information — An Applicative Approach.

Spatial constraint systems are algebraic structures from concurrent constraint programming to specify spatial and epistemic behavior in multi-agent system. In [21], [15] we studied the applicability of declarative models to encode and describe structured information by means of semantics. Specifically, we introduced D-SPACES, an implementation of constraint systems with space and extrusion operators. D-SPACES provides property-checking methods as well as an implementation of a specific type of constraint systems (a spatial boolean algebra). We showed the applicability of this framework with two examples; a scenario in the form of a social network where users post their beliefs and utter their opinions, and a semantical interpretation of a logical language to express time behaviors and properties.

### 6.2.2. Characterizing Right Inverses for Spatial Constraint Systems with Applications to Modal Logic

In [23] spatial constraint systems were used to give an abstract characterization of the notion of normality in modal logic and to derive right inverse/reverse operators for modal languages. In particular, a necessary and sufficient condition for the existence of right inverses was identified and the abstract notion of normality is shown to correspond to the preservation of finite suprema. Furthermore, a taxonomy of normal right inverses was provided, identifying the greatest normal right inverse as well as the complete family of minimal right inverses. These results were applied to existing modal languages such as the weakest normal modal logic, Hennessy-Milner logic, and linear-time temporal logic. Some implications of these results were also discussed in the context of modal concepts such as bisimilarity and inconsistency invariance.

### 6.2.3. Observational and Behavioural Equivalences for Soft Concurrent Constraint Programming

In citegadducci:hal-01675060 we presented a labelled semantics for Soft Concurrent Constraint Programming (SCCP), a meta-language where concurrent agents may synchronise on a shared store by either posting or checking the satisfaction of (soft) constraints. SCCP generalises the classical formalism by parametrising the constraint system over an order-enriched monoid, thus abstractly representing the store with an element of the monoid, and the standard unlabelled semantics just observes store updates. The novel operational rules were shown to offer a sound and complete co-inductive technique to prove the original equivalence over the unlabelled semantics. Based on this characterisation, we provided an axiomatisation for finite agents.

### 6.2.4. On the Expressiveness of Spatial Constraint Systems

The dissertation [11] focused on the expressiveness of spatial constraint systems in the broader perspective of modal and epistemic behaviour. It was shown that that spatial constraint systems are sufficiently robust to capture inverse modalities and to derive new results for modal logics. It was shown that one can use scs's to express a fundamental epistemic behaviour such as knowledge. The dissertation also provided an algebraic characterization of the notion of distributed information by means of constructors over scs's.

## DATASHAPE Project-Team

## 7. New Results

### 7.1. Algorithmic aspects of topological and geometric data analysis

#### 7.1.1. Variance Minimizing Transport Plans for Inter-surface Mapping

**Participant:** David Cohen-Steiner.

*In collaboration with Manish Mandad, Leik Kobbelt (RWTH Aachen), Pierre Alliez (Inria), and Mathieu Desbrun (Caltech).*

We introduce an efficient computational method for generating dense and low distortion maps between two arbitrary surfaces of same genus. Instead of relying on semantic correspondences or surface parameterization, we directly optimize a variance-minimizing transport plan between two input surfaces that defines an as-conformal-as-possible inter-surface map satisfying a user-prescribed bound on area distortion. The transport plan is computed via two alternating convex optimizations, and is shown to minimize a generalized Dirichlet energy of both the map and its inverse. Computational efficiency is achieved through a coarse-to-fine approach in diffusion geometry, with Sinkhorn iterations modified to enforce bounded area distortion. The resulting inter-surface mapping algorithm applies to arbitrary shapes robustly, with little to no user interaction.

#### 7.1.2. Approximating the spectrum of a graph

**Participant:** David Cohen-Steiner.

*In collaboration with Weihao Kong, Gregory Valiant (Stanford), and Christian Sohler (TU Dortmund).*

The spectrum of a network or graph  $G = (V, E)$  with adjacency matrix  $A$  consists of the eigenvalues of the normalized Laplacian  $L = I - D^{-1/2} A D^{-1/2}$ . This set of eigenvalues encapsulates many aspects of the structure of the graph, including the extent to which the graph possesses community structures at multiple scales. We study the problem of approximating the spectrum  $\lambda = (\lambda_1, \dots, \lambda_{|V|})$ ,  $0 \leq \lambda_1 \leq \dots \leq \lambda_{|V|} \leq 2$  of  $G$  in the regime where the graph is too large to explicitly calculate the spectrum. We present a sublinear time algorithm that, given the ability to query a random node in the graph and select a random neighbor of a given node, computes a succinct representation of an approximation  $\tilde{\lambda}$  such that  $\|\tilde{\lambda} - \lambda\|_1 \leq \varepsilon|V|$ . Our algorithm has query complexity and running time  $\exp(O(1/\varepsilon))$ , independent of the size of the graph,  $|V|$ . We demonstrate the practical viability of our algorithm on 15 different real-world graphs from the Stanford Large Network Dataset Collection, including social networks, academic collaboration graphs, and road networks. For the smallest of these graphs, we are able to validate the accuracy of our algorithm by explicitly calculating the true spectrum; for the larger graphs, such a calculation is computationally prohibitive. In addition we study the implications of our algorithm to property testing in the bounded degree graph model.

#### 7.1.3. Anisotropic triangulations via discrete Riemannian Voronoi diagrams

**Participants:** Jean-Daniel Boissonnat, Mathijs Wintraecken.

*In collaboration with mael Rouxel-Labbé (GeometryFactory).*

The construction of anisotropic triangulations is desirable for various applications, such as the numerical solving of partial differential equations and the representation of surfaces in graphics. To solve this notoriously difficult problem in a practical way, we introduce the discrete Riemannian Voronoi diagram, a discrete structure that approximates the Riemannian Voronoi diagram. This structure has been implemented and was shown to lead to good triangulations in  $\mathbb{R}^2$  and on surfaces embedded in  $\mathbb{R}^3$  as detailed in our experimental companion paper.

In [23], [32], [34], we study theoretical aspects of our structure. Given a finite set of points  $\mathcal{P}$  in a domain  $\Omega$  equipped with a Riemannian metric, we compare the discrete Riemannian Voronoi diagram of  $\mathcal{P}$  to its Riemannian Voronoi diagram. Both diagrams have dual structures called the discrete Riemannian Delaunay and the Riemannian Delaunay complex. We provide conditions that guarantee that these dual structures are identical. It then follows from previous results that the discrete Riemannian Delaunay complex can be embedded in  $\Omega$  under sufficient conditions, leading to an anisotropic triangulation with curved simplices. Furthermore, we show that, under similar conditions, the simplices of this triangulation can be straightened.

#### 7.1.4. Only distances are required to reconstruct submanifolds

**Participants:** Jean-Daniel Boissonnat, Ramsay Dyer, Steve Oudot.

*In collaboration with Arijit Ghosh (Indian Statistical Institute).*

In [14], we give the first algorithm that outputs a faithful reconstruction of a submanifold of Euclidean space without maintaining or even constructing complicated data structures such as Voronoi diagrams or Delaunay complexes. Our algorithm uses the witness complex and relies on the stability of *power protection*, a notion introduced in this paper. The complexity of the algorithm depends exponentially on the intrinsic dimension of the manifold, rather than the dimension of ambient space, and linearly on the dimension of the ambient space. Another interesting feature of this work is that no explicit coordinates of the points in the point sample is needed. The algorithm only needs the *distance matrix* as input, i.e., only distance between points in the point sample as input.

#### 7.1.5. An obstruction to Delaunay triangulations in Riemannian manifolds

**Participants:** Jean-Daniel Boissonnat, Ramsay Dyer.

*In collaboration with Arijit Ghosh (Indian Statistical Institute) and Nikolay Martynchuk (University of Groningen).*

Delaunay has shown that the Delaunay complex of a finite set of points  $P$  of Euclidean space  $\mathbb{R}^m$  triangulates the convex hull of  $P$ , provided that  $P$  satisfies a mild genericity property. Voronoi diagrams and Delaunay complexes can be defined for arbitrary Riemannian manifolds. However, Delaunay's genericity assumption no longer guarantees that the Delaunay complex will yield a triangulation; stronger assumptions on  $P$  are required. A natural one is to assume that  $P$  is sufficiently dense. Although results in this direction have been claimed, we show that sample density alone is insufficient to ensure that the Delaunay complex triangulates a manifold of dimension greater than 2 [13].

#### 7.1.6. Local criteria for triangulation of manifolds

**Participants:** Jean-Daniel Boissonnat, Ramsay Dyer, Mathijs Wintraecken.

*In collaboration with Arijit Ghosh (Indian Statistical Institute).*

We present criteria for establishing a triangulation of a manifold [40]. Given a manifold  $M$ , a simplicial complex  $\mathcal{A}$ , and a map  $H$  from the underlying space of  $\mathcal{A}$  to  $M$ , our criteria are presented in local coordinate charts for  $M$ , and ensure that  $H$  is a homeomorphism. These criteria do not require a differentiable structure, or even an explicit metric on  $M$ . No Delaunay property of  $\mathcal{A}$  is assumed. The result provides a triangulation guarantee for algorithms that construct a simplicial complex by working in local coordinate patches. Because the criteria are easily checked algorithmically, they are expected to be of general use.

#### 7.1.7. Triangulating stratified manifolds I: a reach comparison theorem

**Participants:** Jean-Daniel Boissonnat, Mathijs Wintraecken.

In [42], we define the reach for submanifolds of Riemannian manifolds, in a way that is similar to the Euclidean case. Given a  $d$ -dimensional submanifold  $S$  of a smooth Riemannian manifold  $M$  and a point  $p \in M$  that is not too far from  $S$  we want to give bounds on local feature size of  $\exp_p^{-1}(S)$ . Here  $\exp_p^{-1}$  is the inverse exponential map, a canonical map from the manifold to the tangent space. Bounds on the local feature size of  $\exp_p^{-1}(S)$  can be reduced to giving bounds on the reach of  $\exp_p^{-1}(B)$ , where  $B$  is a geodesic ball, centred at  $c$  with radius equal to the reach of  $S$ . Equivalently we can give bounds on the reach of  $\exp_p^{-1} \circ \exp_c(B_c)$ , where now  $B_c$  is a ball in the tangent space  $T_c M$ , with the same radius. To establish bounds on the reach of  $\exp_p^{-1} \circ \exp_c(B_c)$  we use bounds on the metric and on its derivative in Riemann normal coordinates.

This result is a first step towards answering the important question of how to triangulate stratified manifolds.

### 7.1.8. *The reach, metric distortion, geodesic convexity and the variation of tangent spaces*

**Participants:** Jean-Daniel Boissonnat, Mathijs Wintraecken.

*In collaboration with André Lieutier (Dassault Syst me).*

In [41], we discuss three results. The first two concern general sets of positive reach: We first characterize the reach by means of a bound on the metric distortion between the distance in the ambient Euclidean space and the set of positive reach. Secondly, we prove that the intersection of a ball with radius less than the reach with the set is geodesically convex, meaning that the shortest path between any two points in the intersection lies itself in the intersection. For our third result we focus on manifolds with positive reach and give a bound on the angle between tangent spaces at two different points in terms of the distance between the points and the reach.

### 7.1.9. *Delaunay triangulation of a random sample of a good sample has linear size*

**Participants:** Jean-Daniel Boissonnat, Kunal Dutta, Marc Glisse.

*In collaboration with Olivier Devillers (Inria Nancy Grand Est).*

The *randomized incremental construction* (RIC) for building geometric data structures has been analyzed extensively, from the point of view of worst-case distributions. In many practical situations however, we have to face nicer distributions. A natural question that arises is: do the usual RIC algorithms automatically adapt when the point samples are nicely distributed. We answer positively to this question for the case of the Delaunay triangulation of  $\epsilon$ -nets.

$\epsilon$ -nets are a class of nice distributions in which the point set is such that any ball of radius  $\epsilon$  contains at least one point of the net and two points of the net are distance at least  $\epsilon$  apart. The Delaunay triangulations of  $\epsilon$ -nets are proved to have linear size; unfortunately this is not enough to ensure a good time complexity of the randomized incremental construction of the Delaunay triangulation. In [33], [38], we prove that a uniform random sample of a given size that is taken from an  $\epsilon$ -net has a linear sized Delaunay triangulation in any dimension. This result allows us to prove that the randomized incremental construction needs an expected linear size and an expected  $O(n \log n)$  time.

Further, we also prove similar results in the case of non-Euclidean metrics, when the point distribution satisfies a certain *bounded expansion* property; such metrics can occur, for example, when the points are distributed on a low-dimensional manifold in a high-dimensional ambient space.

### 7.1.10. *Kernelization of the Subset General Position problem in Geometry*

**Participants:** Jean-Daniel Boissonnat, Kunal Dutta.

*In collaboration with Arijit Ghosh (Indian Statistical Institute) and Sudeshna Kolay (Eindhoven University of Technology).*

In [21], we consider variants of the GEOMETRIC SUBSET GENERAL POSITION problem. In defining this problem, a geometric subsystem is specified, like a subsystem of lines, hyperplanes or spheres. The input of the problem is a set of  $n$  points in  $\mathbb{R}^d$  and a positive integer  $k$ . The objective is to find a subset of at least  $k$  input points such that this subset is in general position with respect to the specified subsystem. For example, a set of points is in general position with respect to a subsystem of hyperplanes in  $\mathbb{R}^d$  if no  $d + 1$  points lie on the same hyperplane. In this paper, we study the HYPERPLANE SUBSET GENERAL POSITION problem under two parameterizations. When parameterized by  $k$  then we exhibit a polynomial kernelization for the problem. When parameterized by  $h = n - k$ , or the dual parameter, then we exhibit polynomial kernels which are also tight, under standard complexity theoretic assumptions. We can also conclude similar kernelization results for D-POLYNOMIAL SUBSET GENERAL POSITION, where a vector space of polynomials of degree at most  $d$  are specified as the underlying subsystem such that the size of the basis for this vector space is  $b$ . The objective is to find a set of at least  $k$  input points, or in the dual delete at most  $h = n - k$  points, such that no  $b + 1$  points lie on the same polynomial. Notice that this is a generalization of many well-studied geometric variants of the SET COVER problem, such as CIRCLE SUBSET GENERAL POSITION. We also study the general projective variants of these problems. These problems are also related to other geometric problems like SUBSET DELAUNAY TRIANGULATION problem.

#### **7.1.11. Tight Kernels for Covering and Hitting: Point Hyperplane Cover and Polynomial Point Hitting Set**

**Participants:** Jean-Daniel Boissonnat, Kunal Dutta.

*In collaboration with Arijit Ghosh (Indian Statistical Institute) and Sudeshna Kolay (Eindhoven University of Technology).*

The POINT HYPERPLANE COVER problem in  $\mathbb{R}^d$  takes as input a set of  $n$  points in  $\mathbb{R}^d$  and a positive integer  $k$ . The objective is to cover all the given points with a set of at most  $k$  hyperplanes. The  $D$ -POLYNOMIAL POINTS HITTING SET ( $D$ -POLYNOMIAL POINTS HS) problem in  $\mathbb{R}^d$  takes as input a family  $\mathcal{F}$  of  $D$ -degree polynomials from a vector space  $\mathcal{R}$  in  $\mathbb{R}^d$ , and determines whether there is a set of at most  $k$  points in  $\mathbb{R}^d$  that hit all the polynomials in  $\mathcal{F}$ . In [22], we exhibit tight kernels where  $k$  is the parameter for these problems.

#### **7.1.12. Shallow packings, semialgebraic set systems, Macbeath regions, and polynomial partitioning**

**Participant:** Kunal Dutta.

*In collaboration with Arijit Ghosh (Indian Statistical Institute) and Bruno Jartoux (Université Paris-Est, Laboratoire d'Informatique Gaspard-Monge, ESIEE Paris, France) and Nabil H. Mustafa (Université Paris-Est, Laboratoire d'Informatique Gaspard-Monge, ESIEE Paris, France).*

The packing lemma of Haussler states that given a set system  $(X, \mathbb{R})$  with bounded VC dimension, if every pair of sets in  $\mathbb{R}$  have large symmetric difference, then  $\mathbb{R}$  cannot contain too many sets. Recently it was generalized to the shallow packing lemma, applying to set systems as a function of their shallow-cell complexity. In [29] we present several new results and applications related to packings:

1. an optimal lower bound for shallow packings,
2. improved bounds on Mnets, providing a combinatorial analogue to Macbeath regions in convex geometry,
3. we observe that Mnets provide a general, more powerful framework from which the state-of-the-art unweighted  $\epsilon$ -net results follow immediately, and
4. simplifying and generalizing one of the main technical tools in Fox *et al.* (*J. of the EMS*, to appear).

#### **7.1.13. A Simple Proof of Optimal Epsilon Nets**

**Participant:** Kunal Dutta.

*In collaboration with Nabil H. Mustafa (Université Paris-Est, Laboratoire d'Informatique Gaspard-Monge, ESIEE Paris, France, and Arijit Ghosh (Indian Statistical Institute) ).*



Showing the existence of  $\epsilon$ -nets of small size has been the subject of investigation for almost 30 years, starting from the initial breakthrough of Haussler and Welzl (1987). Following a long line of successive improvements, recent results have settled the question of the size of the smallest  $\epsilon$ -nets for set systems as a function of their so-called shallow-cell complexity.

In [20] we give a short proof of this theorem in the space of a few elementary paragraphs, showing that it follows by combining the  $\epsilon$ -net bound of Haussler and Welzl (1987) with a variant of Haussler's packing lemma (1991).

This implies all known cases of results on unweighted  $\epsilon$ -nets studied for the past 30 years, starting from the result of Matoušek, Seidel and Welzl (1990) to that of Clarkson and Varadajan (2007) to that of Varadarajan (2010) and Chan, Grant, Könemann and Sharpe (2012) for the unweighted case, as well as the technical and intricate paper of Aronov, Ezra and Sharir (2010).

#### 7.1.14. On Subgraphs of Bounded Degeneracy in Hypergraphs

**Participant:** Kunal Dutta.

*In collaboration with Arijit Ghosh (Indian Statistical Institute).*

A  $k$ -uniform hypergraph is  $d$ -degenerate if every induced subgraph has a vertex of degree at most  $d$ . In [48], given a  $k$ -uniform hypergraph  $H = (V(H), E(H))$ , we show there exists an induced subgraph of size at least

$$\sum_{v \in V(H)} \min \left\{ 1, c_k \left( \frac{d+1}{d_H(v)+1} \right)^{1/(k-1)} \right\},$$

where  $c_k = 2^{-(1+\frac{1}{k-1})} (1 - \frac{1}{k})$  and  $d_H(v)$  denotes the degree of vertex  $v$  in the hypergraph  $H$ . This connects, extends, and generalizes results of Alon-Kahn-Seymour (1987), on  $d$ -degenerate sets of graphs, Dutta-Mubayi-Subramanian (2012) on  $d$ -degenerate sets of linear hypergraphs, and Srinivasan-Shachnai (2004) on independent sets in hypergraphs to  $d$ -degenerate subgraphs of hypergraphs. Our technique also gives optimal lower bounds for a more generalized definition of degeneracy introduced by Zaker (2013). We further give a simple non-probabilistic proof of the Dutta-Mubayi-Subramanian bound for linear  $k$ -uniform hypergraphs, which extends the Alon-Kahn-Seymour proof technique to hypergraphs. Finally we provide several applications in discrete geometry, extending results of Payne-Wood (2013) and Cardinal-Tóth-Wood (2016). We also address some natural algorithmic questions. The proof of our main theorem combines the *random permutation* technique of Bopanna-Caro-Wei and Beame and Luby, together with a new *local density* argument which may be of independent interest.

## 7.2. Statistical aspects of topological and geometric data analysis

### 7.2.1. The DTM-signature for a geometric comparison of metric-measure spaces from samples

**Participant:** Claire Bréchet.

In [43], we introduce the notion of DTM-signature, a measure on  $\mathbb{R}_+$  that can be associated to any metric-measure space. This signature is based on the distance to a measure (DTM) introduced by Chazal, Cohen-Steiner and Mérigot. It leads to a pseudo-metric between metric-measure spaces, upper-bounded by the Gromov-Wasserstein distance. Under some geometric assumptions, we derive lower bounds for this pseudo-metric. Given two  $N$ -samples, we also build an asymptotic statistical test based on the DTM-signature, to reject the hypothesis of equality of the two underlying metric measure spaces, up to a measure-preserving isometry. We give strong theoretical justifications for this test and propose an algorithm for its implementation.

#### 7.2.2. Estimating the Reach of a Manifold

**Participants:** Eddie Aamari, Frédéric Chazal, Bertrand Michel.

*In collaboration with J. Kim, A. Rinaldo, L. Wasserman (Carnegie Mellon University)*

Various problems of computational geometry and manifold learning encode geometric regularity through the so-called reach, a generalized convexity parameter. The reach  $\tau_M$  of a submanifold  $M \subset \mathbb{R}^D$  is the maximal offset radius on which the projection onto  $M$  is well defined. The quantity  $\tau_M$  renders a certain minimal scale of  $M$ , giving bounds on both maximum curvature and possible bottleneck structures. In [35], we study the geometry of the reach through an approximation perspective. We derive new geometric results on the reach for submanifolds without boundary. An estimator  $\hat{\tau}$  of  $\tau_M$  is proposed in a framework where tangent spaces are known, and bounds assessing its efficiency are derived. In the case of i.i.d. random point cloud  $\mathbb{X}_n$ ,  $\hat{\tau}(\mathbb{X}_n)$  is showed to achieve uniform expected loss bounds over a  $\mathcal{C}^3$ -like model. Minimax upper and lower bounds are derived, and we conclude with the extension to a model with unknown tangent spaces.

### 7.2.3. *Robust Topological Inference: Distance To a Measure and Kernel Distance*

**Participants:** Frédéric Chazal, Bertrand Michel.

*In collaboration with B. Fasy, F. Lecci, A. Rinaldo, L. Wasserman.*

Let  $P$  be a distribution with support  $S$ . The salient features of  $S$  can be quantified with persistent homology, which summarizes topological features of the sublevel sets of the distance function (the distance of any point  $x$  to  $S$ ). Given a sample from  $P$  we can infer the persistent homology using an empirical version of the distance function. However, the empirical distance function is highly non-robust to noise and outliers. Even one outlier is deadly. The distance-to-a-measure (DTM) and the kernel distance are smooth functions that provide useful topological information but are robust to noise and outliers. In [17], we derive limiting distributions and confidence sets, and we propose a method for choosing tuning parameters.

### 7.2.4. *Statistical analysis and parameter selection for Mapper*

**Participants:** Steve Oudot, Bertrand Michel, Mathieu Carrière.

In [44] we study the question of the statistical convergence of the 1-dimensional Mapper to its continuous analogue, the Reeb graph. We show that the Mapper is an optimal estimator of the Reeb graph, which gives, as a byproduct, a method to automatically tune its parameters and compute confidence regions on its topological features, such as its loops and flares. This allows to circumvent the issue of testing a large grid of parameters and keeping the most stable ones in the brute-force setting, which is widely used in visualization, clustering and feature selection with the Mapper.

### 7.2.5. *Sliced Wasserstein Kernel for Persistence Diagrams*

**Participants:** Steve Oudot, Mathieu Carrière.

*In collaboration with M. Cuturi (ENSAE)*

Persistence diagrams (PDs) play a key role in topological data analysis (TDA), in which they are routinely used to describe succinctly complex topological properties of complicated shapes. PDs enjoy strong stability properties and have proven their utility in various learning contexts. They do not, however, live in a space naturally endowed with a Hilbert structure and are usually compared with specific distances, such as the bottleneck distance. To incorporate PDs in a learning pipeline, several kernels have been proposed for PDs with a strong emphasis on the stability of the RKHS distance w.r.t. perturbations of the PDs. In [27], we use the Sliced Wasserstein approximation of the Wasserstein distance to define a new kernel for PDs, which is not only provably stable but also provably discriminative w.r.t. the Wasserstein distance  $W_{1\infty}$  between PDs. We also demonstrate its practicality, by developing an approximation technique to reduce kernel computation time, and show that our proposal compares favorably to existing kernels for PDs on several benchmarks.

### 7.2.6. *An introduction to Topological Data Analysis: fundamental and practical aspects for data scientists*

**Participants:** Frédéric Chazal, Bertrand Michel.

Topological Data Analysis (TDA) is a recent and fast growing field providing a set of new topological and geometric tools to infer relevant features for possibly complex data. In [45], we propose a brief introduction, through a few selected recent and state-of-the-art topics, to basic fundamental and practical aspects of TDA for non experts.



### 7.3. Topological approach for multimodal data processing

#### 7.3.1. *On the Stability of Functional Maps and Shape Difference Operators*

**Participants:** Frédéric Chazal, Ruqi Huang, Maks Ovsjanikov.

In this paper, we provide stability guarantees for two frameworks that are based on the notion of functional maps. We consider two types of perturbations in our analysis: one is on the input shapes and the other is on the change in *scale*. In theory, we formulate and justify the robustness that has been observed in practical implementations of those frameworks. Inspired by our theoretical results, we propose a pipeline for constructing shape difference operators on point clouds and show numerically that the results are robust and informative. In particular, we show that both the shape difference operators and the derived areas of highest distortion are stable with respect to changes in shape representation and change of scale. Remarkably, this is in contrast with the well-known instability of the eigenfunctions of the Laplace-Beltrami operator computed on point clouds compared to those obtained on triangle meshes.

#### 7.3.2. *Local Equivalence and Intrinsic Metrics Between Reeb Graphs*

**Participants:** Steve Oudot, Mathieu Carrière.

As graphical summaries for topological spaces and maps, Reeb graphs are common objects in the computer graphics or topological data analysis literature. Defining good metrics between these objects has become an important question for applications, where it matters to quantify the extent by which two given Reeb graphs differ. Recent contributions emphasize this aspect, proposing novel distances such as functional distortion or interleaving that are provably more discriminative than the so-called bottleneck distance, being true metrics whereas the latter is only a pseudo-metric. Their main drawback compared to the bottleneck distance is to be comparatively hard (if at all possible) to evaluate. In [28] we take the opposite view on the problem and show that the bottleneck distance is in fact good enough locally, in the sense that it is able to discriminate a Reeb graph from any other Reeb graph in a small enough neighborhood, as efficiently as the other metrics do. This suggests considering the intrinsic metrics induced by these distances, which turn out to be all globally equivalent. This novel viewpoint on the study of Reeb graphs has a potential impact on applications, where one may not only be interested in discriminating between data but also in interpolating between them.

#### 7.3.3. *Structure and Stability of the One-Dimensional Mapper*

**Participants:** Steve Oudot, Mathieu Carrière.

Given a continuous function  $f : X \rightarrow R$  and a cover  $I$  of its image by intervals, the Mapper is the nerve of a refinement of the pullback cover  $f^{-1}(I)$ . Despite its success in applications, little is known about the structure and stability of this construction from a theoretical point of view. As a pixelized version of the Reeb graph of  $f$ , it is expected to capture a subset of its features (branches, holes), depending on how the interval cover is positioned with respect to the critical values of the function. Its stability should also depend on this positioning. In [16] we propose a theoretical framework relating the structure of the Mapper to that of the Reeb graph, making it possible to predict which features will be present and which will be absent in the Mapper given the function and the cover, and for each feature, to quantify its degree of (in-)stability. Using this framework, we can derive guarantees on the structure of the Mapper, on its stability, and on its convergence to the Reeb graph as the granularity of the cover  $I$  goes to zero.

### 7.4. Experimental research and software development

#### 7.4.1. *Stride detection for pedestrian trajectory reconstruction: a machine learning approach based on geometric patterns*

**Participants:** Frédéric Chazal, Bertrand Michel, Bertrand Beauflis.

*In collaboration with M. Grelet (Sysnav)*

A strides detection algorithm is proposed using inertial sensors worn on the ankle. This innovative approach based on geometric patterns can detect both normal walking strides and atypical strides such as small steps, side steps and backward walking that existing methods struggle to detect. It is also robust in critical situations, when for example the wearer is sitting and moving the ankle, while most algorithms in the literature would wrongly detect strides.

## DEDUCTEAM Project-Team

## 6. New Results

### 6.1. $\lambda\Pi$ -calculus modulo theory

G. Dowek has given a semantic criterion for the termination of the  $\lambda\Pi$ -calculus modulo theory. This result has been published in [23].

A. Assaf, G. Dowek, J.-P. Jouannaud and J. Liu have given a confluence criterion for untyped higher-order rewrite systems, and demonstrated some applications to the  $\lambda\Pi$ -calculus modulo theory.

G. Dowek has given an invited talk at PxTP where he has presented a state of the art of the production of system-independent proof libraries. This paper has been published in the proceedings of PxTP [12].

### 6.2. Dedukti

During his internship [22], A. Defourné extended F. Blanqui's prototype of proof assistant based on Dedukti by developing a tactic for calling external provers through Why3 [28]. He also started to study a simple rewriting tactic.

During his internship, R. Bocquet studied unification in the  $\lambda\Pi$ -calculus modulo rewriting, and started to implement a prototype.

During his internship [24], G. Genestier studied the possibility to use the Size-Change Principle [34] in order to prove termination in the  $\lambda\Pi$ -calculus modulo rewriting. This work led to an adaptation of the criterion developed in his thesis by Wahlstedt [40] to a calculus containing dependant types. He also implemented a prototype of a weak version of the criterion.

During the first three months of his postdoc, R. Lepigre proposed a new implementation of Dedukti [36], based on the Bindlib library for the representation of structures with binders [38]. The libraries generated for Dedukti are compatible with this new implementation, and can be type-checked with minor modifications.

During the first months of his PhD, G. Férey adapted the higher-order pattern matching and convertibility checking algorithms to implemented support for rewriting modulo associative-commutative (AC) symbols in Dedukti.

### 6.3. Interoperability

F. Thiré has finished to implement a translation of an arithmetic library from Matita to OpenTheory. This work can be decomposed in two steps: A first step goes from Matita to a new logic called STTforall while a second step goes from STTforall to OpenTheory. This translation will be described in two separate papers. The first paper that will be submitted to FSCD 2018 describe the logic STTforall and its translation to HOL while the second paper explains the translation from Matita to STTforall. STTforall is a very simple logic and so, it is easy to translate proofs from this logic to other proofs assistants. For example, a translation from STTforall to Coq has also been implemented by F. Thiré. Two new tools have been implemented to make these translations:

- Dkmeta is a tool that translates terms thanks to the rewrite engine of Dedukti
- Ediloh is a tool that translates terms from STTforall them in OpenTheory

F. Gilbert developed a first prototype for the extraction of proofs from the proof assistant PVS that can be verified externally. The system PVS is based on the dichotomy between a *type-checker* and a *prover*. This proof extraction mechanism is built by instrumenting the PVS *prover*, but does not contain any typing information from the *type-checker* at this stage. Proofs can be built for any PVS theory. However, some reasoning steps rely on unverified assumptions. For a restricted fragment of PVS, the proofs are exported to Dedukti, and the unverified assumptions are proved externally using the automated theorem prover MetiTarski. This work has been published and presented in [15].

## 6.4. Termination

F. Blanqui revised his paper on “size-based termination of higher-order rewrite systems” submitted to the Journal of Functional Programming [19]. This paper provides a general and modular criterion for the termination of simply-typed  $\lambda$ -calculus extended with function symbols defined by user-defined rewrite rules. Following a work of Hughes, Pareto and Sabry for functions defined with a fixpoint operator and pattern-matching [33], several criteria use typing rules for bounding the height of arguments in function calls. In this paper, we extend this approach to rewriting-based function definitions and more general user-defined notions of size.

R. Lepigre worked on his paper “Practical Subtyping for System F with Sized (Co-)Induction” [39] (joint work with C. Raffalli), which was submitted to the journal Transactions on Programming Languages and Systems (TOPLAS) and is now under revision. This paper proposes a practical type system for a rich, normalizing, extension of (Curry-style) System F. The termination of recursive programs is established using a new mechanism based on circular proofs, which is also used to deal with (sized) inductive and coinductive types (in subtyping). The idea is to build (possibly ill-formed) infinite, circular typing (resp. subtyping) derivations, and to check for their well-foundedness a posteriori. The normalization proof then follows using standard realizability (or reducibility) techniques, the main point being that the adequacy lemma can still be proved by (well-founded) induction on the structure of the “circular” typing (resp. subtyping) derivations.

## 6.5. Proof theory

G. Burel developed a general framework, focusing with selection, of which various logical systems are instances: ordinary focusing, refinements of resolution, deduction modulo theory, superdeduction and beyond [20]. This strengthens links between sequent calculi and resolution methods.

F. Gilbert developed a constructivization algorithm, taking as input the classical proof of some formula and generating as output, whenever possible, a constructive proof of the same formula. This result has been published and presented in [14].

F. Gilbert submitted his PhD dissertation (work document [25]), centered on the extension of higher-order logic with predicate subtyping. Predicate subtyping is a key feature of the proof assistant PVS, allowing to define types from predicates – for instance, using this feature, the type of even numbers can be defined from the corresponding predicate. The core of this work is the definition of a language of verifiable certificates for predicate subtyping, as well as the proof of two properties of this language: a cut-elimination theorem, a theorem of conservativity over higher-order logic. F. Gilbert presented this language of certificates as well as the cut-elimination theorem at the workshop TYPES 2017.

## 6.6. Automated theorem proving

G. Bury presented the mSAT library at the OCaml workshop during the International Conference on Functional Programming [21]. This library provides an efficient SAT/SMT solver core written in OCaml, and presented as a functor to allow instantiation with different theories.

## 6.7. Program verification

R. Lepigre submitted a paper describing the PML<sub>2</sub> programming language and proof assistant [35], which was the main object of his recently defended PhD thesis [37].

## 6.8. Quantum computing

A. Díaz-Caro and G. Dowek have developed a type system for the  $\lambda$ -calculus that permits to distinguish duplicable terms from non duplicable ones. This work has been presented at Theory and Practice of Natural Computing [13].

## GRACE Project-Team

## 6. New Results

### 6.1. qDSA: Compact signatures for IoT

B. Smith and Joost Renes (Radboud University, NL) developed **qDSA**, a new digital signature scheme targeting constrained devices, typically microcontrollers with extremely limited memory. An article describing qDSA was presented at ASIACRYPT 2017, and a reference implementation software package has been placed into the public domain.

### 6.2. PIR based on transversal designs

J. Lavauzelle presented a construction of Private Information Retrieval (PIR) protocols from combinatorial structures called transversal designs. The construction features low computation and low storage overhead for the servers. For some instances, adequate communication between servers and user is achieved. The PIR scheme also generalizes to colluding servers. The construction has been presented during WCC 2017 [17], and in a poster session in the Munich Workshop in Coding and Applications.

### 6.3. On the security of compact McEliece keys

E. Barelli presented at WCC 2017 (Workshop on Coding and Cryptography, St Petersburg, Russia) her recent results on the analysis of McEliece scheme based on alternant codes with a non trivial automorphism group [16]. These codes were suggested for public key encryption since, compared to codes with trivial automorphism group, they could provide shorter keys.

If the security with respect to generic decoding attacks is almost unchanged when considering codes with non trivial automorphisms, E. Barelli proved that the security with respect to key recovery attacks is highly reduced since, it reduces to recover the structure of the subcode of fixed elements by the automorphism group.

### 6.4. Two-points codes on the generalized Giuletti Korchmaros curve

In a collaboration with Peter Beelen, Mrinmoy Datta, Vincent Neiger and Johan Rosenkilde (DTU Copenhagen), E. Barelli obtained improved lower bounds for the minimum distance of some algebraic geometry codes from Giuletti Korchmaros curves [20].

### 6.5. Towards a function field version of Freiman's theorem

In a collaboration with Christine Bachoc and Gilles Zémor (University of Bordeaux), A. Couvreur obtained a characterisation of subspaces  $S$  of a function field  $F$  over an algebraically closed field satisfying

$$\dim S^2 = 2 \dim S$$

where  $S^2$  denotes the space spanned by all the products of two elements of  $S$ . They obtained the following result [18]:

**Theorem.** *Let  $F$  be a function field over an algebraically closed field, and  $S$  be a finite dimensional subspace of  $F$  which spans  $F$  as an algebra and such that*

$$\dim S^2 = 2 \dim S.$$

Then  $F$  is a function field of transcendence degree 1 and

- either  $F$  has genus 1 and  $S$  is a Riemann Roch space
- or  $F$  has genus 0 and  $S$  is a subspace of codimension 1 in a Riemann Roch space.

## 6.6. BIG QUAKE

In the context of NIST's call for post quantum cryptosystems:

<https://csrc.nist.gov/Projects/Post-Quantum-Cryptography>

A. Couvreur and E. Barelli participated to the submission BIG QUAKE [19] (BINARY Goppa QUASI-cyclic Key Encapsulation). The proposal consists in a public key encryption scheme (with a conversion to a Key Encapsulation Mechanism) using binary quasi-cyclic Goppa codes.

The details on the proposal are on the following website.

<https://bigquake.inria.fr/>

## 6.7. Discrete Logarithm computations in finite fields with the NFS algorithm

The best discrete logarithm record computations in prime fields and large characteristic finite fields are obtained with Number Field Sieve algorithm (NFS) at the moment.

### 6.7.1. Computing discrete logarithms in $GF(p^6)$

A. Guillevic, L. Grémy, F. Morain and E. Thomé (from CARAMBA EPC in LORIA) computed a discrete log on a curve of embedding degree 6 and cryptographic size. This clearly showed that curves with small embedding degrees are indeed weak. The article [23] was presented by L. Grémy during the SAC 2017 conference in Ottawa.

### 6.7.2. Identity management on Bitcoin's blockchain

D. Augot and W. George in collaboration with Hervé Chabanne (Safran Identity and Security, ex Morpho, now Idemia) designed two schemes to allow users to authenticate using so-called anonymous credentials, issued by an identity provider. We used Brands anonymous credentials with selective disclosure each time, first for a finely tuned, user managed, identity scheme [12], second for a more classical high throughput scheme [13], inspired by CONIKS <https://coniks.cs.princeton.edu>.

### 6.7.3. Law and Blockchain smart contracts

D. Augot, with Célia Zolynski, is co-advising Hanna-Mae Bissierier, a PhD student law, on the impact of blockchains on legal systems. The PhD is in law, and D. Augot only gives scientific and technological explanations, while the direction of the thesis is done by Célia Zolynski.

## MEXICO Project-Team

## 7. New Results

### 7.1. Optimal constructions for active diagnosis

Published in [4].

Diagnosis is the task of detecting fault occurrences in a partially observed system. Depending on the possible observations, a discrete-event system may be diagnosable or not. Active diagnosis aims at controlling the system to render it diagnosable. Past research has proposed solutions for this problem, but their complexity remains to be improved. Here, we solve the decision and synthesis problems for active diagnosability, proving that (1) our procedures are optimal with respect to computational complexity, and (2) the memory required for our diagnoser is minimal. We then study the delay between a fault occurrence and its detection by the diagnoser. We construct a memory-optimal diagnoser whose delay is at most twice the minimal delay, whereas the memory required to achieve optimal delay may be highly greater. We also provide a solution for parametrized active diagnosis, where we automatically construct the most permissive controller respecting a given delay.

### 7.2. Diagnosability of Repairable Faults

Published in [3].

The diagnosis problem for discrete event systems consists in deciding whether some fault event occurred or not in the system, given partial observations on the run of that system. Diagnosability checks whether a correct diagnosis can be issued in bounded time after a fault, for all faulty runs of that system. This problem appeared two decades ago and numerous facets of it have been explored, mostly for permanent faults. It is known for example that diagnosability of a system can be checked in polynomial time, while the construction of a diagnoser is exponential. The present paper examines the case of transient faults, that can appear and be repaired. Diagnosability in this setting means that the occurrence of a fault should always be detected in bounded time, but also before the fault is repaired, in order to prepare for the detection of the next fault or to take corrective measures while they are needed. Checking this notion of diagnosability is proved to be PSPACE-complete. It is also shown that faults can be reliably counted provided the system is diagnosable for faults and for repairs.

### 7.3. Diagnostic et contrôle de la dégradation des systèmes probabilistes

Published in [18].

Le diagnostic actif est opéré par un contrôleur en vue de rendre un système diagnosticable. Afin d'éviter que le contrôleur ne dégrade trop fortement le système, on lui affecte généralement un second objectif en termes de qualité de service. Dans le cadre des systèmes probabilistes, une spécification possible consiste à assurer une probabilité positive qu'une exécution infinie soit correcte, ce qu'on appelle le diagnostic actif sûr. Nous introduisons ici deux spécifications alternatives. La gamma-correction du système affecte à une exécution une valeur de correction dépendant d'un facteur de décote gamma et le contrôleur doit assurer une valeur moyenne supérieure à un seuil fixé. La alpha-dégradation requiert qu'asymptotiquement, à chaque unité de temps une proportion supérieure à alpha des exécutions jusqu'alors correctes le demeure. D'un point de vue sémantique, nous explicitons des liens significatifs entre les différentes notions. Algorithmiquement, nous établissons la frontière entre décidabilité et indécidabilité des problèmes et dans le cas positif nous exhibons la complexité précise ainsi qu'une synthèse, potentiellement à mémoire infinie.

### 7.4. The Complexity of Diagnosability and Opacity Verification for Petri Nets

Published in [7].

Diagnosability and opacity are two well-studied problems in discrete-event systems. We revisit these two problems with respect to expressiveness and complexity issues. We first relate different notions of diagnosability and opacity. We consider in particular fairness issues and extend the definition of Germanos et al. [ACM TECS, 2015] of weakly fair diagnosability for safe Petri nets to general Petri nets and to opacity questions. Second, we provide a global picture of complexity results for the verification of diagnosability and opacity. We show that diagnosability is NL-complete for finite state systems, PSPACE-complete for safe Petri nets (even with fairness), and EXSPACE-complete for general Petri nets without fairness, while non diagnosability is inter-reducible with reachability when fault events are not weakly fair. Opacity is ESPACE-complete for safe Petri nets (even with fairness) and undecidable for general Petri nets already without fairness.

## 7.5. Probabilistic Disclosure: Maximisation vs. Minimisation

Published in [8].

We consider opacity questions where an observation function provides to an external attacker a view of the states along executions and secret executions are those visiting some state from a fixed subset. Disclosure occurs when the observer can deduce from a finite observation that the execution is secret, the  $\varepsilon$ -disclosure variant corresponding to the execution being secret with probability greater than  $1 - \varepsilon$ . In a probabilistic and non deterministic setting, where an internal agent can choose between actions, there are two points of view, depending on the status of this agent: the successive choices can either help the attacker trying to disclose the secret, if the system has been corrupted, or they can prevent disclosure as much as possible if these choices are part of the system design. In the former situation, corresponding to a worst case, the disclosure value is the supremum over the strategies of the probability to disclose the secret (maximisation), whereas in the latter case, the disclosure is the infimum (minimisation). We address quantitative problems (comparing the optimal value with a threshold) and qualitative ones (when the threshold is zero or one) related to both forms of disclosure for a fixed or finite horizon. For all problems, we characterise their decidability status and their complexity. We discover a surprising asymmetry: on the one hand optimal strategies may be chosen among deterministic ones in maximisation problems, while it is not the case for minimisation. On the other hand, for the questions addressed here, more minimisation problems than maximisation ones are decidable.

## 7.6. D-SPACES: Implementing Declarative Semantics for Spatially Structured Information

Published in [13].

We introduce in this paper D-SPACES, an implementation of constraint systems with space and extrusion operators. Constraint systems are algebraic models that allow for a semantic language-like representation of information in systems where the concept of space is a primary structural feature. We give this information mainly an epistemic interpretation and consider various agents as entities acting upon it. D-SPACES is coded as a c++11 library providing implementations for constraint systems, space functions and extrusion functions. The interfaces to access each implementation are minimal and thoroughly documented. D-SPACES also provides property-checking methods as well as an implementation of a specific type of constraint systems (a boolean algebra). This last implementation serves as an entry point for quick access and proof of concept when using these models. Furthermore, we offer an illustrative example in the form of a small social network where users post their beliefs and utter their opinions.

## 7.7. Unbounded product-form Petri nets

Published in [14].



Computing steady-state distributions in infinite-state stochastic systems is in general a very difficult task. Product-form Petri nets are those Petri nets for which the steady-state distribution can be described as a natural product corresponding, up to a normalising constant, to an exponentiation of the markings. However, even though some classes of nets are known to have a product-form distribution, computing the normalising constant can be hard. The class of (closed)  $\Pi^3$ -nets has been proposed in an earlier work, for which it is shown that one can compute the steady-state distribution efficiently. However these nets are bounded. In this paper, we generalise queuing Markovian networks and closed  $\Pi^3$ -nets to obtain the class of open  $\Pi^3$ -nets, that generate infinite-state systems. We show interesting properties of these nets: (1) we prove that liveness can be decided in polynomial time, and that reachability in live  $\Pi^3$ -nets can be decided in polynomial time; (2) we show that we can decide ergodicity of such nets in polynomial time as well; (3) we provide a pseudo-polynomial time algorithm to compute the normalising constant.

## 7.8. Statistical Model-Checking for Autonomous Vehicle Safety Validation

Published in [20].

We present an application of statistical model-checking to the verification of an autonomous vehicle controller. Our goal is to check safety properties in various traffic situations. More specifically, we focus on a traffic jam situation.

The controller is specified by a C++ program. Using sensors, it registers positions and velocities of nearby vehicles and modifies the position and velocity of the controlled vehicle to avoid collisions. We model the environment using a stochastic high level Petri net, where random behaviors of other vehicles can be described. We use HASL, a quantitative variant of linear temporal logic, to express the desired properties. A large family of performance indicators can be specified in HASL and we target in particular the expectation of travelled distance or the collision probability.

We evaluate the properties of this model using COSMOS1. This simulation tool implements numerous statistical techniques such as sequential hypothesis testing and most confidence range computation methods. Its efficiency allowed us to conduct several experiments with success.

## 7.9. Une sémantique formelle pour les modèles Simulink

Published in [19].

De nombreux projets industriels, notamment dans la construction automobile, font appel à la suite d'outils Simulink pour la conception et la validation de composants critiques représentant des systèmes hybrides c'est-à-dire combinant des aspects discrets et continus. Cependant les formalismes associés ne disposent pas d'une sémantique formelle ce qui peut diminuer la confiance des ingénieurs vis-à-vis des résultats produits. Nous proposons ici une telle sémantique en procédant en deux étapes. Nous développons d'abord une sémantique exacte mais non exécutable. Puis nous l'enrichissons d'une sémantique opérationnelle approchée avec pour objectif une quantification de l'erreur issue de cette approximation.

## 7.10. The Logical View on Continuous Petri Nets

Published in [5].

Continuous Petri nets are a relaxation of classical discrete Petri nets in which transitions can be fired a fractional number of times, and consequently places may contain a fractional number of tokens. Such continuous Petri nets are an appealing object to study since they over approximate the set of reachable configurations of their discrete counterparts, and their reachability problem is known to be decidable in polynomial time. The starting point of this paper is to show that the reachability relation for continuous Petri nets is definable by a sentence of linear size in the existential theory of the rationals with addition and order. Using this characterization, we obtain decidability and complexity results for a number of classical decision problems for continuous Petri nets. In particular, we settle the open problem about the precise complexity of reachability set inclusion. Finally, we show how continuous Petri nets can be incorporated inside the classical

backward coverability algorithm for discrete Petri nets as a pruning heuristic in order to tackle the symbolic state explosion problem. The cornerstone of the approach we present is that our logical characterization enables us to leverage the power of modern SMT-solvers in order to yield a highly performant and robust decision procedure for coverability in Petri nets. We demonstrate the applicability of our approach on a set of standard benchmarks from the literature.

### 7.11. Memoryless Determinacy of Finite Parity Games: Another Simple Proof

Published in [24].

Memoryless determinacy of (infinite) parity games is an important result with numerous applications. It was first independently established by Emerson and Jutla [1] and Mostowski [2] but their proofs involve elaborate developments. The elegant and simpler proof of Zielonka [3] still requires a nested induction on the finite number of priorities and on ordinals for sets of vertices. There are other proofs for finite games like the one of Bjørklund, Sandberg and Vorobyov [4] that relies on relating infinite and finite duration games. We present here another simple proof that finite parity games are determined with memoryless strategies using induction on the number of relevant states. The closest proof that relies on induction over non absorbing states is the one of Graedel [5]. However instead of focusing on a single appropriate vertex for induction as we do here, he considers two reduced games per vertex, for all the vertices of the game. The idea of reasoning about a single state has been inspired to me by the analysis of finite stochastic priority games by Karelövic and Zielonka [6].

### 7.12. Interval iteration algorithm for MDPs and IMDPs

Markov Decision Processes (MDP) are a widely used model including both non-deterministic and probabilistic choices. Minimal and maximal probabilities to reach a target set of states, with respect to a policy resolving non-determinism, may be computed by several methods including value iteration. This algorithm, easy to implement and efficient in terms of space complexity, iteratively computes the probabilities of paths of increasing length. However, it raises three issues: (1) defining a stopping criterion ensuring a bound on the approximation, (2) analysing the rate of convergence, and (3) specifying an additional procedure to obtain the exact values once a sufficient number of iterations has been performed. The first two issues are still open and, for the third one, an upper bound on the number of iterations has been proposed. Based on a graph analysis and transformation of MDPs, we address these problems. First we introduce an interval iteration algorithm, for which the stopping criterion is straightforward. Then we exhibit its convergence rate. Finally we significantly improve the upper bound on the number of iterations required to get the exact values. We extend our approach to also deal with Interval Markov Decision Processes (IMDP) that can be seen as symbolic representations of MDPs.

### 7.13. Alignment-Based Trace Clustering

Published in [9].

A novel method to cluster event log traces is presented in this paper. In contrast to the approaches in the literature, the clustering approach of this paper assumes an additional input: a process model that describes the current process. The core idea of the algorithm is to use model traces as centroids of the clusters detected, computed from a generalization of the notion of alignment. This way, model explanations of observed behavior are the driving force to compute the clusters, instead of current model agnostic approaches, e.g., which group log traces merely on their vector-space similarity. We believe alignment-based trace clustering provides results more useful for stakeholders. Moreover, in case of log incompleteness, noisy logs or concept drift, they can be more robust for dealing with highly deviating traces. The technique of this paper can be combined with any clustering technique to provide model explanations to the clusters computed. The proposed technique relies on encoding the individual alignment problems into the (pseudo-)Boolean domain, and has been implemented in our tool DarkSider that uses an open-source solver.

### **7.14. Aligning Modeled and Observed Behavior: A Compromise Between Complexity and Quality**

Published in [17].

Certifying that a process model is aligned with the real process executions is perhaps the most desired feature a process model may have: aligned process models are crucial for organizations, since strategic decisions can be made easier on models instead of on plain data. In spite of its importance, the current algorithmic support for computing alignments is limited: either techniques that explicitly explore the model behavior (which may be worst-case exponential with respect to the model size), or heuristic approaches that cannot guarantee a solution, are the only alternatives. In this paper we propose a solution that sits right in the middle in the complexity spectrum of alignment techniques; it can always guarantee a solution, whose quality depends on the exploration depth used and local decisions taken at each step. We use linear algebraic techniques in combination with an iterative search which focuses on progressing towards a solution. The experiments show a clear reduction in the time required for reaching a solution, without sacrificing significantly the quality of the alignment obtained.

### **7.15. Temporal Reprogramming of Boolean Networks**

Published in [15].

Cellular reprogramming, a technique that opens huge opportunities in modern and regenerative medicine, heavily relies on identifying key genes to perturb. Most of computational methods focus on finding mutations to apply to the initial state in order to control which attractor the cell will reach. However, it has been shown, and is proved in this article, that waiting between the perturbations and using the transient dynamics of the system allow new reprogramming strategies. To identify these temporal perturbations, we consider a qualitative model of regulatory networks, and rely on Petri nets to model their dynamics and the putative perturbations. Our method establishes a complete characterization of temporal perturbations, whether permanent (mutations) or only temporary, to achieve the existential or inevitable reachability of an arbitrary state of the system. We apply a prototype implementation on small models from the literature and show that we are able to derive temporal perturbations to achieve trans-differentiation.

### **7.16. Goal-Driven Unfolding of Petri Nets**

Published in [10].

Unfoldings provide an efficient way to avoid the state-space explosion due to interleavings of concurrent transitions when exploring the runs of a Petri net. The theory of adequate orders allows one to define finite prefixes of unfoldings which contain all the reachable markings. In this paper we are interested in reachability of a single given marking, called the goal. We propose an algorithm for computing a finite prefix of the unfolding of a 1-safe Petri net that preserves all minimal configurations reaching this goal. Our algorithm combines the unfolding technique with on-the-fly model reduction by static analysis aiming at avoiding the exploration of branches which are not needed for reaching the goal. We present some experimental results.

### **7.17. Euler's Method Applied to the Control of Switched Systems**

Hybrid systems are a powerful formalism for modeling and reasoning about cyber-physical systems. They mix the continuous and discrete natures of the evolution of computerized systems. Switched systems are a special kind of hybrid systems, with restricted discrete behaviours: those systems only have finitely many different modes of (continuous) evolution, with isolated switches between modes. Such systems provide a good balance between expressiveness and controllability, and are thus in widespread use in large branches of industry such as power electronics and automotive control. The control law for a switched system defines the way of selecting the modes during the run of the system. Controllability is the problem of (automatically) synthesizing a control law in order to satisfy a desired property, such as safety (maintaining the variables within a given zone) or stabilisation (confinement of the variables in a close neighborhood around an objective point).

In order to compute the control of a switched system, we need to compute the solutions of the differential equations governing the modes. Euler's method is the most basic technique for approximating such solutions. We present here an estimation of the Euler's method local error, using the notion of "one-sided Lipschitz constant" for modes. This yields a general control synthesis approach which can encompass several features such as bounded disturbance and compositionality.

## 7.18. An Improved Algorithm for the Control Synthesis of Nonlinear Sampled Switched Systems

Published in [6].

A novel algorithm for the control synthesis for nonlinear switched systems is presented in this paper. Based on an existing procedure of state-space bisection and made available for nonlinear systems with the help of guaranteed integration, the algorithm has been improved to be able to consider longer patterns of modes with a better pruning approach. Moreover, the use of guaranteed integration also permits to take bounded perturbations and varying parameters into account. It is particularly interesting for safety critical applications, such as in aeronautical, military or medical fields. The whole approach is entirely guaranteed and the induced controllers are correct-by-design. Some experimentations are performed to show the important gain of the new algorithm.

## 7.19. Distributed Control Synthesis Using Euler's Method

Published in [22].

In a previous work, we explained how Euler's method for computing approximate solutions of systems of ordinary differential equations can be used to synthesize safety controllers for sampled switched systems. We continue here this line of research by showing how Euler's method can also be used for synthesizing safety controllers in a distributed manner. The global system is seen as an interconnection of two (or more) sub-systems where, for each component, the sub-state corresponding to the other component is seen as an "input"; the method exploits (a variant of) the notions of incremental input-to-state stability ( $\delta$ -ISS) and ISS Lyapunov function. We illustrate this distributed control synthesis method on a building ventilation example.

## 7.20. Control Synthesis of Nonlinear Sampled Switched Systems using Euler's Method

Published in [21].

In this paper, we propose a symbolic control synthesis method for nonlinear sampled switched systems whose vector fields are one-sided Lipschitz. The main idea is to use an approximate model obtained from the forward Euler method to build a guaranteed control. The benefit of this method is that the error introduced by symbolic modeling is bounded by choosing suitable time and space discretizations. The method is implemented in the interpreted language Octave. Several examples of the literature are performed and the results are compared with results obtained with a previous method based on the Runge-Kutta integration method.

## 7.21. Metastability-Aware Memory-Efficient Time-to-Digital Converter

Published in [11].

We propose a novel method for transforming delay- line time-to-digital converters (TDCs) into TDCs that output Gray code without relying on synchronizers. We formally prove that the inevitable metastable memory upsets (Marino, TC'81) do not induce an additional time resolution error. Our modified design provides suitable inputs to the recent metastability-containing sorting networks by Lenzen and Medina (ASYNC'16) and Bund et al. (DATE'17). In contrast, employing existing TDCs would require using thermometer code at the TDC output (followed by conversion to Gray code) or resolving metastability inside the TDC. The former is too restrictive w.r.t. the dynamic range of the TDCs, while the latter loses the advantage of enabling (accordingly much faster) computation without having to first resolve metastability.

Our all-digital designs are also of interest in their own right: they support high sample rates and large measuring ranges at nearly optimal bit-width of the output, yet maintain the original delay-line's time resolution. No previous approach unifies all these properties in a single device.

## **7.22. Brief Announcement: Lower Bounds for Asymptotic Consensus in Dynamic Networks**

Published in [12].

## **7.23. Metastability Tolerant Computing**

Published in [16].

Synchronization using flip-flop chains imposes a latency of a few clock cycles when transferring data and control signals between clock domains. We propose a design scheme that avoids this latency by performing synchronization as part of state/data computations while guaranteeing that metastability is contained and its effects tolerated (with an acceptable failure probability). We present a theoretical framework for modeling synchronous state machines in the presence of metastability and use it to prove properties that guarantee some form of reliability. Specifically, we show that the inevitable state/data corruption resulting from propagating metastable states can be confined to a subset of computations. Applications that can tolerate certain failures can exploit this property to leverage low-latency and quasi-reliable operation simultaneously. We demonstrate the approach by designing a Network-on-Chip router with zero-latency asynchronous ports and show via simulation that it outperforms a variant with two flip-flop synchronizers at a negligible cost in packet transfer reliability.

## PARSIFAL Project-Team

## 6. New Results

### 6.1. Separating Functional Computation from Relations

**Participants:** Ulysse Gérard, Dale Miller.

The logical foundation of arithmetic generally starts with a quantificational logic over relations. Of course, one often wishes to have a formal treatment of functions within this setting. Both Hilbert and Church added choice operators (such as the epsilon operator) to logic in order to coerce relations that happen to encode functions into actual functions. Others have extended the term language with confluent term rewriting in order to encode functional computation as rewriting to a normal form (e.g., the Dedukti proof checking project [46]). It is possible to take a different approach that does not extend the underlying logic with either choice principles or with an equality theory. Instead, we use the familiar two-phase construction of focused proofs and capture functional computation entirely within one of these phases. As a result, computation of functions can remain purely relational even when it is computing functions. This result, which appeared in [22], could be used to add to the Abella theorem prover a primitive method for doing deterministic computations.

### 6.2. Translating between implicit and explicit versions of proof

**Participants:** Roberto Blanco, Zakaria Chihani, Dale Miller.

As we have demonstrated within the Parsifal team, the Foundational Proof Certificate (FPC) framework can be used to define the semantics of a wide range of proof evidence. We have given such definitions for a number of textbook proof systems as well as for the proof evidence output from some existing theorem proving systems. An important decision in designing a proof certificate format is the choice of how many details are to be placed within certificates. Formats with fewer details are smaller and easier for theorem provers to output but they require more sophistication from checkers since checking will involve some proof reconstruction. Conversely, certificate formats containing many details are larger but are checkable by less sophisticated checkers. Since the FPC framework is based on well-established proof theory principles, proof certificates can be manipulated in meaningful ways. In fact, we have shown how it is possible to automate moving from implicit to explicit (*elaboration*) and from explicit to implicit (*distillation*) proof evidence via the proof checking of a *pair of proof certificates*. Performing elaboration makes it possible to transform a proof certificate with details missing into a certificate packed with enough details so that a simple kernel (without support for proof reconstruction) can check the elaborated certificate. This design allows us to trust in only a single, simple checker of explicitly described proofs but trust in a range of theorem provers employing a range of proof structures. Experimental results of using this design appear in

### 6.3. Combinatorial Flows

**Participant:** Lutz Straßburger.

Combinatorial flows are a variation of combinatorial proofs that allow for the substitution of proofs into proofs (instead of just substituting formulas). This makes combinatorial flows p-equivalent to Frege systems with substitution, which are the strongest proof systems with respect to p-simulation, as studied in proof complexity. Since combinatorial flows have a polynomial correctness criterion, they can also be seen as an improvement to atomic flows (which do not have a correctness criterion). This work has been presented at the FCSD 2017 conference [37], [28]

### 6.4. Justification Logic for Constructive Modal Logic

**Participants:** Lutz Straßburger, Sonia Marin.



Justification logic is a family of modal logics generalizing the Logic of Proofs  $LP$ , introduced by Artemov in [45]. The original motivation, which was inspired by works of Kolmogorov and Gödel in the 1930's, was to give a classical provability semantics to intuitionistic propositional logic. The language of the Logic of Proofs can be seen as a modal language where occurrences of the  $\Box$ -modality are replaced with terms, also known as *proof polynomials*, *evidence terms*, or *justification terms*, depending on the setting. The intended meaning of the formula ' $t : A$ ' is '*t* is a proof of  $A$ ' or, more generally, the reason for the validity of  $A$ . Thus, the justification language is viewed as a refinement of the modal language, with one provability construct  $\Box$  replaced with an infinite family of specific proofs. In a joint work with Roman Kuznets (TU Wien), we add a second type of terms, which we call *witness terms* and denote by Greek letters. Thus, a formula  $\Diamond A$  is to be realized by ' $\mu : A$ '. The intuitive understanding of these terms is based on the view of  $\Diamond$  modality as representing consistency (with  $\Box$  still read as provability). The term  $\mu$  justifying the consistency of a formula is viewed as an abstract witnessing model for the formula. We keep these witnesses abstract so as not to rely on any specific semantics. All the operations on witness terms that we employ to ensure the realization theorem for  $CK$ ,  $CD$ ,  $CT$ , and  $CS4$ . This work has been presented at the IMLA 2017 workshop [40]

## 6.5. Proof Theory of Indexed Nested Sequents

**Participants:** Lutz Straßburger, Sonia Marin.

Indexed nested sequents are an extension of nested sequents allowing a richer underlying graph-structure that goes beyond the plain tree-structure of pure nested sequents. For this reason they can be used to give deductive systems to modal logics which cannot be captured by pure nested sequents. In this work we show how the standard cut-elimination procedure for nested sequents can be extended to indexed nested sequents, and we discuss how indexed nested sequents can be used for intuitionistic modal logics. These results have been presented at the TABLEAUX 2017 conference [24], [35]

## 6.6. On the Length of Medial-Switch-Mix Derivations

**Participant:** Lutz Straßburger.

Switch and medial are two inference rules that play a central role in many deep inference proof systems. In specific proof systems, the mix rule may also be present. In a joint work with Paola Bruscoli (University of Bath) we show that the maximal length of a derivation using only the inference rules for switch, medial, and mix, modulo associativity and commutativity of the two binary connectives involved, is quadratic in the size of the formula at the conclusion of the derivation. This shows, at the same time, the termination of the rewrite system. This result has been presented at the International Workshop on Logic, Language, Information, and Computation 2017 [20].

## 6.7. Maehara-style Modal Nested Calculi

**Participant:** Lutz Straßburger.

In a joint work with Roman Kuznets (TU Wien), we develop multi-conclusion nested sequent calculi for the fifteen logics of the intuitionistic modal cube between IK and IS5. The proof of cut-free completeness for all logics is provided both syntactically via a Maehara-style translation and semantically by constructing an infinite birelational countermodel from a failed proof search [83]. Interestingly, the Maehara-style translation for proving soundness syntactically fails due to the hierarchical structure of nested sequents. Consequently, we only provide the semantic proof of soundness. The countermodel construction used to prove completeness required a completely novel approach to deal with two independent sources of non-termination in the proof search present in the case of transitive and Euclidean logics.

## 6.8. Combining inference systems in the CDSAT framework

**Participant:** Stéphane Graham-Lengrand.

In 2016 we had designed a methodology [49], based on *inference systems*, for combining theories in SMT-solving, that supersedes the existing approaches, namely that of Nelson-Oppen [78] and that of MCSAT [86], [66]. While soundness and completeness of our approach were proved in 2016, we further developed, in 2017, the meta-theory of this system, now called CDSAT for *Conflict-Driven Satisfiability*, in particular with

- a proof of termination for the CDSAT system, and the identification of sufficient conditions, on the theory modules to be combined, for the global termination of the system to hold;
- a learning mechanism, whereby the system discovers lemmas along the run, which can be used later to speed-up the rest of the run;
- an enrichment of the CDSAT system with proof-object generation, and the identification of proof-construction primitives that can be used to make the answers produced by CDSAT correct-by-construction.

The first result, together with the introduction of the CDSAT framework, was publishing this year in [19]. The last two results are described in a paper accepted for publication at CPP in 2018.

## 6.9. Theory modules for CDSAT

**Participant:** Stéphane Graham-Lengrand.

The CDSAT system described above is a framework for the combination of theory modules, so it is only useful inasmuch many theories can be captured as CDSAT theory modules. Theory modules are essentially given by a set of inference rules and, for each input problem, a finite set of expressions that are allowed to be used by CDSAT at runtime. These ingredients need to satisfy some requirement for soundness, completeness, and termination of CDSAT. In 2017 we identified such theory modules for the following theories

- Boolean logic;
- Linear Rational Arithmetic;
- Equality with Uninterpreted Function symbols;
- Any theory whose ground satisfiability is decidable, if one is willing to give up the fine-grained aspect of inference rules;
- Bitvectors (core fragment).

The first four cases of theories were published in [19], while the Bitvector theory was published in [21].

## 6.10. Environments and the Complexity of Abstract Machines

**Participant:** Beniamino Accattoli.

This joint work with Bruno Barras (Inria) [30] belongs to line of work *Cost Models and Abstract Machines for Functional Languages*, supported by the ANR project COCA HOLA.

We study various notions of environments (local, global, split) for abstract machines for functional languages, from a complexity and implementative point of view.

An environment is a data structure used to implement sharing of subterms. There are two main styles. The most common one is to have many local environments, one for every piece of code in the data structures of the machine. A minority of works uses a single global environment instead. Up to now, the two approaches have been considered equivalent, in particular at the level of the complexity of the overhead: they have both been used to obtain bilinear bounds, that is, linear in the number of beta steps and in the size of the initial term.

Our main result is that local environments admit implementations that are asymptotically faster than global environments, lowering the dependency from the size of the initial term from linear to logarithmic, thus improving the bounds in the literature. We also show that a third style, split environments, that are in between local and global ones, has the benefits of both. Finally, we provide a call-by-need machine with split environments for which we prove the new improved bounds on the overhead.



## 6.11. The Negligible and Yet Subtle Cost of Pattern Matching

**Participant:** Beniamino Accattoli.

This joint work with Bruno Barras (Inria) [31] belongs to line of work *Cost Models and Abstract Machines for Functional Languages*, supported by the ANR project COCA HOLA.

In this work we extend results about time cost models for the  $\lambda$ -calculus to a larger language, namely the  $\lambda$ -calculus with constructors and pattern matching. We consider all natural evaluation strategies, that is, call-by-name, call-by-value, and call-by-need.

The results are expected, and considered folklore, but we show that the question is subtler than it seems at first sight, by exhibiting some counter-example for naive formulations of the extensions. The, we show the actual results for the right extensions.

## 6.12. Implementing Open Call-by-Value

This joint work with Giulio Guerrieri (Oxford University) [32] belongs to line of work *Cost Models and Abstract Machines for Functional Languages*, supported by the ANR project COCA HOLA.

The theory of the call-by-value  $\lambda$ -calculus relies on weak evaluation and closed terms, that are natural hypotheses in the study of programming languages. To model proof assistants, however, strong evaluation and open terms are required. Open call-by-value is the intermediate setting of weak evaluation with open terms, on top of which Grégoire and Leroy designed the abstract machine of Coq. This paper provides a theory of abstract machines for open call-by-value. The literature contains machines that are either simple but inefficient, as they have an exponential overhead, or efficient but heavy, as they rely on a labelling of environments and a technical optimization. We introduce a machine that is simple and efficient: it does not use labels and it implements open call-by-value within a bilinear overhead. Moreover, we provide a new fine understanding of how different optimizations impact on the complexity of the overhead.

## 6.13. Further Formalizing the Meta-Theory of Linear Logic

**Participants:** Kaustuv Chaudhuri, Leonardo Lima, Giselle Reis.

We have continued our formalization of the meta-theory of substructural logics by giving a fully formal proof of cut-elimination (and hence of completeness) for focused classical first-order linear logic. This is the first time that this complete system has had a fully formalized proof.

This formalization serves as a *tour de force* of Abella's ability to reason about mutual induction and support sophisticated binding constructs.

An extended invited paper is currently under review, to possibly appear in a special issue of *Theoretical Computer Science* in 2018.

## 6.14. Formalized Meta-Theory of Simultaneous Substitutions

**Participant:** Kaustuv Chaudhuri.

It has long been claimed that a logical framework must have sophisticated built-in support for reasoning about formal substitutions in order to formalize relational meta-theorems such as strong normalization (using a logical relations style argument) or that applicative simulation is a pre-congruence. A number of type-theoretic frameworks in recent years, such as Beluga, have indeed started to incorporate such constructs in their core systems.

We have recently shown how to implement the meta-theory of simultaneous substitutions in the Abella system without any modification or extension of the (trusted) kernel, and without sacrificing any expressivity. The results of this paper will appear in the ACM Conference on Certified Programming in January 2018.

Our hope is that this work will be continued in the near future to build a specification language based on contextual LF in Abella, similar to how Abella/LF handles (ordinary) LF.

## 6.15. Hybrid Linear Logic Revisited

**Participants:** Kaustuv Chaudhuri, Joëlle Despeyroux, Carlos Olarte, Elaine Pimentel.

We have written a comprehensive account of hybrid linear logic (HyLL) and its relation to a number of related linear logic variants such as subexponential logic. One of the new and novel examples that we have fully worked out is how to encode CTL and CTL\* in HyLL, which shows that HyLL can indeed serve as a logical framework for representing and reasoning about constrained transition systems, such as biochemical networks.

This account will appear in a special issue of MSCS in 2018.

## 6.16. Correctness of Speculative Optimizations with Dynamic Deoptimization

**Participant:** Gabriel Scherer.

This joint work with Olivier Flückiger, Ming-Ho Yee Ming-Ho, Aviral Goel, Amal Ahmed and Jan Vitek was initiated during Gabriel Scherer's post-doctoral stay at Northeastern University, Boston, USA.

Practitioners from the software industry find it difficult to implement Just-In-Time (JIT) compilers for dynamic programming languages, such as Javascript: they don't know how to reason on the correctness of their optimizations in the context of Just-In-Time code generation and deoptimization. We explain how to adapt reasoning approaches and proof techniques from standard compiler research to this new setting.

This work [14] will appear in POPL 2018.

## SPECFUN Project-Team

## 6. New Results

### 6.1. Efficient Algorithms in Computer Algebra

This year has seen the end of the writing and the publication of a book on computer-algebra algorithms [8]. The course at Master 2 level *Algorithmes efficaces en calcul formel* is a course that Alin Bostan and Frédéric Chyzak have set up progressively since 2005 together with Marc Giusti (LIX), Bruno Salvy (today AriC), as well as, initially, Éric Schost (LIX at the time) and François Ollivier (LIX), and, more recently, Grégoire Lecerf (LIX). The course is very strongly focused to presenting the design of algorithms guided by complexity analysis, with the goal to lead the students to the understanding of all algorithmic aspects that are necessary to the “creative telescoping” used for symbolic computations of sums and integrals. Their lecture notes had been circulating in and used by the (French) computer-algebra community, while they long had the goal of turning them into a book. They could publish it in 2017 (686 pages), after a big finalization effort in 2016 and 2017. The first parts of the book present fast algorithms for basic objects (integers, polynomials, series, matrices, linear recurrences), insisting on general principles to design efficient algorithms. The next parts of the work build on them to address topics that have made recent progress: factorization of polynomials, algorithms for polynomial systems, definite summation and integration. The work [8] is online as a HAL collection<sup>0</sup>. It is available for free in pdf format and is otherwise sold at a very low price (via print-on-demand). Over the first three months after publication, the book has sold roughly 60 printed copies and the pdf has been downloaded 265 times.

### 6.2. Hypergeometric Expressions for Generating Functions of Walks with Small Steps in the Quarter Plane

In [2], Alin Bostan and Frédéric Chyzak, together with Mark van Hoeij (Florida State University), Manuel Kauers (Johannes Kepler University), and Lucien Pech, have studied nearest-neighbors walks on the two-dimensional square lattice, that is, models of walks on  $\mathbb{Z}^2$  defined by a fixed step set that consists of non-zero vectors with coordinates 0, 1 or  $-1$ . They concerned themselves with the enumeration of such walks starting at the origin and constrained to remain in the quarter plane  $\mathbb{N}^2$ , counted by their length and by the position of their ending point. In earlier works, Bousquet-Mélou and Mishna had identified 19 models of walks that possess a D-finite generating function, and linear differential equations had then been guessed in these cases by Bostan and Kauers. Here, we have given the first proof that these equations are indeed satisfied by the corresponding generating functions. As a first corollary, we have proved that all these 19 generating functions can be expressed in terms of Gauss’ hypergeometric functions, with specific parameters that relate them intimately to elliptic integrals. As a second corollary, we have shown that all the 19 generating functions are transcendental, and that among their  $19 \times 4$  combinatorially meaningful specializations only four are algebraic functions.

### 6.3. Multiple Binomial Sums

Multiple binomial sums form a large class of multi-indexed sequences, closed under partial summation, which contains most of the sequences obtained by multiple summation of products of binomial coefficients, as well as all the sequences with algebraic generating function. Alin Bostan and Pierre Lairez, together with Bruno Salvy (AriC), have studied in [7] the representation of the generating functions of binomial sums by integrals of rational functions. The outcome is twofold. Firstly, we have shown that a univariate sequence is a multiple binomial sum if and only if its generating function is the diagonal of a rational function. Secondly, we have proposed algorithms that decide the equality of multiple binomial sums and that compute recurrence relations for them. In conjunction with geometric simplifications of the integral representations, this approach behaves well in practice. The process avoids the computation of certificates and the problem of the appearance of spurious singularities that afflicts discrete creative telescoping, both in theory and in practice.

<sup>0</sup><https://hal.archives-ouvertes.fr/AECF/>

## 6.4. Algebraic Diagonals and Walks

The diagonal of a multivariate power series  $F$  is the univariate power series  $\text{Diag} F$  generated by the diagonal terms of  $F$ . Diagonals form an important class of power series; they occur frequently in number theory, theoretical physics and enumerative combinatorics. In [28], Alin Bostan and Louis Dumont, together with Bruno Salvy (AriC), have studied algorithmic questions related to diagonals in the case where  $F$  is the Taylor expansion of a bivariate rational function. It is classical that in this case  $\text{Diag} F$  is an algebraic function. They have proposed an algorithm for computing an annihilating polynomial of  $\text{Diag} F$ . They have given a precise bound on the size of this polynomial and show that generically, this polynomial is the minimal polynomial of  $\text{Diag} F$  and that its size reaches the bound. Their algorithm runs in time quasi-linear in this bound, which grows exponentially with the degree of the input rational function. They have also addressed the related problem of enumerating directed lattice walks. The insight given by their study has led to a new method for expanding the generating power series of bridges, excursions and meanders. They have shown that their first  $N$  terms can be computed in quasi-linear complexity in  $N$ , without first computing a very large polynomial equation. An extended version of this work has been presented in [4].

## 6.5. A Human Proof of the Gessel Conjecture

Counting lattice paths obeying various geometric constraints is a classical topic in combinatorics and probability theory. Many recent works deal with the enumeration of 2-dimensional walks with prescribed steps confined to the positive quadrant. A notoriously difficult case concerns the so-called *Gessel walks*: they are planar walks confined to the positive quarter plane, which move by unit steps in any of the West, North-East, East, and South-West directions. In 2001, Ira Gessel conjectured a closed-form expression for the number of such walks of a given length starting and ending at the origin. In 2008, Kauers, Koutschan and Zeilberger gave a computer-aided proof of this conjecture. The same year, Bostan and Kauers showed, using again computer algebra tools, that the trivariate generating function of Gessel walks is algebraic. This year, Alin Bostan, together with Irina Kurkova (Univ. Paris 6) and Kilian Raschel (CNRS and Univ. Tours), proposed in [6] the first “human proofs” of these results. They are derived from a new expression for the generating function of Gessel walks in terms of special functions.

## 6.6. Subresultants in Multiple Roots

In [3], we have provided explicit formulae for the coefficients of the order- $d$  polynomial subresultant of  $(x - \alpha)^m$  and  $(x - \beta)^n$  with respect to the set of Bernstein polynomials  $\{(x - \alpha)^j(x - \beta)^{d-j}, 0 \leq j \leq d\}$ . They are given by hypergeometric expressions arising from determinants of binomial Hankel matrices.

## 6.7. On Matrices with Displacement Structure: Generalized Operators and Faster Algorithms

For matrices with displacement structure, basic operations like multiplication, inversion, and linear-system solving can all be expressed in terms of a single task: evaluating the product  $AB$ , where  $A$  is a structured  $n \times n$  matrix of displacement rank  $\alpha$ , and  $B$  is an arbitrary  $n \times \alpha$  matrix. Given  $B$  and a so-called *generator* of  $A$ , this product is classically computed with a cost ranging from  $O(\alpha^2 M(n))$  to  $O(\alpha^2 M(n) \log(n))$  arithmetic operations, depending on the specific structure of  $A$ . (Here,  $M$  is a cost function for polynomial multiplication.) In [5], Alin Bostan, jointly with Claude-Pierre Jeannerod (AriC), Christophe Moulleron (ENSIIE), and Éric Schost (University of Waterloo), has generalized classical displacement operators, based on block diagonal matrices with companion diagonal blocks, and has also designed fast algorithms to perform the task above for this extended class of structured matrices. The cost of these algorithms ranges from  $O(\alpha^{\omega-1} M(n))$  to  $O(\alpha^{\omega-1} M(n) \log(n))$ , with  $\omega$  such that two  $n \times n$  matrices over a field can be multiplied using  $O(n^\omega)$  field operations. By combining this result with classical randomized regularization techniques, he has obtained faster Las Vegas algorithms for structured inversion and linear system solving.

## 6.8. Quasilinear Average Complexity for Solving Polynomial Systems

How many operations do we need on the average to compute an approximate root of a random Gaussian polynomial system? Beyond Smale's 17th problem that asked whether a polynomial bound is possible, Pierre Lairez has proved in [10] a quasi-optimal bound  $(\text{input size})^{1+o(1)}$ , which improves upon the previously known  $(\text{input size})^{3/2+o(1)}$  bound. His new algorithm relies on numerical continuation along *rigid continuation paths*. The central idea is to consider rigid motions of the equations rather than line segments in the linear space of all polynomial systems. This leads to a better average condition number and allows for bigger steps. He showed that on the average, one approximate root of a random Gaussian polynomial system of  $n$  equations of degree at most  $D$  in  $n + 1$  homogeneous variables can be computed with  $O(n^5 D^2)$  continuation steps. This is a decisive improvement over previous bounds, which prove no better than  $\sqrt{2}^{\min(n,D)}$  continuation steps on the average.

## 6.9. Computing the Homology of Basic Semialgebraic Sets in Weak Exponential Time

In [9], Pierre Lairez, jointly with Peter Bürgisser (TU Berlin) and Felipe Cucker (City University of Hong Kong), has described and analyzed an algorithm for computing the homology (Betti numbers and torsion coefficients) of basic semialgebraic sets. The algorithm works in weak exponential time, that is, out of a set of exponentially small measure in the space of data, the cost of the algorithm is exponential in the size of the data. All algorithms previously proposed for this problem have a complexity that is doubly exponential (and this is so for almost all data).

## 6.10. Formally Certified Computation of Improper Definite Integrals

Assia Mahboubi and Thomas Sibut-Pinote, in collaboration with Guillaume Melquiond (Toccata), have pursued their work on the certified computation of intervals approximating the values of definite integrals involving elementary mathematical functions. This library provides an automated tool that builds a formal proof of the correctness of the output, that is, a formal proof that the interval contains the mathematical values and a formal proof of the integrability of the input function on the input interval. This tool has been extended this year, and it can now deal with improper integrals, that is, integrals whose bounds are infinite or singularities of the integrand. The methodology, the implementation and benchmarks have been described in [13].

## 6.11. A Complete Formal Proof of the Irrationality of $\zeta(3)$

Assia Mahboubi and Thomas Sibut-Pinote have completed a formal proof of the irrationality of the constant  $\zeta(3)$ . The missing step in a previous work [32] with Frédéric Chyzak and Enrico Tassi was to obtain a formal proof of the asymptotic behaviour of the least common multiple of the first  $n$  integers. They have written a report on this work, which is included as a chapter in Thomas Sibut-Pinote's PhD manuscript.

## TOCCATA Project-Team

## 7. New Results

### 7.1. Deductive Verification

**Synthetic topology in HoTT for probabilistic programming.** F. Faissole and B. Spitters have developed a mathematical formalism based on synthetic topology and homotopy type theory to interpret probabilistic algorithms. They suggest to use proof assistants to prove such programs [39] [31]. They also have formalized synthetic topology in the Coq proof assistant using the HoTT library. It consists of a theory of lower reals, valuations and lower integrals. All the results are constructive. They apply their results to interpret probabilistic programs using a monadic approach [28].

**Defunctionalization for proving higher-order programs.** J.-C. Filliâtre and M. Pereira proposed a new approach to the verification of higher-order programs, using the technique of defunctionalization, that is, the translation of first-class functions into first-order values. This is an early experimental work, conducted on examples only within the Why3 system. This work was published at JFLA 2017 [29].

**Extracting Why3 programs to C programs.** R. Rieu-Helft, C. Marché, and G. Melquiond devised a simple memory model for representing C-like pointers in the Why3 system. This makes it possible to translate a small fragment of Why3 verified programs into idiomatic C code [30]. This extraction mechanism was used to turn a verified Why3 library of arbitrary-precision integer arithmetic into a C library that can be substituted to part of the GNU Multi-Precision (GMP) library [23].

**Verification of highly imperative OCaml programs with Why3** J.-C. Filliâtre, M. Pereira and S. Melo de Sousa proposed a new methodology for proving highly imperative OCaml programs with Why3. For a given OCaml program, a specific memory model is built and one checks a Why3 program that operates on it. Once the proof is complete, they use Why3's extraction mechanism to translate its programs to OCaml, while replacing the operations on the memory model with the corresponding operations on mutable types of OCaml. This method is evaluated on several examples that manipulate linked lists and mutable graphs [20].

### 7.2. Automated Reasoning

**A Three-tier Strategy for Reasoning about Floating-Point Numbers in SMT.** The SMT-LIB standard defines a formal semantics for a theory of floating-point (FP) arithmetic (FPA). This formalization reduces FP operations to reals by means of a rounding operator, as done in the IEEE-754 standard. Closely following this description, S. Conchon, M. Iguernlala, K. Ji, G. Melquiond and C. Fumex propose a three-tier strategy to reason about FPA in SMT solvers. The first layer is a purely axiomatic implementation of the automatable semantics of the SMT-LIB standard. It reasons with exceptional cases (e.g. overflows, division by zero, undefined operations) and reduces finite representable FP expressions to reals using the rounding operator. At the core of the strategy, a second layer handles a set of lemmas about the properties of rounding. For these lemmas to be used effectively, the instantiation mechanism of SMT solvers is extended to tightly cooperate with the third layer, the NRA engine of SMT solvers, which provides interval information. The strategy is implemented in the Alt-Ergo SMT solver and validated on a set of benchmarks coming from the SMT-LIB competition, and also from the deductive verification of C and Ada programs. The results show that the approach is promising and compete with existing techniques implemented in state-of-the-art SMT solvers. This work was presented at the CAV conference [18].



**Lightweight Approach for Declarative Proofs.** M. Clochard designed an extension of first-order logic, for describing reasoning steps needed to discharge a proof obligation. The extension is under the form of two new connectives, called proof indications, that allow the user to encode reasoning steps inside a logic formula. This extension makes possible to use the syntax of formulas as a proof language. The approach was presented at the JFLA conference [26] and implemented in Why3. It brings a lightweight mechanism for declarative proofs in an environment like Why3 where provers are used as black boxes. Moreover, this mechanism restricts the scope of auxiliary lemmas, reducing the size of proof obligations sent to external provers.

### 7.3. Certification of Algorithms, Languages, Tools and Systems

**Formalization and closedness of finite dimensional subspaces.** F. Faissole formalized a theory of finite dimensional subspaces of Hilbert spaces in order to apply the Lax-Milgram Theorem on such subspaces. He had to prove, in the Coq proof assistant, that finite dimensional subspaces of Hilbert spaces are closed in the context of general topology using filters [19]. He also formalized both finite dimensional modules and finite dimensional subspaces of modules. He compared the two formalizations and showed a complementarity between them. He proved that the product of two finite dimensional modules is a finite dimensional module [27].

**Verified numerical approximations of improper definite integrals.** The CoqInterval library provides some tactics for computing and formally verifying numerical approximations of real-valued expressions inside the Coq system. In particular, it is able to compute reliable bounds on proper definite integrals [111]. A. Mahboubi, G. Melquiond, and T. Sibut-Pinote extended these algorithms to also cover some improper integrals, e.g., those with an unbounded integration domain [40]. This makes CoqInterval one of the very few tools able to produce reliable results for improper integrals, be they formally verified or not.

**A Coq Formal Proof of the Lax–Milgram theorem.** S. Boldo, F. Clément, F. Faissole, V. Martin, and M. Mayero worked on a Coq formal proof of the Lax–Milgram theorem. It is one of the theoretical cornerstone for the correctness of the Finite Element Method. It required many results from linear algebra, geometry, functional analysis, and Hilbert spaces [13] [24].

**Formalization of numerical filters** S. Boldo, D. Gallois-Wong, and T. Hilaire developed a formalization in the Coq proof assistant of numerical filters. It includes equivalences between several expressions and the formal proof of the Worst-Case Peak Gain Theorem to bound the magnitude of the outputs (and every intern variable) of stable filters.

**A Verified OCaml Library.** Abstract Libraries are the basic building blocks of any realistic programming project. It is thus of utmost interest for a programmer to build her software on top of bug-free libraries. At the ML family workshop [38], A. Charguéraud, J.-C. Filliâtre, M. Pereira and F. Pottier presented the ongoing VOCAL project, which aims at building a mechanically verified library of general-purpose data structures and algorithms, written in the OCaml language. A key ingredient of VOCAL is the design of a specification language for OCaml, independently of any verification tool.

**Formal Analysis of shell scripts.** The shell language is widely used for various system administration tasks on UNIX machines. The CoLiS project aims at applying formal methods for verifying scripts used for installation of packages of software distributions. The syntax and semantics of shell are particularly treacherous. They proposed a new language called CoLiS which, on the one hand, has well-defined static semantics and avoids some of the pitfalls of the shell, and, on the other hand, is close enough to the shell to be the target of an automated translation of the scripts in our corpus. In collaboration with N. Jeannerod and R. Treinen, C. Marché formalized the syntax and semantics of CoLiS in Why3, defined an interpreter for the language in the WhyML programming language, and present an automated proof in the Why3 proof environment of soundness and completeness of this interpreter with respect to the formal semantics [22]. The development is available in Toccata's gallery [http://toccata.lri.fr/gallery/colis\\_interpreter.en.html](http://toccata.lri.fr/gallery/colis_interpreter.en.html). This formalized interpreter is extracted to OCaml and the verified code is integrated into a prototype software toolset developed by I. Dami and C. Marché [36].

**A verified yet efficient arbitrary-precision integer library.** R. Rieu-Helft used the Why3 system to implement, specify, and verify a library of arbitrary-precision integer arithmetic: comparison, addition, multiplication, shifts, division. A lot of efforts were put into replicating and verifying the numerous implementation tricks the GMP library uses to achieve state-of-the-art performances, especially for the division algorithm. While the resulting library is nowhere near as fast as the hand-written assembly code GMP uses, it is competitive with the generic C code of GMP for small integers (i.e., mini-GMP) [23]. The development is available in Toccata's gallery <http://toccata.lri.fr/gallery/multiprecision.en.html>.

**Case study: algorithms for matrix multiplication.** M. Clochard, L. Gondelman and M. Pereira worked on a case study about matrix multiplication. Two variants for the multiplication of matrices are proved: a naive version using three nested loops and Strassen's algorithm. To formally specify the two multiplication algorithms, they developed a new Why3 theory of matrices, and they applied a reflection methodology to conduct some of the proofs. A first version of this work was presented at the VSTTE Conference in 2016 [78]. An extended version that considers arbitrary rectangular matrices instead of square ones is published in the Journal of Automated Reasoning [12]. The development is available in Toccata's gallery [http://toccata.lri.fr/gallery/verifythis\\_2016\\_matrix\\_multiplication.en.html](http://toccata.lri.fr/gallery/verifythis_2016_matrix_multiplication.en.html).

**Case studies: Strongly Connected Components in Directed Graphs** As part of a larger set of case studies on algorithms on graphs <http://pauillac.inria.fr/~levy/why3/>, R. Chen and J.-J. Lévy work on formal verification of algorithms for computing strongly connected components of directed graphs. The formal proofs are conducted using Why3. The formal proof of Tarjan's algorithm was presented at the French-speaking symposium JFLA 2017 [25] and then at the VSTTE 2017 international conference [17]

**A Formally Proved, Complete Algorithm for Path Resolution with Symbolic Links** In the context of file systems like those of Unix, path resolution is the operation that given a character string denoting an access path, determines the target object (a file, a directory, etc.) designated by this path. This operation is not trivial because of the presence of symbolic links. Indeed, the presence of such links may induce infinite loops in the resolution process. R. Chen, M. Clochard and C. Marché consider a path resolution algorithm that always terminates, detecting if it enters an infinite loop and reports a resolution failure in such a case. They propose a formal specification of path resolution and they formally prove that their algorithm terminates on any input, and is correct and complete with respect to this formal specification. [11]. The development is available in Toccata's gallery [http://toccata.lri.fr/gallery/path\\_resolution.en.html](http://toccata.lri.fr/gallery/path_resolution.en.html).

## 7.4. Floating-Point and Numerical Programs

### Computer Arithmetic and Formal Proofs: Verifying Floating-point Algorithms with the Coq System

S. Boldo and G. Melquiond published a book that provides a comprehensive view of how to formally specify and verify tricky floating-point algorithms with the Coq proof assistant. It describes the Flocq formalization of floating-point arithmetic and some methods to automate theorem proofs. It then presents the specification and verification of various algorithms, from error-free transformations to a numerical scheme for a partial differential equation. The examples cover not only mathematical algorithms but also C programs as well as issues related to compilation [32].

**Automating the Verification of Floating-Point Programs.** The level of proof success and proof automation highly depends on the way the floating-point operations are interpreted in the logic supported by back-end provers. C. Fumex, C. Marché and Y. Moy addressed this challenge by combining multiple techniques to separately prove different parts of the desired properties. They use abstract interpretation to compute numerical bounds of expressions, and use multiple automated provers, relying on different strategies for representing floating-point computations. One of these strategies is based on the native support for floating-point arithmetic recently added in the SMT-LIB standard. The approach is implemented in the Why3 environment and its front-end SPARK 2014.



It is validated experimentally on several examples originating from industrial use of SPARK 2014 [37], [21].

**Round-off Error Analysis of Explicit One-Step Numerical Integration Methods.** S. Boldo, A. Chapoutot, and F. Faissolle provided bounds on the round-off errors of explicit one-step numerical integration methods, such as Runge-Kutta methods. They developed a fine-grained analysis that takes advantage of the linear stability of the scheme, a mathematical property that vouches the scheme is well-behaved [14].

**Robustness of 2Sum and Fast2Sum.** S. Boldo, S. Graillat, and J.-M. Muller worked on the 2Sum and Fast2Sum algorithms, that are important building blocks in numerical computing. They are used (implicitly or explicitly) in many compensated algorithms or for manipulating floating-point expansions. They showed that these algorithms are much more robust than it is usually believed: the returned result makes sense even when the rounding function is not round-to-nearest, and they are almost immune to overflow [10].

**Formal Verification of a Floating-Point Expansion Renormalization Algorithm.** Many numerical problems require a higher computing precision than the one offered by standard floating-point formats. A common way of extending the precision is to use floating-point expansions. S. Boldo, M. Joldes, J.-M. Muller, and V. Popescu proved one of the algorithms used as a basic brick when computing with floating-point expansions: renormalization that “compresses” an expansion [15].

## COMMANDS Project-Team

## 7. New Results

### 7.1. Deterministic Optimal Control

#### 7.1.1. *Galerkin approximations of nonlinear optimal control problems in Hilbert spaces*

**Participant:** Axel Kroner.

With Mickaël D. Chekroun (UCLA), and Honghu Liu (Virginia Tech). Nonlinear optimal control problems in Hilbert spaces are considered for which we derive approximation theorems for Galerkin approximations. Approximation theorems are available in the literature. The originality of our approach relies on the identification of a set of natural assumptions that allows us to deal with a broad class of nonlinear evolution equations and cost functionals for which we derive convergence of the value functions associated with the optimal control problem of the Galerkin approximations. This convergence result holds for a broad class of nonlinear control strategies as well. In particular, we show that the framework applies to the optimal control of semilinear heat equations posed on a general compact manifold without boundary. The framework is then shown to apply to geoengineering and mitigation of greenhouse gas emissions formulated for the first time in terms of optimal control of energy balance climate models posed on the sphere  $S^2$ . See [12].

#### 7.1.2. *Galerkin approximations for the optimal control of nonlinear delay differential equations*

**Participant:** Axel Kroner.

With Mickaël D. Chekroun (UCLA), and Honghu Liu (Virginia Tech).

Optimal control problems of nonlinear delay differential equations (DDEs) are considered for which we propose a general Galerkin approximation scheme built from Koornwinder polynomials. Error estimates for the resulting Galerkin-Koornwinder approximations to the optimal control and the value function, are derived for a broad class of cost function-als and nonlinear DDEs. The approach is illustrated on a delayed logistic equation set not far away from its Hopf bifurcation point in the parameter space. In this case, we show that low-dimensional controls for a standard quadratic cost functional can be efficiently computed from Galerkin-Koornwinder approximations to reduce at a nearly optimal cost the oscillation amplitude displayed by the DDE's solution. Optimal controls computed from the Pontryagin's maximum principle (PMP) and the Hamilton-Jacobi-Bellman equation (HJB) associated with the corresponding ODE systems, are shown to provide numerical solutions in good agreement. It is finally argued that the value function computed from the corresponding reduced HJB equation provides a good approximation of that obtained from the full HJB equation. See [16].

### 7.2. Stochastic Control

#### 7.2.1. *On the time discretization of stochastic optimal control problems: the dynamic programming approach*

**Participant:** Frederic Bonnans.

With Justina Gianatti (U. Rosario) and Francisco J. Silva (U. Limoges) In this work we consider the time discretization of stochastic optimal control problems. Under general assumptions on the data, we prove the convergence of the value functions associated with the discrete time problems to the value function of the original problem. Moreover, we prove that any sequence of optimal solutions of discrete problems is minimizing for the continuous one. As a consequence of the Dynamic Programming Principle for the discrete problems, the minimizing sequence can be taken in discrete time feedback form. See [17].

### 7.2.2. *Variational analysis for options with stochastic volatility and multiple factors*

**Participants:** Frederic Bonnans, Axel Kroner.

We perform a variational analysis for a class of European or American options with stochastic volatility models, including those of Heston and Achdou-Tchou. Taking into account partial correlations and the presence of multiple factors, we obtain the well-posedness of the related partial differential equations, in some weighted Sobolev spaces. This involves a generalization of the commutator analysis introduced by Achdou and Tchou. See [18].

### 7.2.3. *Infinite Horizon Stochastic Optimal Control Problems with Running Maximum Cost*

**Participant:** Axel Kroner.

With Athena Picarelli (U. Oxford) and Hasna Zidani (ENSTA).

An infinite horizon stochastic optimal control problem with running maximum cost is considered. The value function is characterized as the viscosity solution of a second-order HJB equation with mixed boundary condition. A general numerical scheme is proposed and convergence is established under the assumptions of consistency, monotonicity and stability of the scheme. A convergent semi-Lagrangian scheme is presented in detail. See [19].

## 7.3. Applications

### 7.3.1. *On the Design of Optimal Health Insurance Contracts under Ex Post Moral Hazard*

**Participant:** Pierre Martinon.

With Pierre Picard and Anasuya Raj (Ecole Polytechnique, Econ. dpt).

We analyze in [20] the design of optimal medical insurance under ex post moral hazard, i.e., when illness severity cannot be observed by insurers and policyholders decide on their health expenditures. We characterize the trade-off between ex ante risk sharing and ex post incentive compatibility, in an optimal revelation mechanism under hidden information and risk aversion.

We establish that the optimal contract provides partial insurance at the margin, with a deductible when insurers rates are affected by a positive loading, and that it may also include an upper limit on coverage. We show that the potential to audit the health state leads to an upper limit on out-of-pocket expenses. Numerical simulations indicate that these qualitative results tend to be robust with respect to the health parameter.

## DEFI Project-Team

## 6. New Results

### 6.1. Methods for inverse problems

#### 6.1.1. *The Generalized Linear Sampling Method for limited aperture measurements*

L. Audibert and H. Haddar

We extend the so-called Generalized Linear Sampling Method (GLSM) to the case of limited aperture data at a fixed frequency. In this case the factorization of the sampling operator does not obey the symmetry required in the justification of the GLSM introduced in Audibert-Haddar [Inverse Problems, 2014]. We propose a new formulation by adding an extra penalty term that asymptotically correct the non symmetry of the GLSM original penalty term. The analysis of the new formulation is first presented in an abstract framework. We then show how to apply our setting to the scalar problem with far field measurements or near field measurements on a limited aperture. We finally validate the method through some numerical tests in two dimensions and for far field measurements.

#### 6.1.2. *A synoptic approach to the seismic sensing of heterogeneous fractures: from geometric reconstruction to interfacial characterization*

B. Guzina, H. Haddar and F. Pourahmadian

A non-iterative waveform sensing approach is proposed toward (i) geometric reconstruction of penetrable fractures, and (ii) quantitative identification of their heterogeneous contact condition by seismic i.e. elastic waves. To this end, the fracture support  $\Gamma$  (which may be non-planar and unconnected) is first recovered without prior knowledge of the interfacial condition by way of the recently established approaches to non-iterative waveform tomography of heterogeneous fractures, e.g. the methods of generalized linear sampling and topological sensitivity. Given suitable approximation  $\tilde{\Gamma}$  of the fracture geometry, the jump in the displacement field across  $\tilde{\Gamma}$  i.e. the fracture opening displacement (FOD) profile is computed from remote sensory data via a regularized inversion of the boundary integral representation mapping the FOD to remote observations of the scattered field. Thus obtained FOD is then used as input for solving the traction boundary integral equation on  $\tilde{\Gamma}$  for the unknown (linearized) contact parameters. In this study, linear and possibly dissipative interactions between the two faces of a fracture are parameterized in terms of a symmetric, complex-valued matrix  $K$  collecting the normal, shear, and mixed-mode coefficients of specific stiffness. To facilitate the high-fidelity inversion for  $K$ , a 3-step regularization algorithm is devised to minimize the errors stemming from the inexact geometric reconstruction and FOD recovery. The performance of the inverse solution is illustrated by a set of numerical experiments where a cylindrical fracture, endowed with two example patterns of specific stiffness coefficients, is illuminated by plane waves and reconstructed in terms of its geometry and heterogeneous (dissipative) contact condition.

#### 6.1.3. *Sampling methods for reconstructing the geometry of a local perturbation in unknown periodic layers*

H. Haddar and T.P Nguyen

The aim of this work is the design and analysis of sampling methods to reconstruct the shape of a local perturbation in a periodic layer from measurements of scattered waves at a fixed frequency. We first introduce the model problem that corresponds with the semi-discretized version of the continuous model with respect to the Floquet-Bloch variable. We then present the inverse problem setting where (propagative and evanescent) plane waves are used to illuminate the structure and measurements of the scattered wave at a parallel plane to the periodicity directions are performed. We introduce the near field operator and analyze two possible factorizations of this operator. We then establish sampling methods to identify the defect and the periodic

background geometry from this operator measurement. We also show how one can recover the geometry of the background independently from the defect. We then introduce and analyze the single Floquet-Bloch mode measurement operators and show how one can exploit them to build an indicator function of the defect independently from the background geometry. Numerical validating results are provided for simple and complex backgrounds.

#### **6.1.4. Nanoparticles volume determination from SAXS measurements**

M. Bakry and H. Haddar

The aim of this work is to develop a fully automatic method for the reconstruction of the volume distribution of polydisperse non-interacting nanoparticles with identical shapes from Small Angle X-ray Scattering measurements. In the case of diluted systems we proposed a method that solves a maximum likelihood problem with a positivity constraint on the solution by means of an Expectation Maximization iterative scheme coupled with a robust stopping criterion. We prove that the stopping rule provides a regularization method according to an innovative notion of regularization specifically defined for inverse problems with Poisson data. Such a regularization, together with the positivity constraint results in high fidelity quantitative reconstructions of particle volume distributions making the method particularly effective in real applications. We tested the performance of the method on synthetic data in the case of uni- and bi-modal particle volume distributions. We extended the method to the case of dense solutions where the inverse problem becomes non linear. The development of this research topic is ongoing under the framework of Saxsize.

#### **6.1.5. Identification of small objects with near-field data in quasi-backscattering configurations**

H. Haddar and M. Lakhali

We present a new sampling method for detecting targets (small inclusions or defects) immersed in a homogeneous medium in three-dimensional space, from measurements of acoustic scattered fields created by point source incident waves. We consider the harmonic regime and a data setting that corresponds with quasi-backscattering configuration: the data is collected by a set of receivers that are distributed on a segment centered at the source position and the device is swept along a path orthogonal to the receiver line. We assume that the aperture of the receivers is small compared with the distance to the targets. Considering the asymptotic form of the scattered field as the size of the targets goes to zero and the small aperture approximation, one is able to derive a special expression for the scattered field. In this expression a separation of the dependence of scattered field on the source location and the distance source-target is performed. This allows us to propose a sampling procedure that characterizes the targets location in terms of the range of a near-field operator constructed from available data. Our procedure is similar to the one proposed by Haddar-Rezac for far-field configurations. The reconstruction algorithm is based on the MUSIC (Multiple Signal Classification) algorithm.

### **6.2. Invisiblity and transmission eigenvalues**

#### **6.2.1. Trapped modes and reflectionless modes as eigenfunctions of the same spectral problem**

A.-S. Bonnet-Ben Dhia, L. Chesnel and V. Pagneux

We consider the reflection-transmission problem in a waveguide with obstacle. At certain frequencies, for some incident waves, intensity is perfectly transmitted and the reflected field decays exponentially at infinity. We show that such reflectionless modes can be characterized as eigenfunctions of an original non-selfadjoint spectral problem. In order to select ingoing waves on one side of the obstacle and outgoing waves on the other side, we use complex scalings (or Perfectly Matched Layers) with imaginary parts of different signs. We prove that the real eigenvalues of the obtained spectrum correspond either to trapped modes (or bound states in the continuum) or to reflectionless modes. Interestingly, complex eigenvalues also contain useful information on weak reflection cases. When the geometry has certain symmetries, the new spectral problem enters the class of  $\mathcal{PT}$ -symmetric problems.

### 6.2.2. *Transmission eigenvalues with artificial background for explicit material index identification*

L. Audibert, L. Chesnel and H. Haddar

We are interested in the problem of retrieving information on the refractive index  $n$  of a penetrable inclusion embedded in a reference medium from farfield data associated with incident plane waves. Our approach relies on the use of transmission eigenvalues (TEs) that carry information on  $n$  and that can be determined from the knowledge of the farfield operator  $F$ . We explain how to modify  $F$  into a farfield operator  $F^a = F - \tilde{F}$ , where  $\tilde{F}$  is computed numerically, corresponding to well chosen artificial background and for which the associated TEs provide more accessible information on  $n$ .

### 6.2.3. *Simple examples of perfectly invisible and trapped modes in waveguides*

L. Chesnel and V. Pagneux

We consider the propagation of waves in a waveguide with Neumann boundary conditions. We work at low wavenumber focusing our attention on the monomode regime. We assume that the waveguide is symmetric with respect to an axis orthogonal to the longitudinal direction and is endowed with a branch of height  $L$  whose width coincides with the wavelength of the propagating modes. In this setting, tuning the parameter  $L$ , we prove the existence of simple geometries where the transmission coefficient is equal to one (perfect invisibility). We also show that these geometries, for possibly different values of  $L$ , support so called trapped modes (non zero solutions of finite energy of the homogeneous problem) associated with eigenvalues embedded in the continuous spectrum.

### 6.2.4. *Invisibility and perfect reflectivity in waveguides with finite length branches*

L. Chesnel, S.A. Nazarov and V. Pagneux

We consider a time-harmonic wave problem, appearing for example in water-waves theory, in acoustics or in electromagnetism, in a setting such that the analysis reduces to the study of a 2D waveguide problem with a Neumann boundary condition. The geometry is symmetric with respect to an axis orthogonal to the direction of propagation of waves. Moreover, the waveguide contains one branch of finite length. We analyse the behaviour of the complex scattering coefficients  $\mathcal{R}$ ,  $\mathcal{T}$  as the length of the branch increases and we exhibit situations where non reflectivity ( $\mathcal{R} = 0$ ,  $|\mathcal{T}| = 1$ ), perfect reflectivity ( $|\mathcal{R}| = 1$ ,  $\mathcal{T} = 0$ ) or perfect invisibility ( $\mathcal{R} = 0$ ,  $\mathcal{T} = 1$ ) hold. Numerical experiments illustrate the different results.

### 6.2.5. *Invisibility in scattering theory*

L. Chesnel, A.-S. Bonnet-Ben Dhia and S.A. Nazarov

We are interested in a time harmonic acoustic problem in a waveguide with locally perturbed sound hard walls. We consider a setting where an observer generates incident plane waves at  $-\infty$  and probes the resulting scattered field at  $-\infty$  and  $+\infty$ . Practically, this is equivalent to measure the reflection and transmission coefficients respectively denoted  $R$  and  $T$ . In a recent work, a technique has been proposed to construct waveguides with smooth walls such that  $R = 0$  and  $|T| = 1$  (non reflection). However the approach fails to ensure  $T = 1$  (perfect transmission without phase shift). First we establish a result explaining this observation. More precisely, we prove that for wavenumbers smaller than a given bound  $k_{\star}$  depending on the geometry, we cannot have  $T = 1$  so that the observer can detect the presence of the defect if he/she is able to measure the phase at  $+\infty$ . In particular, if the perturbation is smooth and small (in amplitude and in width),  $k_{\star}$  is very close to the threshold wavenumber. Then, in a second step, we change the point of view and, for a given wavenumber, working with singular perturbations of the domain, we show how to obtain  $T = 1$ . In this case, the scattered field is exponentially decaying both at  $-\infty$  and  $+\infty$ . We implement numerically the method to provide examples of such undetectable defects.

### 6.2.6. *New sets of eigenvalues in inverse scattering for inhomogeneous media and their determination from scattering data*

F. Cakoni, H. Haddar and L. Audibert

We developed a general mathematical framework to determine interior eigenvalues from a knowledge of the modified far field operator associated with an unknown (anisotropic) inhomogeneity. The modified far field operator is obtained by subtracting from the measured far field operator the computed far field operator corresponding to a well-posed scattering problem depending on one (possibly complex) parameter. Injectivity of this modified far field operator is related to an appropriate eigenvalue problem whose eigenvalues can be determined from the scattering data, and thus can be used to obtain information about material properties of the unknown inhomogeneity. We discuss here two examples of such modification leading to a Steklov eigenvalue problem, and a new type of the transmission eigenvalue problem. We present some numerical examples demonstrating the viability of our method for determining the interior eigenvalues from far field data.

### ***6.2.7. The Asymptotic of Transmission Eigenvalues for a Domain with a Thin Coating***

H. Boujlida, H Haddar and M. Khenissi

We consider the transmission eigenvalue problem for a medium surrounded by a thin layer of inhomogeneous material with different refractive index. We derive explicit asymptotic expansion for the transmission eigenvalues with respect to the thickness of the thin layer. We prove error estimate for the asymptotic expansion up to order 1 for simple eigenvalues. This expansion can be used to obtain explicit expressions for constant index of refraction.

## **6.3. Shape and topology optimization**

### ***6.3.1. Structural optimization under overhang constraints imposed by additive manufacturing technologies***

G. Allaire, C. Dapogny, R. Estevez, A. Faure and G. Michailidis.

This work addresses one of the major constraints imposed by additive manufacturing processes on shape optimization problems - that of overhangs, i.e. large regions hanging over void without sufficient support from the lower structure. After revisiting the ‘classical’ geometric criteria used in the literature, based on the angle between the structural boundary and the build direction, we propose a new mechanical constraint functional, which mimics the layer by layer construction process featured by additive manufacturing technologies, and thereby appeals to the physical origin of the difficulties caused by overhangs. This constraint, as well as some variants, are precisely defined; their shape derivatives are computed in the sense of Hadamard’s method, and numerical strategies are extensively discussed, in two and three space dimensions, to efficiently deal with the appearance of overhang features in the course of shape optimization processes.

### ***6.3.2. Shape optimisation with the level set method for contact problems in linearised elasticity***

G. Allaire, F. Jouve and A. Maury

This work is devoted to shape optimisation of contact problems in linearised elasticity, thanks to the level set method. We circumvent the shape non-differentiability, due to the contact boundary conditions, by using penalised and regularised versions of the mechanical problem. This approach is applied to five different contact models: the frictionless model, the Tresca model, the Coulomb model, the normal compliance model and the Norton-Hoff model. We consider two types of optimisation problems in our applications: first, we minimise volume under a compliance constraint, second, we optimise the normal force, with a volume constraint, which is useful to design compliant mechanisms. To illustrate the validity of the method, 2D and 3D examples are performed, the 3D examples being computed with an industrial software.

### ***6.3.3. Elasto-plastic shape optimization using the level set method***

G. Allaire, F. Jouve and A. Maury



This work is concerned with shape optimization of structures made of a material obeying Hencky's laws of plasticity, with the stress bound expressed by the von Mises effective stress. The ill-posedness of the model is circumvented by using two regularized versions of the mechanical problem. The first one is the classical Perzyna formulation which is regularized, the second one is a new regularized formulation proposed for the von Mises criterion. Shape gradients are calculated thanks to the adjoint method. The optimal shape is numerically computed by using the level set method. To illustrate the validity of the method, 2D examples are performed.

## 6.4. Numerical methods for wave problems

### 6.4.1. Finite element methods for eigenvalue problems with sign-changing coefficients

C. Carvalho, P. Ciarlet and L. Chesnel

We consider a class of eigenvalue problems involving coefficients changing sign on the domain of interest. We analyse the main spectral properties of these problems according to the features of the coefficients. Under some assumptions on the mesh, we study how one can use classical finite element methods to approximate the spectrum as well as the eigenfunctions while avoiding spurious modes. We also prove localisation results of the eigenfunctions for certain sets of coefficients.

### 6.4.2. Linearized Navier-Stokes equations for Aeroacoustics using Stabilized Finite Elements : Boundary Conditions and Industrial Application to Aft-Fan Noise Propagation.

A. Bissuel, G. Allaire, L. Daumas, S., Barré and F. Rey

A numerical method for solving the linearized Navier-Stokes equations is presented for aeroacoustic sound propagation problem. The Navier-Stokes equations are linearized in the frequency domain. The fan noise of jet engine is emitted nearly selectively on some frequencies, which depend on the rotation velocity of the fan. A frequency domain approach is highly suitable for this kind of problems, instead of a costly time-dependent simulation which can handle a large range of frequencies depending on the time step and the mesh. The calculations presented here were all made using Aether, a Navier-Stokes code which uses finite elements stabilized with SUPG (Streamline Upwind Galerkin). Automatic code differentiation was used to linearize this code. Entropy variables bring interesting mathematical properties to the numerical scheme, but also prevent the easy implementation of boundary conditions. For instance, the pressure is a non-linear combination of the entropy variables. Imposing a pressure variation needs a linearization of this relation which is detailed herein. The performance of different types of boundary conditions used to impose the acoustic pressure variation inside the engine is studied in detail. Finally, a very surprising effect of the SUPG scheme was to transform a homogeneous Dirichlet boundary condition on all variables to a transparent one which is able to let only outgoing waves pass through with no incoming wave. A one-dimensional toy model is given to explain how SUPG brings about this transformation.

We finally treated an industrial test case. The geometry of a model turbine from the Clean Sky European project was used for sound propagation of the fan exhaust noise of a jet engine. Computations on several modes with increasing complexities were done and the results compared to a boundary element method which served as a reference when no mean flow is present. Results of a computation with a mean flow are shown.

## 6.5. Diffusion MRI

J.R. Li, K. V. Nguyen and I. Mekkaoui

Diffusion Magnetic Resonance Imaging (DMRI) is a promising tool to obtain useful information on microscopic structure and has been extensively applied to biological tissues.

We obtained the following results.

- The Bloch-Torrey equation describes the evolution of the spin (usually water proton) magnetization under the influence of applied magnetic field gradients and is commonly used in numerical simulations for diffusion MRI and NMR. Microscopic heterogeneity inside the imaging voxel is modeled by interfaces inside the simulation domain, where a discontinuity in the magnetization across the interfaces is produced via a permeability coefficient on the interfaces. To avoid having to simulate on a computational domain that is the size of an entire imaging voxel, which is often much larger than the scale of the microscopic heterogeneity as well as the mean spin diffusion displacement, smaller representative volumes of the imaging medium can be used as the simulation domain. In this case, the exterior boundaries of a representative volume either must be far away from the initial positions of the spins or suitable boundary conditions must be found to allow the movement of spins across these exterior boundaries.

Many approaches have been taken to solve the Bloch-Torrey equation but an efficient high performance computing framework is still missing. We present formulations of the interface as well as the exterior boundary conditions that are computationally efficient and suitable for arbitrary order finite elements and parallelization. In particular, the formulations use extended finite elements with weak enforcement of real (in the case of interior interfaces) and artificial (in the case of exterior boundaries) permeability conditions as well as operator splitting for the exterior boundary conditions. The method is straightforward to implement and it is available in the FEniCS for moderate-scale simulations and in the FEniCS-HPC for large-scale simulations.

- The nerve cells of the *Aplysia* are much larger than mammalian neurons. Using the *Aplysia* ganglia to study the relationship between the cellular structure and the diffusion MRI signal can potentially shed light on this relationship for more complex organisms. We measured the dMRI signal of chemically-fixed abdominal ganglia of the *Aplysia* at several diffusion times. At the diffusion times measured, the dMRI signal is mono-exponential and can be accurately represented by the parameter ADC.

We analyzed the diffusion time-dependent ADC using a well-known analytical formula that is valid in the short diffusion time regime. We performed this analysis for the largest sized cells of the ganglia to satisfy the short diffusion time requirement. We noted that a naive application of the short time formula is not adequate because of the presence of the cell nucleus, making the effective cell size much smaller than the actual cell size.

We went on to perform numerical simulation of the ADC for several cell types of the abdominal ganglia. To create the simulation geometries, for the largest cells, we segmented a high resolution T2-weighted images and incorporated a manually generated nucleus. For small cells and nerve cells, we created spherical and cylindrical geometrical domains that are consistent with known information about the cellular structures from the literature. Using the library of simulation results, we fitted for the intrinsic diffusivities of the small cells and the nerve cells.

- We participated in providing simulation results for the Parietal team in their work on sensing Spindle Neurons in the Insula with Multi-shell Diffusion MRI.
- We started a new direction in the simulation and modeling of heart diffusion MRI with the post-doc project of Imen Mekkaoui, funded by Inria-EPFL lab. The project is co-supervised with Jan Hesthaven, Chair of Computational Mathematics and Simulation Science (MCSS), EPFL.

## 6.6. Mathematical tools for Psychology

J. R. Li and J. Hao

This is the start of a collaborative effort between the Defi team and the mental health professionals at the centre hospitalier Sainte Anne and l'Université Paris Diderot.

- We started a new research direction in algorithm and software development for analysis and classification of EEG measurements during the administration of neuropsychological tests for AD/HD with the PhD project of Jingjing Hao, co-supervised with Dr. Hassan Rahioui, Chef du pôle psychiatrique du 7e arrondissement de Paris rattaché au centre hospitalier Sainte-Anne.

## DISCO Project-Team

## 7. New Results

### 7.1. Maximal-multiplicity-based rightmost-root assignment for retarded TDS

**Participants:** Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [L2S], Hakki Unal [Anadolu University], Toma Vyhlidal [Czech Technical University].

The proposed approach is a stabilizing delayed state-feedback design guaranteeing an appropriate (admissible) convergence rate to the trivial solution of the controlled dynamical system. Unlike methods based on finite spectrum assignment, our method does not render the closed loop system finite dimensional but consists in controlling its rightmost spectral value. First, it consists in characterizing the root of the characteristic quasipolynomial function to be of maximal multiplicity by mean of an analytical necessary and sufficient condition. Then, conditions on such a root (of maximal multiplicity) to be stable and dominant are established. These results are obtained for reduced-orders time-delay system (scalar and quadratic cases), see [69].

### 7.2. Migration of multiple roots under parameters/delays perturbation

**Participants:** Islam Boussaada, Dina Irofti, Silviu-Iulian Niculescu, Wim Michiels [KU Leuven].

In the context of the perturbation theory of nonlinear eigenvalue problem, the sensitivity of multiple eigenvalues with respect to parameters' variations is studied. In the complete regular splitting case, explicit expressions for the leading coefficients of the Puiseux series of the eigenvalue are provided [22]. In contrast to existing analysis of multiple roots of delay equations the developed results are in a matrix framework, i.e., without reduction of the problem to the analysis of a scalar characteristic quasipolynomial.

### 7.3. A generalized $\tau$ —decomposition for TDS with delay-dependent coefficients

**Participants:** Chi Jin [L2S], Keqin Gu [Illinois State University], Islam Boussaada, Silviu-Iulian Niculescu.

The standard frequency domain approaches for Time-delay systems analysis do not apply when the coefficients of the system are delay-dependent. Given a system with delay-dependent coefficients as well as a delay interval of interest, a method is proposed to find all the delay subintervals guaranteeing the asymptotic stability of the trivial solution. The crossing direction criteria is proposed which can be clearly interpreted from a geometrical two-parameter perspective [36], [52].

### 7.4. State and Output-feedback control design for (possibly fractional) time-delay systems

**Participants:** Catherine Bonnet, Caetano Cardeliquio, André Fioravanti [FEM-UNICAMP, Brazil].

We obtained this year new results for  $H_\infty$ -control synthesis via output-feedback through a finite order LTI system, called comparison system [42].

We also generalised those results for fractional systems.

The fractional comparison system was obtained and through LMIs we were able to calculate the  $H_\infty$ -norm for the fractional system and design a state-feedback control through the comparison system approach.

### 7.5. Stability and Stabilisability Through Envelopes for Retarded and Neutral Time-Delay Systems

**Participants:** Catherine Bonnet, Caetano Cardeliquio, Silviu Niculescu, André Fioravanti [FEM-UNICAMP, Brazil].

We presented a new approach to develop an envelope that engulfs all poles of a time-delay system.

Through LMIs we determined envelopes for retarded and neutral time-delay systems.

The envelopes proposed were not only tighter than the ones in the literature but they can also be applied to verify the stability of the system.

The approach was also used to design state-feedback controllers which cope with design requirements regarding  $\alpha$  – stability.

## 7.6. Backstepping with artificial delays

**Participants:** Frederic Mazenc, Michael Malisoff [LSU, USA], Laurent Burlion [ONERA], Victor Gibert [Airbus], Jerome Weston [LSU, USA].

We worked on the problem of improving a fundamental control design technique called backstepping.

We provided in [54] a new backstepping control design for time-varying systems with input delays. The result was obtained by the introduction of a constant 'artificial' pointwise delay in the input and a dynamic extension. Thus it is significantly different from backstepping results for systems with delay in the input as presented in previous contributions. The result in [54] ensures global asymptotic convergence for a broad class of partially linear systems with an arbitrarily large number of integrators. We used only one artificial delay, and we assumed that the nonlinear subsystems satisfy a converging-input-converging-state assumption. When the nonlinear subsystem is control affine with the state of the first integrator as the control, we provided sufficient conditions for our converging-input- converging-state assumption to hold.

## 7.7. Stability of time-varying systems with delay and Switched Nonlinear Systems

**Participants:** Frederic Mazenc, Hitay Ozbay [Blikent University, Turkey], Saeed Ahmed [Blikent University, Turkey], Silviu Niculescu, Michael Malisoff [LSU, USA].

Switched systems is a family of systems which is frequently encountered in practice and can be used to approximate time-varying systems to ease their stability analysis or control. In the two works [20] and [17], we provided results that are useful when it comes to analyze the stability of time-varying or switched systems with delay. In [20] we provided several significant applications of the trajectory approach developed recently by Mazenc and Malisoff. In two results, we used a Lyapunov function for a corresponding undelayed system to provide a new method for proving stability of linear continuous-time time-varying systems with bounded time-varying delays. Our main results used upper bounds on an integral average involving the delay. We also provided a novel reduction model approach that ensures global exponential stabilization of linear systems with a time-varying pointwise delay in the input, which allows the delay to be discontinuous and uncertain.

Three of our other works are devoted to switched systems. In [55] and [21], a new technique is proposed to ensure global asymptotic stability for nonlinear switched time-varying systems with time-varying discontinuous delays. It uses an adaptation of Halanay's inequality to switched systems and the trajectory based technique mentioned above. The result is applied to a family of linear time-varying systems with time-varying delays. In [53], we presented an extension of the trajectory based approach mentioned above for state feedback stabilization of switched linear continuous-time systems with a time-varying input delay. In contrast with finding classical common Lyapunov function or multiple Lyapunov functions for establishing the stability of the closed-loop switched system, the new trajectory based approach relies on verifying certain inequalities along the solution of a supplementary system. This study does not make any assumption regarding the stabilizability of all of the constituent modes of the switched system. Moreover, no assumption is needed about the differentiability of the delay and no constraint is imposed on the upper bound of the delay derivative.

In [17], we proved extensions of the celebrated Razumikhin's theorem for a general family of time-varying continuous and discrete-time nonlinear systems. Our results include a novel "strictification" technique for converting a nonstrict Lyapunov function into a strict one. We also provided new constructions of Lyapunov-Krasovskii functionals that can be used to prove robustness to perturbations. Our examples include a key model from identification theory, and they show how our method can sometimes allow broader classes of delays than the results in the literature.

## 7.8. Systems with Long Delays

**Participants:** Frederic Mazenc, Silviu Niculescu, Michael Malisoff [LSU,USA], Jerome Weston [LSU,USA], Ali Zemouche, Bin Zhou [Harbin Institute of Technology], Qingsong Liu [Harbin Institute of Technology].

We solved several problems of observer and control designs pertaining to the fundamental (and difficult) case where a delay in the input is too long for being neglected.

In [35], we studied the stabilization of linear systems with both state and input delays where the input delay can be arbitrarily large but exactly known. Observer-predictor based controllers are designed to predict the future states so that the input delay can be properly compensated. Necessary and sufficient conditions guaranteeing the stability of the closed-loop system are provided in terms of the stability of some simple linear time-delay systems referred to as observer-error systems. Moreover, linear matrix inequalities are used to design both the state feedback gains and observer gains. Finally, a numerical example illustrates that the proposed approaches are more effective and safe to implement than the existing methods.

In [57], for a particular family of systems, we constructed observers in the case where the measured variables are affected by the presence of a point-wise time-varying delay. The key feature of the proposed observers is that the size of their gains is proportional to the inverse of the largest value taken by the delay. The main result is first presented in the case of linear chain of integrators and next is extended to nonlinear systems with specific nonlinearities (systems of feedforward form).

Two of our works are devoted to the development of the prediction technique based on sequential predictors. Let us recall that one of the key advantages of this method is that it circumvents the problem of constructing and estimating distributed terms in the control laws: instead of using distributed terms, our approach to handling longer delays is to increase the number of predictors. In [61], we provided a significant generalization of our previous results to cases with arbitrarily large feedback delay bounds, and where, in addition, current values of the plant state are not available to use in the sequential predictors. We illustrate our work in a pendulum example. In [18], we provided a new sequential predictors approach for the exponential stabilization of linear time-varying systems. Our method allows arbitrarily large input delay bounds, pointwise time-varying input delays and uncertainties. We obtain explicit formulas to find lower bounds for the number of required predictors.

## 7.9. Nonlinear Observer Design via LMIs

**Participants:** Ali Zemouche, Rajesh Rajamani [University of Minneapolis, USA], Hieu Trinh [Deakin University, Australia], Yan Wang [University of Minneapolis, USA], Michel Zasadzinski [CRAN], Hugues Rafaralahy [CRAN], Boulaïd Boulkroune [Flanders Make, Lommel, Belgium], Gridsada Phanomchoeng [Chulalongkorn University, Thailand], Khadidja Chaib-Draa [University of Luxembourg], Mohamed Darouach [CRAN], Marouane Alma [CRAN], Holger Voos [University of Luxembourg].

- Observer Design for Lipschitz and Monotonic nonlinear systems using LMIs:

New LMI (Linear Matrix Inequality) design techniques have been developed to address the problem of designing performant observers for a class of nonlinear systems. The developed techniques apply to both locally Lipschitz as well as monotonic nonlinear systems, and allows for nonlinear functions in both the process dynamics and output equations [59], [34]. The LMI design conditions obtained are less conservative than all previous results proposed in literature for these classes of nonlinear systems. By judicious use of Young's relation, additional degrees of freedom are included in the observer design. These additional decision variables enable improvements in the feasibility of the

obtained LMI. Several recent results in literature are shown to be particular cases of the more general observer design methodology developed in this paper. Illustrative examples are used to show the effectiveness of the proposed methodology. The application of the method to slip angle estimation in automotive applications is discussed and experimental results are presented. Although this application was the main motivation of this work, the proposed techniques have been applied to an anaerobic digestion model for different contexts [43], [44], [45].

- **HG/LMI Observer:**

A new high-gain observer design method with lower gain compared to the standard high-gain observer was proposed [62]. This new observer, called "HG/LMI" observer is obtained by combining the standard high-gain methodology with the LPV/LMI-based technique. Through analytical developments, it is shown how the new observer provides a lower gain. A numerical example was used to illustrate the performance of the new "HG/LMI" observer that we can call "smart high-gain observer". The aim of this research is the application of this new observer design to estimate some variables in vehicle applications and other real-world applications.

- **Dual Spatially Separated Sensors for Enhanced Estimation:**

Inspired by the function of spatially separated sensory organs found in nature, we explored the use of dual spatially separated sensors for enhanced estimation in modern engineering applications [26]. To illustrate the interest of dual spatially separated sensors, some real applications have been considered: 1) Adaptive parameter and state estimation in magnetic sensors; 2) Estimation of an unknown disturbance input in an automotive suspension; 3) Separation of inputs based on their direction of action in a digital stethoscope. Both analytical observer design developments and experimental evaluation of the results have been provided.

## 7.10. Observer-Based Stabilization of Uncertain Nonlinear Systems

**Participants:** Ali Zemouche, Rajesh Rajamani [University of Minneapolis, USA], Yan Wang [University of Minneapolis, USA], Fazia Bedouhne [University of Tizi-Ouzou, Algeria], Hamza Bibi [University of Tizi-Ouzou, Algeria], Abdel Aitouche [CRISTAL, Lille].

- **Relaxed LMI conditions for switched systems and LPV systems:**

By exploiting the Finsler's lemma in a non-standard way, we derived new LMI conditions. This technique has been applied to linear switched systems with uncertain parameters [10], [40] and LPV (Linear Parameter Varying) systems with inexact parameters [39], respectively. In each case, the Finsler's inequality is exploited in a convenient way to get additional decision variables which render the LMIs less conservative than those existing in the literature. In addition to analytical comparisons, several numerical examples have been used to show the superiority of the proposed new LMI conditions.

- **From LMI relaxations to sequential LMI algorithm:**

Recently, motivated by autonomous vehicle control problem, a robust observer based estimated state feedback control design method for an uncertain dynamical system that can be represented as a LTI system connected with an IQC-type nonlinear uncertainty was developed [28]. Different from existing design methodologies in which a convex semidefinite constraint is obtained at the cost of conservatism and unrealistic assumptions, the design of the robust observer state feedback controller is formulated in this paper as a feasibility problem of a bilinear matrix inequality (BMI) constraint. Unfortunately, the search for a feasible solution of a BMI constraint is a NP hard problem in general. The applicability of the linearization method, such as variable change method or congruence transformation, depends on the specific structure of the problem at hand and cannot be generalized. A new sequential LMI optimization method to search for a feasible solution was established. In the application part, a vehicle lateral control problem is presented to demonstrate the applicability of the proposed algorithm to a real-world estimated state feedback control design.



### 7.11. Analysis of PWA control of discrete-time linear dynamics in the presence of variable input delay

**Participants:** Sorin Olaru, Mohammed Laraba [CentraleSupélec], Silviu Niculescu.

We have addressed the robustness of a specific class of control laws, namely the piecewise affine (PWA) controllers, defined over a bounded region of the state-space. More precisely, we were interested in closed-loop systems emerging from linear dynamical systems controlled via feedback channels in the presence of varying transmission delays by a PWA controller defined over a polyhedral partition of the state-space. We exploit the fact that the variable delays are inducing some particular model uncertainty. Our objective was to characterize the delay invariance margins: the collection of all possible values of the time-varying delays for which the positive invariance of the corresponding region is guaranteed with respect to the closed-loop dynamics. These developments are proving to be useful for the analysis of different design methodologies and, in particular, for model predictive control (MPC) approaches. The proposed delay margin describes the admissible transmission delays for an MPC implementation. From a different perspective, the delay margin further characterizes the fragility of an embedded MPC implementation via the on-line optimization and subject to variable computational time.

### 7.12. On the precision in polyhedral partition representation and the fragility of PWA control

**Participants:** Sorin Olaru, Rajesh Koduri [CentraleSupélec], Pedro Rodriguez [CentraleSupélec].

Explicit model predictive control (EMPC) solves a multi-parametric Quadratic Programming (mp-QP) problem for a class of discrete-time linear system with linear inequality constraints. The solution of the EMPC problem in general is a piecewise affine control function defined over non-overlapping convex polyhedral regions composing a polyhedral partition of the feasible region. In this work, we considered the problem of perturbations on the representation of the vertices of the polyhedral partition. Such perturbations may affect some of the structural characteristics of the PWA controller such as *non-overlapping within the regions* or *the closed-loop invariance*. We first showed how a perturbation affects the polyhedral regions and evoked the overlapping within the modified polyhedral regions. The major contribution of this work is to analyze to what extend the non-overlapping and the invariance characteristics of the PWA controller can be preserved when the perturbation takes place on the vertex representation. We determined a set called sensitivity margin to characterize for admissible perturbation preserving the non-overlapping and the invariance property of the controller. Finally, we show how to perturb multiple vertices sequentially and reconfigure the entire polyhedral partition

### 7.13. Convex Lifting: Theory and Control Applications

**Participants:** Sorin Olaru, Martin Gulán [STU, Bratislava, Slovaquie], Ngoc Anh Nguyen [J. Kepler Univ., Linz, Austria], Pedro Rodriguez [CentraleSupélec].

We introduced the *convex lifting* concept which was proven to enable significant implementation benefits for the class of piecewise affine controllers. Accordingly, two different algorithms to construct a convex lifting for a given polyhedral/polytopic partition were presented. These two algorithms rely on either the vertex or the halfspace representation of the related polyhedra. Also, we introduced an algorithm to refine a polyhedral partition, which does not admit a convex lifting, into a convexly liftable one. Furthermore, two different schemes are put forward to considerably reduce both the memory footprint and the runtime complexity which play a key role in implementation of piecewise affine controllers. These results have been illustrated via a numerical example and a complexity analysis.

### 7.14. Attitude control

**Participants:** Frederic Mazenc, Maruthi Akella [Univ. of Texas, USA], Sungpil Yang [Univ. of Texas, USA].

In [31], we addressed adaptive control of specific Euler-Lagrange systems: rigid-body attitude control, and the  $n$ -link robot manipulator. For each problem, the model parameters are unknown but the lower bound of the smallest eigenvalue of the inertia matrix is assumed to be known. The dynamic scaling Immersion and Invariance (I&I) adaptive controller is proposed to stabilize the system without employing a filter for the regressor matrix. A scalar scaling factor is instead implemented to overcome the integrability obstacle that arises in I&I adaptive control design. First, a filter-free controller is proposed for the attitude problem such that the rate feedback gain is proportional to the square of the scaling factor in the tracking error dynamics. The gain is then shown to be bounded through state feedback while achieving stabilization of the tracking error. The dynamic scaling factor increases monotonically by design and may end up at a finite but arbitrarily large value. However, by introducing three more dynamic equations, the non-decreasing scaling factor can be removed from the closed-loop system. Moreover, the behavior of dynamic gain is dictated by design parameters so that its upper bound is limited by a known quantity and its final value approaches the initial value. A similar approach for the dynamic gain design is also applied to a filter-dependent controller where a filter for the angular rate is utilized to build a parameter estimator. Unlike the filter-free design, the filter-dependent controller admits a constant gain for the rate feedback while the dynamic scaling factor rather appears in the filter. Finally, the proposed design is applied to robot manipulator systems. Spacecraft attitude and 2-link planar robot tracking problems are considered to demonstrate the performance of the controllers through simulations.

The work [32] builds on the preliminary results by generalizing to the tracking case and some further analysis of the filter-free case. Extending the strictification technique, a partially strict Lyapunov function is constructed toward establishment of stability and ultimate boundedness properties for the closed-loop system. With known upper bounds of the magnitude of measurement errors, disturbance torques, and parameter uncertainties, a feasible range for the feedback gains is derived in terms of bounds on the initial conditions in such a way to ensure asymptotic convergence of all closed-loop signals to within a residual set. In spite of the nonlinear structure of the kinematics and dynamics of the problem, however, the closed-loop system is rigorously analyzed through the standard Lyapunov analysis methods. This is achieved owing to the fact that the strictified Lyapunov function allows us to deal with this nontrivial problem in a standard way. As the passivity-based controller is not new for the attitude control problem, the key contribution of this paper is a theoretical analysis of the ideal case design in the presence of uncertainties through Lyapunov stability analysis.

### 7.15. Active Vibration Control of thin structures

**Participants:** Islam Boussaada, Silviu-Iulian Niculescu, Sami Tliba [L2S], Hakki Unal [Anadolu University], Toma Vyhldal [Czech Technical University].

The problem of active vibrations damping of thin mechanical structures is a topic that has received great attention by the control community for several years, especially, when actuators and sensors are based on piezoelectric materials. For mechanical structures that are deformable, piezoelectric materials are used as strain sensors or strain actuators. With an appropriate controller, they allow to achieve shape control or the active damping of multi-modal vibrations thanks to their very large bandwidth. In this area, the major challenge is the design of controllers able to damp the most vibrating modes in a specified low-frequency bandwidth while ensuring robustness against high-frequency modes, outside the bandwidth of interest, often unmodelled or weakly modelled. The inherent feature of this kind of systems is that they arise robustness issues when they are tackled with finite dimensional control tools. A delayed state-feedback control strategies based on rightmost spectral values assignment allowing a fast vibration damping are proposed in [69], [41], [11].

### 7.16. Automatic Train Supervision for a CBTC Suburban Railway Line Using Multiobjective Optimization

**Participants:** Guillaume Sandou, Juliette Pochet [SNCF], Sylvain Baro [SNCF].

Communication-based train control (CBTC) systems have been deployed on subway lines to increase capacities on existing infrastructures. For the same purpose, CBTC systems are to be deployed on suburban railway lines where operating principles and constraints are significantly different. A regulation method for CBTC trains on a suburban line has been developed. This method is designed to combine CBTC functionalities with suburban operating principles. It includes a traffic management method in station, and a rescheduling method in case of disturbances. The proposed regulation method is integrated into the railway system simulation tool SIMONE developed by SNCF. This simulation tool includes models of the whole CBTC system, as well as the classic signaling system, train dynamics and railway infrastructures. Models of these different agents are described. The integration of the proposed regulation method into the tool SIMONE allows evaluating performances while taking into account the functional complexity of a CBTC railway system. The approach is illustrated with a realistic case: simulations of a CBTC traffic on the urban part of a railway line in the Paris region network are described. The proposed regulation method shows interesting results in disturbed situations according to the railway operating principles [60].

### 7.17. A Distributed Consensus Control Under Disturbances for Wind Farm Power Maximization

**Participants:** Guillaume Sandou, Nicolo Gionfra [CentraleSupélec], Houria Siguerdidjane [Centrale-Supélec], Damien Faille [EDF], Philippe Loevenbruck [CentraleSupélec].

We have addressed the problem of power sharing among the wind turbines (WTs) belonging to a wind farm. The objective is to maximize the power extraction under the wake effect, and in the presence of wind disturbances. Because of the latter, WTs may fail in respecting the optimal power sharing gains. These are restored by employing a consensus control among the WTs. In particular, under the assumption of discrete-time communication among the WTs, we propose a distributed PID-like consensus approach that enhances the rejection of the wind disturbances by providing the power references to the local WT controllers. The latter are designed by employing a novel feedback linearization control that, acting simultaneously on the WT rotor speed and the pitch angle, guarantees the tracking of general deloaded power references. The obtained results are validated on a 6-WT wind farm example. [50].

### 7.18. Distributed Particle Swarm Optimization Algorithm for the Optimal Power Flow Problem

**Participants:** Guillaume Sandou, Nicolo Gionfra [CentraleSupélec], Houria Siguerdidjane [Centrale-Supélec], Damien Faille [EDF], Philippe Loevenbruck [CentraleSupélec].

The distributed optimal power flow problem has been addressed. No assumptions on the problem cost function, and network topology are needed to solve the optimization problem. A particle swarm optimization algorithm is proposed, based on Deb's rule to handle hard constraints. Moreover, the approach enables to treat a class of distributed optimization problems, via a population based algorithm, in which the agents share a common optimization variable. A simulation example is provided, based on a 5-bus electric grid. [51].

### 7.19. Chemostat

**Participants:** Frederic Mazenc, Michael Malisoff [LSU,USA], Gonzalo Robledo [Univ. de Chile,Chile].

A chemostat is a fundamental bioreactor used to study the behavior of microorganisms. Many different types of chemostats exist, and many different types of models represent them.

We studied in [56] a chemostat model with an arbitrary number of competing species, one substrate, and constant dilution rates. We allowed delays in the growth rates and additive uncertainties. Using constant inputs of certain species, we derived bounds on the sizes of the delays that ensure asymptotic stability of an equilibrium when the uncertainties are zero, which can allow persistence of multiple species. Under delays and uncertainties, we provided bounds on the delays and on the uncertainties that ensure a robustness property of input-to-state stability with respect to uncertainties.

In [16], we provided a new control design for chemostats, under constant substrate input concentrations, using piecewise constant delayed measurements of the substrate concentration. Our growth functions can be uncertain and are not necessarily monotone. The dilution rate is the control. We use a new Lyapunov approach to derive conditions on the largest sampling interval and on the delay length to ensure asymptotic stabilization properties of a componentwise positive equilibrium point.

## 7.20. Qualitative/quantitative analysis of a delayed chemical model

**Participants:** Islam Boussaada, Silviu-Iulian Niculescu, Hakki Unal [Anadolu University].

The Belousov-Zhabotinsky reaction is a complex chemical reaction exhibiting sustained oscillations observed in some real biological oscillators. However, its oscillatory behavior is represented by a simple mechanism, called the Oregonator. A qualitative/quantitative analysis of a two-delay Oregonator based chemical oscillator is considered where the delay effect in dynamics is investigated; the existence of positive equilibrium point, the stability and boundedness of solutions for positive initial conditions are explored [27].

## 7.21. Mathematical Modelling of Acute Myeloid Leukemia

**Participants:** Catherine Bonnet, Jean Clairambault [MAMBA project-team], François Delhommeau [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Walid Djema, Emilia Fridman [Tel-Aviv University], Pierre Hirsch [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Frédéric Mazenc, Hitay Özbay [Bilkent University].

The ALMA3-project is about the modeling and analysis of healthy and unhealthy cell population dynamics, with a particular focus on hematopoiesis, which is the process of blood cell production and continuous replenishment. We point out that medical research is now looking for new combined targeted therapies able to overcome the challenge of cancer cells (e.g. to stop overproliferation, to restore normal apoptosis rates and differentiation of immature cells, and to avoid the high toxicity effects that characterize heavy non-selective chemotherapy). In that quest, the ultimate goal behind mathematical studies is to provide some inputs that should help biologists to suggest and test new treatment, and to contribute within multi-disciplinary groups in the opening of new perspectives against cancer. Thus, our research project is imbued within a similar spirit and fits the expectations of a better understanding of the behavior of healthy and unhealthy blood cell dynamics. It involve intensive collaboration with hematologists from Saint Antoine hospital in Paris, and aims to analyze the cell fate evolution in treated or untreated leukemia, allowing for the suggestion of new anti-leukemic combined chemotherapy.

In 2017, we have discussed some of the issues that are related to the modeling of the cell cycle, with particular insight into hematopoietic systems. For instance, i) we introduced and studied for the first time the effect of cell plasticity (dedifferentiation and transdifferentiation mechanisms) in the class of models that we focus on, and ii) we considered the effect of cell-arrest (i.e. some cells can be arrested during their cell-cycle) in models with several maturity stages. Stability features of the resulting biological models are highlighted, since systems trajectories reflect the most prominent healthy or unhealthy behaviors of the biological process under study. We indeed perform stability analysis of systems describing healthy and unhealthy situations, particularly in the case of acute myeloblastic leukemia (AML). More precisely, these are nonlinear time-delay systems that involve finite or infinite distributed delay terms, with possibly time-varying parameters. We pursue the objectives of earlier works in order to understand the interactions between the various parameters and functions involved in the mechanisms we study. Sometimes, we extend the stability analysis and the application of some already existing models, whereas news models and variants are other times introduced to cover novel biological evidences, such as: mutations accumulation and cohabitation between ordinary and mutated cells in niches, control and eradication of cancer stem cells, cancer dormancy and cell plasticity. In fact, the challenging problem that we are facing is to steadily extend both modelling and analysis aspects to constantly better represent this complex physiological mechanism, which is not yet fully understood. So, this year, we have progressed on our project and we have extended our works in order to develop the modeling and analysis aspects in cancer dormancy by including the effects of immuno-therapies in AML [48]. Lyapunov-like techniques have been used in this work in order to derive global or local exponential stability conditions

for that class of differential-difference systems. Finally, in [49], we have modeled the role played by growth factors -these are hormone-like molecules- or drugs on the regulation of various biological features that are involved in hematopoiesis.

## 7.22. Analysis of Dengue Fever SIR Model with time-varying parameters

**Participants:** Stefanella Boatto [Univ Feder Rio de Janeiro], Catherine Bonnet, Frédéric Mazenc, Le Ha Vy Nguyen.

Dengue fever is an infectious viral disease occurring in humans that is prevalent in parts of Central and South America, Africa, India and South-east Asia and which causes 390 millions of infections worldwide. We continued this year our study on modeling of dengue epidemics.

We have first considered a SIR model with birth and death terms and time-varying infectivity parameter  $\beta(t)$ . In the particular case of a sinusoidal parameter, we showed that the average Basic Reproduction Number  $R_o$ , introduced in [Bacaër & Guernaoui, 2006], is not the only relevant parameter and we emphasized the rôle played by the initial phase, the amplitude and the period. For a (general) periodic infectivity parameter  $\beta(t)$  a periodic orbit exists, as already proved in [Katriel, 2014]. In the case of a slowly varying  $\beta(t)$  an approximation of such a solution is given, which is shown to be asymptotically stable under an extra assumption on the slowness of  $\beta(t)$ . For a non necessarily periodic  $\beta(t)$ , all the trajectories of the system are proved to be attracted into a tubular region around a suitable curve, which is then an approximation of the underlying attractor. Numerical simulations are given [68].

In other to study the effects of urban human mobility on Dengue epidemics, we have considered a SIR-network model (still with birth and death rates). The same model without these rates was introduced in [72].

In the case of constant infection rates, we first examine networks of two nodes. For arbitrary network topologies, some general properties of the equilibrium points are obtained. Then for several specific topologies, we derive explicit expressions of multiple equilibrium points and characterize their stability properties. We extend the study to networks with an arbitrary number of nodes and obtain sufficient conditions for global asymptotic stability of the disease-free equilibrium point.

In the case of time-varying infection rates and networks of arbitrary number of nodes, we introduce a specific topology which leads to a simplification of the network: the dynamics of the total population is described by the classical SIR model. This fact, together with the results of the team on the SIR model, allows a complete characterization of the stability properties of the system, especially the approximation of the epidemic attractor.

## GAMMA3 Project-Team

## 4. New Results

### 4.1. Element metric, element quality and interpolation error metric

**Participants:** Paul Louis George [correspondant], Houman Borouchaki.

The metric of a simplex of  $\mathbb{R}^d$  is a metric tensor (symmetric positive definite matrix) in which the element is unity (regular with unit edge lengths). This notion is related to the problem of interpolation error of a given field over a mesh. Let  $K$  be a simplex and let us denote by  $v_{ij}$  the vector joining vertex  $i$  and vertex  $j$  of  $K$ . The metric of  $K$  can be written as:

$$\mathcal{M} = \frac{d+1}{2} \left( \sum_{i < j} v_{ij} {}^t v_{ij} \right)^{-1},$$

where  $v_{ij} {}^t v_{ij}$  is a  $d \times d$  rank 1 matrix related to edge  $ij$ .

The metric of a simplex also characterizes the element shape. In particular, if it is the identity, the element is unity. Hence, to define the shape quality of an element, one can determine the gap of the element metric  $\mathcal{M}$  and the identity using different measures based on the eigenvalues  $\lambda_i = \frac{1}{h_i^2}$  of  $\mathcal{M}$  or those of  $\mathcal{M}^{-1}$ , e.g.  $h_i^2$ . Notice that metric  $\mathcal{M}^{-1}$  is directly related to the geometry of the element (edge length, facet area, element volume). The first algebraic shape quality measure ranging from 0 to 1 is defined as the ratio of the geometric average of the eigenvalues of  $\mathcal{M}^{-1}$  and their arithmetic average:

$$q(K) = \frac{\left( \prod_i h_i^2 \right)^{\frac{1}{d}}}{\frac{1}{d} \sum_{i=1}^d h_i^2} = d \frac{(\det(\mathcal{M}^{-1}))^{\frac{1}{d}}}{\text{tr}(\mathcal{M}^{-1})}.$$

As the geometric average is smaller than the arithmetic average, this measure is well defined. In addition, it is the algebraic reading of the well-known quality measure defined by:

$$q^{\frac{d}{2}}(K) = (d!) d^{\frac{d}{2}} (d+1)^{\frac{d-1}{2}} \frac{|K|}{\left( \sum_{i < j} l_{ij}^2 \right)^{\frac{d}{2}}},$$

where the volume and the square of the edge lengths are involved. The algebraic meaning justifies the above geometric measure. The second algebraic shape quality measure is defined as the ratio of the harmonic average of the eigenvalues of  $\mathcal{M}^{-1}$  and their arithmetic average (ranging also from 0 to 1):

$$q(K) = \frac{\left\{ \frac{1}{d} \sum_{i=1}^d \frac{1}{h_i^2} \right\}^{-1}}{\frac{1}{d} \sum_{i=1}^d h_i^2} = \frac{d^2}{\text{tr}(\mathcal{M}) \text{tr}(\mathcal{M}^{-1})}.$$

As above, this measure is well defined, the harmonic average being smaller the arithmetic one. From this measure, one can derive another well-known measure involving the roundness and the size of an element (measure which is widely used for convergence issues in finite element methods).

Note that these measures use the invariants of  $\mathcal{M}^{-1}$  or  $\mathcal{M}$  and thus can be evaluated from the coefficients of the characteristic polynomial of those matrices (avoiding the effective calculation of their eigenvalues). Another advantage of the above algebraic shape measures is their easy extensions in an arbitrary Euclidean space. Indeed, if  $\mathcal{E}$  is the metric of such a space, the algebraic shape measures read:

$$q_{\mathcal{E}}(K) = d \frac{(\det(\mathcal{M}^{-1}\mathcal{E}))^{\frac{1}{d}}}{\text{tr}(\mathcal{M}^{-1}\mathcal{E})} \quad , \quad q_{\mathcal{E}}(K) = \frac{d^2}{\text{tr}(\mathcal{E}^{-1}\mathcal{M})\text{tr}(\mathcal{M}^{-1}\mathcal{E})}.$$

Following this notion of a element metric, a natural work was done regarding how to define the element metric so as to achieve a given accuracy for the interpolation error of a function using a finite element approximation by means of simplices of arbitrary degree.

This is a new approach for the majoration of the interpolation error of a polynomial function of arbitrary degree  $n$  interpolated by a polynomial function of degree  $n - 1$ . From that results a metric, the so-called interpolation metric, which allows for a control of the error. The method is based on the geometric and algebraic properties of the metric of a given element, metric in which the element is regular and unit. The interpolation metric plays an important role in advanced computations based on mesh adaptation. The method relies in a Bezier reading of the functions combined with Taylor expansions. In this way, the error in a given element is fully controlled at the time the edges of the element are controlled.

It is shown that the error is bounded as

$$|e(X)| \leq C \sum_{i < j} f^{(n)}(\cdot)(v_{ij}, v_{ij}, \dots, v_{ij}),$$

where  $C$  is a constant depending on  $d$  and  $n$ ,  $v_{ij}$  is the edge from the vertices of  $K$  of index  $i$  and  $j$ ,  $f^{(n)}(\cdot)$  is the derivative of order  $n$  of  $f$  applied to a  $n$ -uple uniquely composed of  $v_{ij}$ . If we consider the case  $d = 2$  and  $u = (x, y)$  is a vector in  $\mathbb{R}^2$ , we have

$$f^{(n)}(\cdot)(u, u, \dots, u) = \sum_{i=0}^{n-2} x^{n-2-i} y^i {}^t u (C_i^{n-2} \mathcal{H}_{(n-2, n-2-i, i)}) u ,$$

where the quadratic forms  $\mathcal{H}_{(n-2, n-2-i, i)}$  are defined by the matrices of order 2 (with constant entries):

$$\mathcal{H}_{(n-2, n-2-i, i)} = \begin{pmatrix} \frac{\partial^{(n)} f}{\partial x_1^{n-1-i} \partial x_2^i} & \frac{\partial^{(n)} f}{\partial x_1^{n-1-i} \partial x_2^{i+1}} \\ \frac{\partial^{(n)} f}{\partial x_1^{n-1-i} \partial x_2^{i+1}} & \frac{\partial^{(n)} f}{\partial x_1^{n-2-i} \partial x_2^{i+2}} \end{pmatrix},$$

those matrices being the Hessians of the derivatives of  $f$  of order  $n - 2$ .

This work resulted in a paper submitted in a journal and currently under revision.

## 4.2. Realistic modeling of fractured geologic media

**Participants:** Patrick Laug [correspondant], Géraldine Pichot.



This study, in collaboration with project-team Serena, aims to model, in a realistic and efficient manner, natural fractured media. These media are characterized by their diversity of structures and organizations. Numerous studies in the past decades have evidenced the existence of characteristic structures at multiple scales. At fracture scale, the aperture distribution is widely correlated and heterogeneous. At network scale, the topology is complex resulting from mutual mechanical interactions as well as from major stresses. Geometric modeling of fractured networks combines in a non-standard way a large number of 2D fractures interconnected in the 3D space. Intricate local configurations of fracture intersections require original methods of geometric modeling and mesh generation. We have developed in 2016 a software package that automatically builds geometric models and surface meshes of random fracture networks. The results are highly promising and we now want to continue this research to further improve the element quality in complex configurations, take into account multiple size scales in large fracture networks (up to thousands of fractures), and compare several modeling strategies (mixed hybrid finite elements, projected grids, mortar elements).

### 4.3. Parallel meshing of surfaces defined by collections of connected regions

**Participant:** Patrick Laug [correspondant].

In CAD (computer aided design) environments, a surface is commonly modeled as a collection of connected regions represented by parametric mappings. For meshing such a composite surface, a parallelized indirect approach with dynamic load balancing can be used on a shared memory system. However, this methodology can be inefficient in practice because most existing CAD systems use memory caches that are only appropriate to a sequential process. As part of the sabbatical year of P. Laug at Polytechnique Montréal in 2014/2015, two solutions have been proposed, referred to as the Pirate approach and the Discrete approach. In the first approach, the Pirate library can be efficiently called in parallel since no caching is used for the storage or evaluation of geometric primitives. In the second approach, the CAD environment is replaced by internal procedures interpolating a discrete geometric support. In 2016, the dynamic load balancing has been analyzed and improved. Significant modifications to the Pirate library have been made, and new numerical tests on three different computers (4, 8 and 64 cores) have been carried out, now showing an almost linear scaling of the method in all cases.

### 4.4. Discrete CAD model for visualization and meshing

**Participants:** Patrick Laug [correspondant], Houman Borouchaki.

During the design of an object using a CAD (computer aided design) platform, the user can visualize the ongoing model at every moment. Visualization is based on a discrete representation of the model that coexists with the exact analytical representation of the object. Most CAD systems have this discrete representation available, and each of them applies its own construction methodology. We have developed in 2016 a method to build a discrete model for CAD surfaces (the model is quadtree-based and subdivided into quadrilaterals and triangles). The method presents two major particularities: most elements are aligned with iso-parametric curves and the accuracy of the surface approximation is controlled. In addition, we have proposed a new technique of surface mesh generation that is based on this discrete model. This approach has been implemented as a part of a surface mesher called ALIEN, and several examples have demonstrate the robustness and computational efficiency of the program, as well as the quality of the geometric support.

### 4.5. Visualization and modification of high-order curved meshes

**Participants:** Alexis Loyer, Dave Marcum, Adrien Loseille [correspondant].

During the partnership between Inria and Distene, a new visualization software has been designed. It address the typical operations that are required to quickly assess the newly algorithm developed in the team. In particular, interactive modifications of high-order curved mesh and hybrid meshes has been addressed.

### 4.6. Adaptation de maillages pour des écoulements visqueux en turbomachine

**Participants:** Frédéric Alauzet, Loïc Frazza, Adrien Loseille [correspondant].

#### 4.6.1. Calcul.

Les prémices d'une adaptation pour les écoulements Navier-Stokes turbulents ont été testés sur des calculs de turbomachine. Pour ce faire nous avons tout d'abord traité les particularités liées aux calculs en turbomachine: - Les aubes présentent en général une périodicité par rotation et on ne simule donc qu'une période afin d'alléger les calculs. Il faut donc traiter cette périodicité de façon appropriée dans le code CFD et l'adaptation de maillage. - Afin de prendre en compte la rotation des pales sans employer de maillages mobiles et simulations instationnaires on peut se placer dans le référentiel tournant de l'aube en corrigeant les équations. - Les écoulements en turbomachine sont des écoulements clos, les conditions limites d'entrée et de sortie ont donc une influence très forte et peuvent de plus se trouver très près de la turbine afin de simuler la présence d'autres étages en amont ou aval. Des conditions limites bien précises ont donc été développées afin de traiter correctement ces effets.

#### 4.6.2. Adaptation.

Pour l'adaptation de maillages deux particularités doivent être traitées ici, la périodicité du maillage et la couche limite turbulente.

En 2D, la couche limite turbulente est automatiquement adaptée avec la méthode metric orthogonal et la périodicité du maillage est garantie par un traitement spécial des frontières. Les estimateurs d'erreurs Navier-Stokes et RANS n'étant pas encore au point nous avons utilisé la Hessienne du Mach de l'écoulement comme senseur ce qui donne déjà des résultats satisfaisants.

En 3D la méthode metric orthogonal est beaucoup plus complexe à mettre en oeuvre et n'est pas encore au point. La couche limite a donc été exclue de l'adaptation, le maillage est adapté uniquement dans le volume en utilisant la Hessienne du Mach de l'écoulement comme senseur. La périodicité n'étant pas traitée non plus, les frontières périodiques restent inchangées ce qui garantit leur périodicité.

#### 4.6.3. Norm-Oriented.

Dans le cadre de la théorie Norm-Oriented, afin de contrôler l'erreur implicite des schémas numériques, un correcteur a été développé et testé. Etant donné un maillage et la solution numérique obtenue avec, le résidu de cette solution projeté sur un maillage deux fois plus fin est accumulé sur le maillage initial. Ce défaut de résidu est utilisé comme terme source dans une seconde simulation plus courte. La nouvelle solution toujours sur le même maillage est plus proche de la solution exacte et donne une bonne estimation de l'erreur.

### 4.7. Parallel mesh adaptation

**Participants:** Frédéric Alauzet, Adrien Loseille [correspondant].

We devise a strategy in order to generate large-size adapted anisotropic meshes  $O(10^8 - 10^9)$  as required in many fields of application in scientific computing. We target moderate scale parallel computational resources as typically found in R&D units where the number of cores ranges in  $O(10^2 - 10^3)$ . Both distributed and shared memory architectures are handled. Our strategy is based on hierarchical domain splitting algorithm to remesh the partitions in parallel. Both the volume and the surface mesh are adapted simultaneously and the efficiency of the method is independent of the complexity of the geometry. The originality of the method relies on (i) a metric-based static load-balancing, (ii) dedicated hierarchical mesh partitioning techniques to (re)split the (complex) interfaces meshes, (iii) anisotropic Delaunay cavity to define the interface meshes, (iv) a fast, robust and generic sequential cavity-based mesh modification kernel, and (v) out-of-core storing of completing parts to reduce the memory footprint. We are able to generate (uniform, isotropic and anisotropic) meshes with more than 1 billion tetrahedra in less than 20 minutes on 120 cores.

### 4.8. Unsteady adjoint computation on dynamic meshes

**Participants:** Eléonore Gauci, Frédéric Alauzet [correspondant].

Adjoint formulations for unsteady problems are less common due to the extra complexity inherent in the numerical solution and storage but these methods are a great option in engineering because it takes more into account the cost function we want to minimize. Moreover the engineering applications involve moving bodies and this motion must be taken into account by the governing flow equations. We develop a model of unsteady adjoint solver on moving mesh problems. The derivation of the adjoint formulation based on the ALE form of the equations requires consideration of the dynamic meshes. Our model takes into account the DGCL.

#### 4.9. Line solver for efficient stiff parse system resolution

**Participants:** Loïc Frazza, Frédéric Alauzet [correspondant].

Afin d'accélérer la résolution des problèmes raides, un line-solver a été développé. Cette méthode extrait tout d'abord des lignes dans le maillage du problème selon des critères géométriques ou physiques. Le problème peut alors être résolu exactement le long de ces lignes à moindre coût. Cette méthode est particulièrement bien adaptée aux cas où l'information se propage selon une direction privilégiée tels que les chocs, les couches limites ou les sillages. Ces cas sont généralement associés à des maillages très étirés ce qui conduit à des problèmes raides mais quasi-unidimensionnels. Ils peuvent donc être résolus efficacement par un line-solver, réduisant ainsi les temps de calculs tout en gagnant en robustesse.

#### 4.10. Error estimate for high-order solution field

**Participants:** Olivier Coulaud, Adrien Loseille [correspondant].

Afin de produire des solveurs d'ordre élevé, et ainsi répondre aux exigences inhérentes à la résolution de problèmes physiques complexes, nous développons une méthode d'adaptation de maillage d'ordre élevé. Celle-ci est basée sur le contrôle par une métrique de l'erreur d'interpolation induite par le maillage du domaine. Plus précisément, pour une solution donnée, l'erreur d'interpolation d'ordre  $k$  est paramétrée par la forme différentielle  $(k+1)^{\text{ième}}$  de cette solution, et le problème se réduit à trouver la plus grande ellipse incluse dans une ligne de niveau de cette différentielle. La méthode que nous avons mise au point théoriquement et numériquement est appelée "log-simplexe", et permet de produire des maillages adaptés d'ordre élevé dans un temps raisonnable, et ce en dimension 2 et 3. À l'occasion de l'International Meshing Roundtable 2016, ce travail a été présenté et publié. D'autres applications de cette méthode sont en cours d'exploitation, comme par exemple la génération de maillages adaptés courbes de surface, ou le couplage avec un solveur d'ordre élevé.

#### 4.11. Méthode d'immersion de frontières pour la mécanique des fluides

**Participants:** Frédéric Alauzet [correspondant], Rémi Feuillet, Adrien Loseille.

Dans les méthodes de résolution classiques des problèmes d'interaction fluide-structure, il est usuel de représenter l'objet de manière exacte dans le maillage, c'est-à-dire avec des éléments conformes à l'objet : le maillage possède des triangles dont une arête correspond avec le bord de la géométrie immergée. Cette méthode quoique plus précise est très coûteuse en préprocessing. C'est dans ce cadre qu'est introduite la notion d'immersion de frontière (embedded geometry en anglais). Cette méthode consiste à représenter la géométrie de manière fictive. Le maillage de calcul n'est de fait plus nécessairement conforme à la géométrie de l'objet. Il s'agit donc de s'intéresser aux modifications nécessaires sur les méthodes classiques pour faire un calcul dans le cadre de l'immersion de frontières. Cela concerne les conditions aux limites et l'avancée en temps. On s'intéresse également à l'adaptation de maillage pour le cas de l'immersion. La finalité de tout ce travail est d'effectuer des calculs de coefficients aérodynamiques (portance, traînée) et de trouver des résultats du même ordre de précision que ceux en géométrie inscrite.

#### 4.12. Boundary layer mesh generation

**Participants:** Frédéric Alauzet [correspondant], Adrien Loseille, Dave Marcum.

A closed advancing-layer method for generating high-aspect-ratio elements in the boundary layer (BL) region has been developed. This approach provides an answer to the mesh generation robustness issue as it starts from an existing valid mesh and always guarantees a valid mesh in output. And, it handles very efficiently and naturally BL front collisions and it produces a natural smooth anisotropic blending between colliding layers. In addition, it provides a robust strategy to couple unstructured anisotropic mesh adaptation and high-aspect-ratio element pseudo-structured BL meshes. To this end, the mesh deformation is performed using the metric field associated with the given anisotropic meshes to maintain the adaptivity while inflating the BL. This approach utilizes a recently developed connectivity optimization based moving mesh strategy for deforming the volume mesh as the BL is inflated. In regards to the BL mesh generation, it features state-of-art capabilities, including, optimal normal evaluation, normal smoothing, blended BL termination, mixed-elements BL, varying growth rate, and BL imprinting on curved surfaces. Results for typical aerospace configurations are presented to assess the proposed strategy on both simple and complex geometries.

## GECO Project-Team

## 7. New Results

### 7.1. New results

Let us list some the new results in sub-Riemannian geometry and hypoelliptic diffusion obtained by GECO's members.

- On a sub-Riemannian manifold we define two type of Laplacians. The macroscopic Laplacian  $\Delta_\omega$ , as the divergence of the horizontal gradient, once a volume  $\omega$  is fixed, and the microscopic Laplacian, as the operator associated with a geodesic random walk. In [1] we consider a general class of random walks, where all sub-Riemannian geodesics are taken in account. This operator depends only on the choice of a complement  $c$  to the sub-Riemannian distribution, and is denoted  $L_c$ . We address the problem of equivalence of the two operators. This problem is interesting since, on equiregular sub-Riemannian manifolds, there is always an intrinsic volume (e.g. Popp's one  $P$ ) but not a canonical choice of complement. The result depends heavily on the type of structure under investigation:
  - On contact structures, for every volume  $\omega$ , there exists a unique complement  $c$  such that  $\Delta_\omega = L_c$ .
  - On Carnot groups, if  $H$  is the Haar volume, then there always exists a complement  $c$  such that  $\Delta_H = L_c$ . However this complement is not unique in general.
  - For quasi-contact structures, in general,  $\Delta_P = L_c$  for any choice of  $c$ . In particular,  $L_c$  is not symmetric w.r.t. Popp's measure. This is surprising especially in dimension 4 where, in a suitable sense,  $\Delta_P$  is the unique intrinsic macroscopic Laplacian.

A crucial notion that we introduce here is the  $N$ -intrinsic volume, i.e. a volume that depends only on the set of parameters of the nilpotent approximation. When the nilpotent approximation does not depend on the point, a  $N$ -intrinsic volume is unique up to a scaling by a constant and the corresponding  $N$ -intrinsic sub-Laplacian is unique. This is what happens for dimension smaller or equal than 4, and in particular in the 4-dimensional quasi-contact structure mentioned above.

- In sub-Riemannian geometry the coefficients of the Jacobi equation define curvature-like invariants. We show in [4] that these coefficients can be interpreted as the curvature of a canonical Ehresmann connection associated to the metric, first introduced by Zelenko and Li. We show why this connection is naturally nonlinear, and we discuss some of its properties.
- In [6] we study the cut locus of the free, step two Carnot groups  $\mathbb{G}_k$  with  $k$  generators, equipped with their left-invariant Carnot-Carathéodory metric. In particular, we disprove the conjectures on the shape of the cut loci proposed by O. Myasnychenko, by exhibiting sets of cut points  $C_k \subset \mathbb{G}_k$  which, for  $k \geq 4$ , are strictly larger than conjectured ones. While the latter were, respectively, smooth semi-algebraic sets of codimension  $\Theta(k^2)$  and semi-algebraic sets of codimension  $\Theta(k)$ , the sets  $C_k$  are semi-algebraic and have codimension 2, yielding the best possible lower bound valid for all  $k$  on the size of the cut locus of  $\mathbb{G}_k$ . Furthermore, we study the relation of the cut locus with the so-called abnormal set. Finally, and as a straightforward consequence of our results, we derive an explicit lower bound for the small time heat kernel asymptotics at the points of  $C_k$ . The question whether  $C_k$  coincides with the cut locus for  $k \geq 4$  remains open.

New results on complex systems with hybrid or switched components are the following.

- In [2] we address the exponential stability of a system of transport equations with intermittent damping on a network of  $N \geq 2$  circles intersecting at a single point  $O$ . The  $N$  equations are coupled through a linear mixing of their values at  $O$ , described by a matrix  $M$ . The activity of the intermittent damping is determined by persistently exciting signals, all belonging to a fixed class. The main result is that, under suitable hypotheses on  $M$  and on the rationality of the ratios between the lengths of

the circles, such a system is exponentially stable, uniformly with respect to the persistently exciting signals. The proof relies on an explicit formula for the solutions of this system, which allows one to track down the effects of the intermittent damping.

- In [3] we study the relative controllability of linear difference equations with multiple delays in the state by using a suitable formula for the solutions of such systems in terms of their initial conditions, their control inputs, and some matrix-valued coefficients obtained recursively from the matrices defining the system. Thanks to such formula, we characterize relative controllability in time  $T$  in terms of an algebraic property of the matrix-valued coefficients, which reduces to the usual Kalman controllability criterion in the case of a single delay. Relative controllability is studied for solutions in the set of all functions and in the function spaces  $L^p$  and  $C^k$ . We also compare the relative controllability of the system for different delays in terms of their rational dependence structure, proving that relative controllability for some delays implies relative controllability for all delays that are “less rationally dependent” than the original ones, in a sense that we make precise. Finally, we provide an upper bound on the minimal controllability time for a system depending only on its dimension and on its largest delay.

Finally, a new contribution has been proposed in the domain of the control of quantum systems. More precisely, in [5] we consider the bilinear Schrödinger equation with discrete-spectrum drift. We show, for  $n \in \mathbb{N}$  arbitrary, exact controllability in projections on the first  $n$  given eigenstates. The controllability result relies on a generic controllability hypothesis on some associated finite-dimensional approximations. The method is based on Lie-algebraic control techniques applied to the finite-dimensional approximations coupled with classical topological arguments issuing from degree theory.

## POEMS Project-Team

## 7. New Results

### 7.1. New schemes for time-domain simulations

#### 7.1.1. *Solving the Homogeneous Isotropic Linear Elastodynamics Equations Using Potentials*

**Participant:** Patrick Joly.

This work is done in collaboration with Sébastien Impériale (EPI M3DISIM) and Jorge Albella from the University of Santiago de Compostela. We consider the numerical solution of 2D elastodynamic equations using the decomposition of the displacement fields into potentials. This appears as a challenge for finite element methods. We address here the particular question of free boundary conditions. A stable (mixed) variational formulation of the evolution problem is proposed based on a clever choice of Lagrange multipliers. This is expected to be efficient when the velocity of shear waves is much smaller than the velocity of pressure waves, since one can adapt the discretization to each type of waves.

#### 7.1.2. *Discontinuous Galerkin method with high-order absorbing boundary conditions*

**Participant:** Axel Modave.

This work is done in collaboration with Andreas Atle from TOTAL, Jesse Chan from Rice University and Tim Warburton from Virginia Tech.

Discontinuous Galerkin finite element schemes exhibit attractive features for large-scale time-domain wave-propagation simulations on modern parallel architectures (e.g. GPU clusters). For many applications, these schemes must be coupled with non-reflective boundary treatments to limit the size of the computational domain without losing accuracy or computational efficiency, which remains a challenging task.

We propose a combination of a nodal discontinuous Galerkin method with high-order absorbing boundary conditions (HABCs) for cuboidal computational domains. Compatibility conditions are derived for HABCs intersecting at the edges and the corners of a cuboidal domain. We propose a GPU implementation of the computational procedure, which results in a multidimensional solver with equations to be solved on 0D, 1D, 2D and 3D spatial regions. Numerical results demonstrate both the accuracy and the computational efficiency of our approach.

### 7.2. Integral equations

#### 7.2.1. *Mesh adaptation for the fast multipole method in acoustics*

**Participants:** Faisal Amlani, Stéphanie Chaillat.

This work is done in collaboration with Adrien Loseille (EPI Gamma3). We introduce a metric-based anisotropic mesh adaptation strategy for the fast multipole accelerated boundary element method (FM-BEM) applied to exterior boundary value problems of the three-dimensional Helmholtz equation. The present methodology is independent of discretization technique and iteratively constructs meshes refined in size, shape and orientation according to an *optimal* metric reliant on a reconstructed Hessian of the boundary solution. The resulting adaptation is anisotropic in nature and numerical examples demonstrate optimal convergence rates for domains that include geometric singularities such as corners and ridges.

#### 7.2.2. *Coupling integral equations and high-frequency methods*

**Participants:** Marc Bonnet, Marc Lenoir, Eric Lunéville, Laure Pesudo, Nicolas Salles.



This theme concerns wave propagation phenomena which involve two different space scales, namely, on the one hand, a medium scale associated with lengths of the same order of magnitude as the wavelength (medium-frequency regime) and on the other hand, a long scale related to lengths which are large compared to the wavelength (high-frequency regime). Integral equation methods are known to be well suited for the former, whereas high-frequency methods such as geometric optics are generally used for the latter. Because of the presence of both scales, both kinds of simulation methods are simultaneously needed but these techniques do not lend themselves easily to coupling.

A first situation, considered by Marc Lenoir, Eric Lunéville and Nicolas Salles, is the scattering of an acoustic wave by two sound-hard obstacles: a large obstacle subject to high-frequency regime relatively to the wavelength and a small one subject to medium-frequency regime. The technique proposed in this case consists in an iterative method which allows to decouple the two obstacles and to use Geometric Optics for the large obstacle and Boundary Element Method for the small obstacle. The method is implemented on the XLife++ library developed in the lab.

The second situation, undertaken in the context of the PhD thesis of Laure Pesudo, is the subject of a partnership with CEA LIST and a collaboration with Francis Collino. Modelling ultrasonic non destructive testing (NDT) experiments simultaneously involves the scattering of waves by defects of moderate size (for which discretization-based methods such as the BEM are appropriate) and propagation over large distances (requiring high-frequency approximations). A new hybrid strategy between the boundary element method (BEM) and ray tracing is proposed in order to allow the accurate and quick simulation of high frequency Non Destructive Testing (NDT) configurations involving diffraction phenomena. Results from its implementation to 2D acoustic NDT-like diffraction configurations have been obtained. The strategy proposed is however generic, and can be extended to three-dimensional configurations and elastodynamic wave propagation.

### 7.2.3. *Dynamic soil-structure interaction*

**Participants:** Marc Bonnet, Stéphanie Chaillat, Zouhair Adnani.

This work, undertaken in the context of the PhD thesis of Zouhair Adnani (CIFRE partnership with EDF), concerns the simulation of dynamic soil-structure interaction (SSI) in connection with seismic assessment of civil engineering structures. Because of the complementary specificities of the finite element method (FEM) and the boundary element method (BEM), it is natural to use the BEM to model the unbounded soil domain, while the FEM is applied for the bounded region comprising the structure undergoing assessment, and possibly its close-range soil environment.

The originality of this work is to formulate, implement, and evaluate on realistic test examples, a computational strategy that combines the fast multipole accelerated boundary element method (visco-elastodynamic COFFEE solver), and the EDF in-house FEM code Code\_Aster. In a preliminary phase, the evaluation of transient elastodynamic responses via the Fourier synthesis of frequency domain solutions computed using COFFEE (see Section 5.1 ) has been studied on several test problems, achieving substantial improvements of computational efficiency for this component of SSI analysis.

The coupling between the two methods is then done in a black-box fashion with the substructuring method by computing the soil impedance (i.e. elastodynamic Poincaré-Steklov) operator relating forces to displacements on the FEM-BEM coupling interface. One of the main challenges is that this operator cannot be assembled due to the iterative nature of the FM-BEM and the potentially large number of degrees of freedom supported by the interface. To reduce the computational costs, we instead compute its projection on a reduced basis of interface modes, which requires to perform as many FM-BEM calculations as interface modes selected. This approach has so far been compared to reference solutions and validated for superficial and buried foundations on homogeneous or heterogeneous soil.

### 7.2.4. *Volume Integral Formulations*

**Participant:** Marc Bonnet.

Volume integral equations (VIEs), also known as Lippmann-Schwinger integral equations, arise naturally when considering the scattering of waves by penetrable, and possibly heterogeneous, inhomogeneities embedded in a homogeneous background medium (for which a fundamental solution is explicitly known). Their derivation and use in e.g. acoustics, elastodynamics or electromagnetism goes back several decades. Since their geometrical support is confined to the spatial region where material properties differ from the background, VIEs are in particular useful for the derivation and justification of homogenized or asymptotic models (the latter providing our main motivation for this study, in connection with [section gradient topologique]). By directly linking remote measurements to unknown inhomogeneities, VIEs also provide a convenient forward modeling approach for medium imaging inverse problems. However, whereas the theory of boundary integral equations is extensively documented, the mathematical properties of VIEs have undergone a comparatively modest coverage, much of it pertaining to electromagnetic scattering problems.

In this work, we investigate the solvability of VIE formulations arising in elastodynamic scattering by penetrable obstacles. The elasticity tensor and mass density are allowed to be smoothly heterogeneous inside the obstacle and may be discontinuous across the background-obstacle interface, the background elastic material being homogeneous. Both materials may be anisotropic, within certain limitations for the background medium.

Towards this goal, we have introduced a modified version of the singular volume integral equation (SVIE) governing the corresponding elastostatic (i.e. zero frequency) problem, and shown it to be of second kind involving a contraction operator, i.e. solvable by Neumann series, for any background material and inhomogeneity material and geometry. Then, the solvability of VIEs for frequency-domain elastodynamic scattering problems follows by a compact perturbation argument, assuming uniqueness to be established. In particular, in an earlier work, we have established a uniqueness result for the anisotropic background case (where, to avoid difficulties associated with existing radiation conditions for anisotropic elastic media, we have proposed an alternative definition of the radiating character of solutions, which is equivalent to the classical Sommerfeld-Kupradze conditions for the isotropic background case). This investigation extends work by Potthast (1999) on 2D electromagnetic problems (transverse-electric polarization conditions) involving orthotropic inhomogeneities in a isotropic background, and contains recent results on the solvability of Eshelby's equivalent inclusion problem as special cases. The proposed modified SVIE is also useful for fixed-point iterative solution methods, as Neumann series then converge (i) unconditionally for static problems and (ii) on some inhomogeneity configurations for which divergence occurs with the usual SVIE for wave scattering problems.

## 7.3. Domain decomposition methods

### 7.3.1. Transparent boundary conditions with overlap in unbounded anisotropic media

**Participants:** Anne-Sophie Bonnet-Ben Dhia, Sonia Fliss, Yohanes Tjandrawidjaja.

This work is done in the framework of the PhD of Yohanes Tjandrawidjaja, funded by CEA-LIST, in collaboration with Vahan Baronian from CEA. This follows the PhD of Antoine Tonnoir (now Assistant Professor at Insa of Rouen) who developed a new approach, the Half-Space Matching Method, to solve scattering problems in 2D unbounded anisotropic media. The objective is to extend the method to a 3D plate of finite width.

In 2D, our approach consists in coupling several plane-waves representations of the solution in half-spaces surrounding the defect with a FE computation of the solution around the defect. The difficulty is to ensure that all these representations match, in particular in the infinite intersections of the half-spaces. It leads to a Fredholm formulation which couples, via integral operators, the solution in a bounded domain including the defect and some traces of the solution on the edge of the half-planes.

The extension to 3D elastic plates requires some generalizations of the formulation which are not obvious. In particular, we have to use Neumann traces of the solution, which raises difficult theoretical questions.

As a first step, we have considered a scattering problem outside a convex polygonal scatterer for a general class of boundary conditions, using the Half-Space Matching Method. Using the Mellin Transform, we are able to show that this system is coercive + compact in presence of dissipation. We have also proved the convergence of the discrete method with respect to the size of truncation of the Fourier integrals, and with respect to the mesh size. This is the object of a paper that has been submitted.

In parallel, the main ingredient for the numerical method in 3D has been developed. It is the modal/Fourier representation of the elastic field in a semi-infinite plate, as a function of the trace of the displacement and of the normal stress. This has been done in the isotropic case.

### 7.3.2. Domain Decomposition Methods for the neutron diffusion equation

**Participants:** Patrick Ciarlet, Léandre Giret.

This work is done in collaboration with Erell Jamelot (CEA-DEN, Saclay) and Félix Kpadonou (LMV, UVSQ). Studying numerically the steady state of a nuclear core reactor is expensive, in terms of memory storage and computational time. In its simplest form, one must solve a neutron diffusion equation with low-regularity solutions, discretized by mixed finite element techniques, within a loop. Iterating in this loop allows to compute the smallest eigenvalue of the system, which determines the critical, or non-critical, state of the core. This problem fits within the framework of high performance computing so, in order both to optimize the memory storage and to reduce the computational time, one can use a domain decomposition method, which is then implemented on a parallel computer: this is the strategy used for the APOLLO3 neutronics code. The development of non-conforming DD methods for the neutron diffusion equation with low-regularity solutions has recently been finalized, cf. [PC,EJ,FK'1x]. The theory for the eigenvalue problem is also understood. The current research now focuses on the numerical analysis of the full suite of algorithms to prove convergence for the complete multigroup SPN model (which involves coupled diffusion equations).

## 7.4. Wave propagation in complex media

### 7.4.1. Perfectly Matched Layers in plasmas and metamaterials

**Participants:** Eliane Bécache, Maryna Kachanovska.

In this work we consider the problem of the modelling of 2D anisotropic dispersive wave propagation in unbounded domains with the help of perfectly matched layers (PML). We study the Maxwell equations in passive media with the frequency-dependent diagonal tensor of dielectric permittivity and magnetic permeability. An application of the traditional PMLs to this kind of problems often results in instabilities, due to the presence of so-called backward propagating waves. In previous works, this instability was overcome with the help of the frequency-dependent correction of the PML, for isotropic dispersive models.

We show that this idea can be extended to a more general class of models (uniaxial cold plasma, some anisotropic metamaterials). Crucially, we base our considerations on the Laplace-domain techniques. This allows to avoid the analysis of the group and phase velocity (used before) but study (rather formally) coercivity properties of the sesquilinear form corresponding to the PML model in the Laplace domain. The advantage of this method is that it permits to treat problems with dissipation, and provides an intuition on how to obtain explicit energy estimates for the resulting PML models in the time domain. However, such analysis does not allow to obtain easily the necessary stability condition of the PML. We demonstrate that the necessary stability conditions of the PML can be rewritten for a class of models in a form that is easy to verify, and demonstrate that these conditions are sufficient for the stability of the new PMLs with the help of the Laplace-domain techniques. Thanks to the Laplace domain analysis, we are able to rewrite a PML system in the time domain in a form, for which the derivation of energy estimates is simplified (compared to other formulations).

### 7.4.2. Transparent Boundary Conditions for the Wave Propagation in Fractal Trees

**Participants:** Patrick Joly, Maryna Kachanovska.

This work, done in collaboration with Adrien Semin (Postdoctoral student at the Technische Universität of Berlin), is dedicated to an efficient resolution of the wave equation in self-similar trees (e.g. wave propagation in a human lung). In this case it is possible to avoid computing the solution at deeper levels of the tree by using the transparent boundary conditions. The corresponding DtN operator is defined by a functional equation in the frequency domain. In this work we propose and compare two approaches to the discretization of this operator in the time domain. The first one is based on the multistep convolution quadrature, while the second one stems from the rational approximations.

#### **7.4.3. High order transmission conditions between homogeneous and homogenized periodic half-spaces**

**Participants:** Sonia Fliss, Clément Beneteau.

This work is a part of the PhD of Valentin Vinales, and is done in collaboration with Xavier Claeys from Paris 6 University and EPI ALPINE. It is motivated by the fact that classical homogenization theory poorly takes into account interfaces, which is particularly unfortunate when considering negative materials, because important phenomena arise precisely at their surface (plasmonic waves for instance). To overcome this limitation, we want to construct high order transmission conditions. For now, we have treated the case of a plane interface between a homogeneous and a periodic half spaces. Using matched asymptotic techniques, we have derived high order transmission conditions. We have then introduced an approximate model associated to this asymptotic expansions which consists in replacing the periodic media by an effective one but the transmission conditions are not classical. The obtained conditions involve Laplace- Beltrami operators at the interface and requires to solve cell problems in periodicity cell (as in classical homogenisation) and in infinite strips (to take into account the phenomena near the interface). We establish well posedness for the approximate and error estimate which justify that this new model is more accurate near the interface and in the bulk. From a numerical point of view, the only difficulty comes from the problems set in infinite strips (one half is homogeneous and the other is periodic). This is overcome using DtN operators corresponding to the homogeneous and the periodic media. The numerical results confirm the theoretical ones.

### **7.5. Spectral theory and modal approaches for waveguides**

#### **7.5.1. Modal analysis of electromagnetic dispersive media**

**Participants:** Christophe Hazard, Sandrine Paolantoni.

We investigate the spectral effects of an interface between a usual dielectric and a negative-index material (NIM), that is, a dispersive material whose electric permittivity and magnetic permeability become negative in some frequency range. We consider here an elementary situation, namely, 1) the simplest existing model of NIM : the Drude model (for which negativity occurs at low frequencies); 2) a two-dimensional scalar model derived from the complete Maxwell's equations; 3) the case of a simple bounded cavity: a camembert-like domain partially

filled with a portion of non dissipative Drude material. Because of the frequency dispersion (the permittivity and permeability depend on the frequency), the spectral analysis of such a cavity is unusual since it yields a nonlinear eigenvalue problem. Thanks to the use of an additional unknown, we show how to linearize the problem and we present a complete description of the spectrum.

#### **7.5.2. Formulation of invisibility in waveguides as an eigenvalue problem**

**Participants:** Antoine Bera, Anne-Sophie Bonnet-Ben Dhia.

This work is done in collaboration with Lucas Chesnel from EPI DEFI and Vincent Pagneux from Laboratoire d'Acoustique de l'Université du Maine. A scatterer placed in an infinite waveguide may be *invisible* at particular discrete frequencies. We consider two different definitions of invisibility: no reflection (but possible conversion or phase shift in transmission) or perfect invisibility (the scattered field is exponentially decaying at infinity). Our objective is to show that the invisibility frequencies can be characterized as eigenvalues of some spectral problems. Two different approaches are used for the two different definitions of invisibility, leading to non-selfadjoint eigenvalue problems.

More precisely, for the case of no-reflection, we define a new complex spectrum which contains as real eigenvalues the frequencies where perfect transmission occurs and the frequencies corresponding to trapped modes. In addition, we also obtain complex eigenfrequencies which can be exploited to predict frequency ranges of good transmission. Our approach relies on a simple but powerful idea, which consists in using PMLs in an original manner: while in usual PMLs the same stretching parameter is used in the inlet and the outlet, here we take them as two complex conjugated parameters. As a result, they select ingoing waves in the inlet and outgoing waves in the outlet, which is exactly what arises when the transmission is perfect. This simple idea works very well, and provides useful information on the transmission qualities of the system, much faster than any traditional approach.

### 7.5.3. *Transparent boundary conditions for general waveguide problems*

**Participants:** Anne-Sophie Bonnet-Ben Dhia, Sonia Fliss.

In this work, done in collaboration with Antoine Tonnoir from INSA of Rouen, we propose a construction of transparent boundary conditions which can be used for quite general waveguide problems. Classical Dirichlet-to-Neumann maps used for homogeneous acoustic waveguides can be constructed using separation of variables and the orthogonality of the modes on one transverse section. These properties are also important for the mathematical and numerical analysis of problems involving DtN maps. However this framework does not extend directly to stratified, anisotropic or periodic waveguides and for Maxwell's or elastic equations. The difficulties are that (1) the separation of variables is not always possible and (2) the modes of the waveguides are not necessarily orthogonal on the transverse section. We propose an alternative to the DtN maps which uses two artificial boundaries and is constructed using a more general orthogonality property.

## 7.6. Inverse problems

### 7.6.1. *Linear Sampling Method with realistic data in waveguides*

**Participants:** Laurent Bourgeois, Arnaud Recoquillay.

Our activities in the field of inverse scattering in waveguides with the help of sampling methods has now a quite long history. We now intend to apply these methods in the case of realistic data, that is surface data in the time domain. This is the subject of the PhD of Arnaud Recoquillay. It is motivated by Non Destructive Testing activities for tubular structures and is the object of a partnership with CEA List (Vahan Baronian).

Our strategy consists in transforming the time domain problem into a multi-frequency problem by the Fourier transform. This allows us to take full advantage of the established efficiency of modal frequency-domain sampling methods. We have already proved the feasibility of our approach in the 2D acoustic and 2D elastic case. In particular, we have shown how to optimize the number of sources/receivers and the distance between them in order to obtain the best possible identification result. Experiments are currently carried in CEA.

### 7.6.2. *The "exterior approach" to solve inverse obstacle problems*

**Participants:** Laurent Bourgeois, Arnaud Recoquillay.

We consider some inverse obstacle problems in acoustics by using a single incident wave, either in the frequency or in the time domain. When so few data are available, a Linear Sampling type method cannot be applied. In order to solve those kinds of problem, we propose an "exterior approach", coupling a mixed formulation of quasi-reversibility and a simple level set method. In such iterative approach, for a given defect  $D$ , we update the solution  $u$  with the help of a mixed formulation of quasi-reversibility while for a given solution  $u$ , we update the defect  $D$  with the help of a level set method based on a Poisson problem. The case of data in the frequency domain has been studied for the waveguide geometry. We currently investigate the case of data in a finite time domain.

### 7.6.3. *A continuation method for building large invisible obstacles in waveguides*

**Participants:** Antoine Bera, Anne-Sophie Bonnet-Ben Dhia.

In collaboration with Lucas Chesnel (EPI DEFI) and Sergei Nazarov (Saint-Petersburg University), we consider time harmonic acoustic problems in waveguides. We are interested in finding localized perturbations of a straight waveguide which are not detectable in the far field, as they produce neither reflection nor conversion of propagative modes. In other words, such *invisible* perturbation produces a scattered field which is exponentially decaying at infinity in the two infinite outlets of the waveguide.

In our previous contributions, we found a way to build smooth and small perturbations of the boundary which were almost invisible, in the sense that they were producing (in the monomode regime) no reflexions but maybe a phase shift in transmission.

The method is constructive and has been validated numerically. But the drawback is that it is limited to low frequency and small perturbations. During the last year, we have shown that the previous idea can be combined with a continuation method, in order to get larger invisible perturbations at higher frequency.

## 7.7. Aeroacoustics

### 7.7.1. Time-harmonic acoustic scattering in a vortical flow

**Participants:** Antoine Bensalah, Patrick Joly, Jean-François Mercier.

This activity is done in the framework of the PhD of Antoine Bensalah, in partnership with Airbus Group. We study the time-harmonic acoustic radiation in a fluid in a general flow which is not curl free, but has restricted vortical areas. The objective is to take into account the complicated coupling between acoustics and hydrodynamics. The Galbrun approach developed previously in 2D is too expensive in terms of degrees of freedom for 3D simulations. As an alternative, we propose to consider instead the Goldstein equations, which are vectorial only in the vortical areas and remain scalar elsewhere.

To begin with, we aim at determining the acoustic field radiated in 2D by a time-harmonic source in a fluid in flow. Goldstein's equations are proved to be well-posed outside a spectrum of frequencies corresponding to resonant streamlines. This band spectrum is explicitly determined for two simple geometries (an annular domain and a rectangular one with periodic conditions). Then the full model is shown to be well-posed under a coercivity condition, implying a subsonic flow with a small enough vorticity.

### 7.7.2. Propagation of solitons through Helmholtz resonators

**Participant:** Jean-François Mercier.

With Bruno Lombard (Laboratoire de Mécanique et Acoustique of Marseille), we study the propagation of nonlinear solitary acoustic waves in a 1D waveguide connected to a lattice of Helmholtz resonators. We start from an homogenized model of the literature, consisting of two coupled equations evolution: a nonlinear PDE describing acoustic waves (similar to the Burgers equation), and a linear ODE describing oscillations in the Helmholtz resonators. We have already developed a numerical modeling of this model and we have compared simulations with experimental data.

The drawback of the homogenized model is that all the resonators must be the same. In particular the reflection of an incident wave by a defect cannot be considered. To remedy this limitation, we have proposed an extension of the model, predicting two-way propagation across variable resonators. Thanks to a new discrete description of the resonators, the improved model takes into account two important features: resonators of different strengths and back-scattering effects. Comparisons with experimental data show that a closer agreement is obtained.

## RANDOPT Team

## 6. New Results

### 6.1. Theory

**Participants:** Anne Auger, Nikolaus Hansen.

The paper “Information-Geometric Optimization Algorithms: A Unifying Picture via Invariance Principles” has finally been published in the JMLR journal [3]. In this paper in collaboration with Yann Ollivier in particular, we lay the ground of stochastic optimization by means of information geometry. We provide a unified framework for stochastic optimization on arbitrary search spaces that allow to recover well-known algorithms on continuous or discrete search spaces and put them under the same umbrella of Information Geometric Optimization.

When analyzing the stability of Markov chains stemming from comparison-based stochastic algorithms, we are facing difficulties due to the fact that the Markov chains have the following form  $\Phi_{t+1} = F(\Phi_t, U_{t+1})$  where  $\{U_t : t \geq 0\}$  are i.i.d. random vectors and  $F$  is a discontinuous function. The discontinuity comes from the comparison-based property of the algorithms. If  $F$  were  $C^\infty$  or  $C^1$  we could prove easily stability properties like irreducibility and show that compact are small sets by investigating the underlying control model and showing that it has globally attracting states where controllability conditions hold using results developed by Sean Meyn and co-authors.

In the paper [2], we found that we can actually generalize to a great extent the results by Meyn to the case where  $\Phi_{t+1} = F(\Phi_t, \alpha(\Phi_t, U_{t+1}))$  where  $F$  is  $C^1$  and  $\alpha$  is discontinuous but such that  $\alpha(x, U)$  admits a lower-semi continuity density. We have proposed verifiable conditions for the irreducibility and aperiodicity and shown that compact sets are small sets.

The development of evolution strategies has been greatly driven by so-called progress rate or quality gain analysis where simplification assumptions are made to obtain quantitative estimate of progress in one step and deduce from it how to set different parameters like recombination weights, learning rates ...

This theory while very useful often relied on approximations that were not always well appraised, justified or clearly stated. We have been in the past rigorously deriving different progress rate results and related them to bounds on convergence rates. We have investigated rigorously the quality gain (that is progress measured in terms of objective function) on general convex quadratic functions using weighted recombination. This allowed to derive the dependency of the convergence rate of evolution strategies with respect to the eigenspectrum of the Hessian matrix of convex-quadratic function as well as give hints on how to set learning rate [4] and [9].

### 6.2. Novel Constraint Handling

**Participants:** Asma Atamna, Anne Auger, Nikolaus Hansen.

In the context of constrained optimization, we have investigated to use augmented Lagrangian approaches to handle constraints. The originality of the approach is that the parameters of the augmented Lagrangian are adapted online. We have shown sufficient conditions for linear convergence of the ensuing methods with linear constraints [5]. Those sufficient conditions rely on finding a Markov chain candidate to be stable. This Markov chain derives from invariance properties of the algorithm. At the same time we have proposed an algorithm variant for the  $(\mu/\mu, \lambda)$ -CMA-ES and an arbitrary number of constraints.

In [10], we have investigated the linear convergence question on the point of view of invariance. We have analyzed the invariances of adaptive algorithms handling constraints with augmented Lagrangian: we have shown that invariance to monotonic transformation of the objective functions is lost but that a subclass of invariance can and should be preserved, namely affine transformation of the objective function and scaling of the constraint by a positive constant.



### 6.3. Benchmarking

**Participants:** Anne Auger, Dimo Brockhoff, Nikolaus Hansen, Umut Batu, Dejan Tutar.

In his thesis, Ouassim AitElHara has been investigating the benchmarking of algorithms in large dimensions [1]. In this context, the first steps for a testbed of the COCO platform in large dimension have been done. Particularly, the methodology for building a large-scale testbed has been defined: it consists in replacing the usual orthogonal transformation by block-diagonal orthogonal matrices multiplied to the left and to the right by permutation matrices. While still under testing, we expect to be able to release the large-scale testbed in the coming year.

The population size is one of the few parameters, a user is supposed to touch in the state-of-the-art optimizer CMA-ES. In [7], a new approach to also adapt the population size in CMA-ES is proposed and benchmarked on the bbob test suite of our COCO platform. The method is based on tracking the non-decrease of the median of the objective function values in each slot of  $S$  successive iterations to decide whether to increase or decrease or keep the population size in the next slot of  $S$  iterations. The experimental results show the efficiency of our approach on some multi-modal functions with adequate global structure.

Benchmarking budget-dependent algorithms (for which parameters might depend on the given budget of function evaluations) is typically done for a fixed (set of) budget(s). This, however, has the disadvantage that the reported function values at this budget are difficult to interpret. Furthermore, assessing performance in this way does not give any hints how an algorithm would behave for other budgets. Instead, we proposed in [8] a new way to do “Anytime Benchmarking of Budget-Dependent Algorithms” and implemented this functionality in our COCO platform. The idea is to run several experiments for varying budgets and report target-based runtimes in the form of empirical cumulative distribution functions (aka data profiles) as in the case of anytime algorithms.

### 6.4. Performance Assessment in Multiobjective Optimization

In the context of performance assessment in multiobjective optimization, two contributions have been made in 2017. First, we proposed a new visualization method to quantitatively assess the performance of multiobjective optimizers (for 2-objective problems) in the form of average runtime attainment functions [6]. The main idea is to display, for each point in objective space, when (in terms of the average runtime) it has been attained or in other words when it has been dominated by the algorithm. Second, we continued our effort towards automated benchmarking via our COCO platform and described a generic test suite generator that can produce test suites like the previous bbob-biobj test suite for an arbitrary number of objectives<sup>0</sup>.

### 6.5. Comparing Continuous Optimizers Platform

**Participants:** Anne Auger, Dimo Brockhoff, Nikolaus Hansen, Umut Batu, Dejan Tutar.

Thanks to the ADT support for Dejan Tušar (since November, previously supported by ESA) and Umut Batu (since July), as well as due to an increased effort from the core development team, we could progress on several aspects regarding our Comparing Continuous Optimizers platform (COCO, <https://github.com/numbbbo/coco>) in 2017.

Most notably, we provide the new functionality of data archives which allows to access the available data of 200+ algorithms much easier. We also made significant progress towards a first constrained test suite—in particular did we add logging support for constrained problems. The postprocessing module is finally python 3 compatible and zip files are supported as input files. The reference worst f-values-of-interest are exposed to the (multiobjective) solver, algorithms can now be displayed in the background, and simplified example experiment scripts (in python) are available (for both anytime, and budget-dependent algorithms, see also [8]). We also improved our continuous integration support, now using also CircleCI and AppVeyor in addition to Inria’s Jenkins system. Version 2.0, released in January 2017, saw new functionality of reference algorithms for the multiobjective test suite, a new format of reference algorithms that allow to use any existing data set

<sup>0</sup>Paper to be submitted to the Evolutionary Computation journal and to arXiv/HAL in January 2018.

as reference, improved HTML output and navigation, the COCO version number being part of the plots now, and new regression tests for all provided test suites.

COCO facts for 2017

- 218 issues closed
- major release 2.0 in January plus three additional releases, version 2.2 planned for January 2018
- 10 new contributors outside the main development team
- 14 new algorithm data sets made public (total: 233)

Currently, we are working on an entire rewrite of the postprocessing (ADT COCOPost project of Umut Batu), an improved cocoex module for proposing test suites, functions, data loggers etc. in python (ADT COCOPysuites of Dejan Tušar), a first constrained test suite (in particular Asma Atamna via the PGM0 project NumBER), and a large-scale test suite (part of Konstantinos Varelas' PhD thesis, based on the PhD work of Ouassim AitElHara).

Finally, we continued to use COCO also for teaching, in particular for the group project ("contrôle continue") of our Introduction to Optimization (about 40 Master students) and the Derivative-Free Optimization lectures at Université Paris-Sud (about 30 Master students).

## SELECT Project-Team

## 6. New Results

### 6.1. Model selection in Regression and Classification

**Participants:** Gilles Celeux, Pascal Massart, Sylvain Arlot, Jean-Michel Poggi, Kevin Bleakley.

The well-documented and consistent variable selection procedure in model-based cluster analysis and classification that Cathy Maugis (INSA Toulouse) designed during her PhD thesis in SELECT, makes use of stepwise algorithms which are painfully slow in high dimensions. In order to circumvent this drawback, Gilles Celeux, in collaboration with Mohammed Sedki (Université Paris XI) and Cathy Maugis, have recently submitted an article where variables are sorted using a lasso-like penalization adapted to the Gaussian mixture model context. Using this ranking to select variables, they avoid the combinatory problem of stepwise procedures. The performances on challenging simulated and real data sets are similar to the standard procedure, with a CPU time divided by a factor of more than a hundred.

In collaboration with Jean-Michel Marin (Université de Montpellier) and Olivier Gascuel (LIRMM), Gilles Celeux has continued research aiming to select a short list of models rather a single model. This short list is declared to be compatible with the data using a  $p$ -value derived from the Kullback-Leibler distance between the model and the empirical distribution. Furthermore, the Kullback-Leibler distances at hand are estimated through nonparametric and parametric bootstrap procedures. Different strategies are compared through numerical experiments on simulated and real data sets.

### 6.2. Estimator selection and statistical tests

**Participants:** Sylvain Arlot, Matthieu Lerasle.

G. Maillard, S. Arlot and M. Lerasle studied a method mixing cross-validation with aggregation, called aggregated hold-out (Agghoo), which is already used by several practitioners. Agghoo can also be related to bagging. According to numerical experiments, Agghoo can improve significantly cross-validation's prediction error, at the same computational cost; this makes it very promising as a general-purpose tool for prediction. This work provides the first theoretical guarantees on Agghoo, in the supervised classification setting, ensuring that one can use it safely: at worst, Agghoo performs like hold-out, up to a constant factor. A non-asymptotic oracle inequality is also proved, in binary classification under the margin condition, which is sharp enough to get (fast) minimax rates.

With G. Lecué, Matthieu Lerasle working on "learning from MOM's principles", showing that a recent procedure by Lugosi and Mendelson can be derived by applying Le Cam's "estimation from tests" procedure to MOM's tests. They also showed some robustness properties of these estimators, proving that the rates of convergence of this estimator are not downgraded even if some "outliers" have corrupted the dataset, and the other data have only first and second moments equal to that of the targeted probability distribution.

### 6.3. Statistical learning methodology and theory

**Participants:** Gilles Celeux, Serge Cohen, Christine Keribin, Michel Prenat, Kaniav Kamary, Sylvain Arlot, Benjamin Auder, Jean-Michel Poggi, Neska El Haouij, Kevin Bleakley, Matthieu Lerasle.

Gilles Celeux and Serge Cohen have started research in collaboration with Agnès Grimaud (UVSQ) to perform clustering of hyperspectral images which respects spatial constraints. This is a one-class classification problem where distances between spectral images are given by the  $\chi^2$  distance, while spatial homogeneity is associated with a single link distance.

Gilles Celeux continued his collaboration with Jean-Patrick Baudry on model-based clustering. This year, they started work on assessing model-based clustering methods on cytometry data sets. The interest of these is that they involve combining clustering and classification tasks in a unified framework.

Gillies Celeux and Julie Josse have started research on missing data for model-based clustering in collaboration with Christophe Biernacki (Modal, Inria Lille). This year, they have proposed a model for mixture analysis involving not missing-at-random mixtures.

In the framework of MASSICCC, Benjamin Auder and Gilles Celeux have started research on the graphical representation of model-based clusters. The aim of this is to better-display proximity between clusters.

For a long time unsolved, the consistency and asymptotic normality of the maximum likelihood and variational estimators of the latent block model were finally tackled and obtained in a joint work with V. Brault and M. Mariadassou.

J-M. Poggi (with R. Genuer, C. Tuleau-Malot, N. Villa-Vialaneix), have published an article on random forests in “big data” classification problems, and have performed a review of available proposals about random forests in parallel environments as well as on online random forests. Three variants involving subsampling, Big Data-bootstrap and MapReduce respectively were tested on two massive datasets, one simulated one, and the other, real-world data.

With G. Lecué, Matthieu Lerasle worked on robust machine learning by median-of-means, providing an alternative to the Lugosi and Mendelson approach based on median of means for learning. This alternative is easier to present and to analyse theoretically. Furthermore, they proposed an algorithm to approximate this estimator, which could not be done for Lugosi and Mendelson’s champions of tournaments (submitted).

## 6.4. Estimation for conditional densities in high dimension

**Participants:** Claire Lacour, Jeanne Nguyen.

Jeanne Nguyen is working on estimation for conditional densities in high dimension. Much more informative than the regression function, conditional densities are of high interest in recent methods, particularly in the Bayesian framework (studying the posterior distribution). Considering a specific family of kernel estimators, she is studying a greedy algorithm for selecting the bandwidth. Her method addresses several issues: avoiding the curse of high dimensionality under some suitably defined sparsity conditions, being computationally efficient using iterative procedures, and early variable selection, providing theoretical guarantees on the minimax risk.

## 6.5. Reliability

**Participants:** Gilles Celeux, Florence Ducros, Patrick Pamphile.

Since June 2015, in the framework of a CIFRE convention with Nexter, Florence Ducros has begun a thesis on the modeling of aging of vehicles, supervised by Gilles Celeux and Patrick Pamphile. This thesis should lead to designing an efficient maintenance strategy according to vehicle use profiles. Moreover, warranty cost calculations are made in the context of heterogeneous usages. This required estimations of mixtures and competing risk models in a highly-censored setting.

This year, Patrick Pamphile and Florence Ducros have published an article which proposes a two-component Weibull mixture model for modelling unobserved heterogeneity in heavily censored lifetime data collection. Performance of classical estimation methods (maximum of likelihood, EM, full Bayes and MCMC) are poor due to the high number of parameters and the heavy censoring. Thus, a Bayesian bootstrap method called Bayesian Restoration Maximization, was used. Sampling from the posterior distribution was obtained thanks to an importance sampling technique. Simulation results showed that, even with heavy censoring, BRM is effective both in term of estimate’s precision and computation times.

## 6.6. Statistical analysis of genomic data

**Participants:** Gilles Celeux, Christine Keribin, Yann Vasseur, Kevin Bleakley.

The subject of Yann Vasseur's PhD Thesis, supervised by Gilles Celeux and Marie-Laure Martin-Magniette (INRA URGV), was the inference of a regulatory network for Transcriptions Factors (TFs), which are specific genes, of *Arabidopsis thaliana*. For this, a transcriptome dataset with a similar number of TFs and statistical units was available. They reduced the dimension of the network to avoid high-dimensional difficulties. Representing this network with a Gaussian graphical model, the following procedure was defined:

1. *Selection step*: choose the set of TF regulators (supports) of each TF.
2. *Classification step*: deduce co-factor groups (TFs with similar expression levels) from these supports.

Thus, the reduced network would be built on the co-factor groups. Currently, several selection methods based on Gauss-LASSO and resampling procedures have been applied to the dataset. The study of stability and parameter calibration of these methods is in progress. The TFs are clustered with the Latent Block Model into a number of co-factor groups, selected with BIC or the exact ICL criterion. Since these models are built in an ad hoc way, Yann Vasseur has defined complex simulation tools to assess their performances in a proper way.

In collaboration with Benno Schwikowski, Iryna Nikolayeva and Anavaj Sakuntabhai (Pasteur Institute, Paris), Kevin Bleakley worked on using 2-d isotonic regression to predict dengue fever severity at hospital arrival using high-dimensional microarray gene expression data. Important marker genes for dengue severity have been detected, some of which now have been validated in external lab trials, and an article has now been submitted.

In collaboration with researchers from the Pasteur Institute, Kevin Bleakley worked on statistical tests in the context of research into what leads to dengue fever *without symptoms* as opposed to *with symptoms*. This work was published in *Science Translational Medicine*.

Kevin Bleakley has also collaborated with Inserm/Paris-Saclay researchers at Kremlin-Bicêtre hospital on cyclic transcriptional clocks and renal corticosteroid signaling, and has developed novel statistical tests for detecting synchronous signals. This work is submitted.

## 6.7. Model-based clustering for pharmacovigilance data

**Participants:** Gilles Celeux, Christine Keribin, Valérie Robert.

In collaboration with Pascale Tubert-Bitter, Ismael Ahmed and Mohamed Sedki, Gilles Celeux and Christine Keribin worked on the detection of associations between drugs and adverse events in the framework of the PhD of Valerie Robert, which was defended this year. At first, this team developed model-based clustering inspired by latent block models (LBMs), which consists of co-clustering rows and columns of two binary tables, imposing the same row ranking. This enabled it to highlight subgroups of individuals sharing the same drug profile, and subgroups of adverse effects and drugs with strong interactions. Furthermore, some sufficient conditions are provided to obtain identifiability of the model, and some results are shown for simulated data. The exact ICL criterion has been extended to this double block latent model. Through computer experiments, Valérie Robert demonstrated the interest of the proposed model, compared with standard contingency table analysis, to detect co-prescription and masking effects.

Furthermore, with V. Robert, C. Kerebin and G. Celeux showed that it can be useful to use an LBM model on a contingency table of drugs and adverse effects to do cluster initialization for dealing with individual's data.

## 6.8. Statistical rating and ranking of scientific journals

**Participants:** Gilles Celeux, Julie Josse, Jean-Louis Foulley.

In collaboration with Jean-Louis Foulley (Montpellier University), Gilles Celeux and Julie Josse have done research on the statistical rating and ranking of scientific journals. They have proposed Dirichlet multinomial Bayesian models for pagerank-type algorithms allowing self-citations to be excluded. The resulting methods were tested on a set of 47 scientific journals.

## 6.9. Statistical mathematics

**Participant:** Matthieu Lerasle.

In collaboration with R. Diel, Matthieu Lerasle published an article on nonparametric estimation for random walks in random environments. They proposed a non-parametric approach for estimating the distribution of the environment from the observation of one trajectory of a random walk in it. They obtained risk bounds in sup-norm for the cumulative distribution function of the environment.

## 6.10. Random graph theory

**Participant:** Matthieu Lerasle.

In collaboration with R. Chetrite and R. Diel, Matthieu Lerasle published an article on the number of potential winners in the Bradley-Terry model in random environments. They proposed the first mathematical study of the Bradley-Terry model where the values of players are i.i.d. realisations of some distribution. They proved that a Bradley-Terry tournament is fair (in the sense that the best player ends up with the largest number of victories) under a certain convexity condition on the tail distribution of the values. They also showed that this condition is sharp and provided sharp estimate of the number of potential winners when the condition fails.

He also collaborated with R. Diel and S. Le Corff on learning latent structures of large random graphs, investigating the possibility of estimating latent structure in sparsely observed random graphs. The main example was a Bradley-Terry tournament where each team has only played a few games. It is well known that individual values of the teams cannot be consistently estimated in this setting. They showed that their distribution on the other hand can be, and provide general tools for bounding the risk of the maximum likelihood estimator (submitted).

## TAU Team

## 7. New Results

### 7.1. Causality, Explainability, and Reliability

As said, the fairness, accountability and transparency of AI/ML need be assessed, measured and enforced to address the ethical impacts of data science on industry and society. TAU has started working toward improving the confidence in ML algorithms through three research directions.

#### 7.1.1. Causality

**Links between quality of life at work and company performance** Within the Amiqap project, a new approach to functional causal modeling from observational data called *Causal Generative Neural Networks* (CGNN) has been developed [45]. CGNN learns a generative model of the joint distribution of the observed variables, by minimizing the Maximum Mean Discrepancy between generated and observed data. An approximate learning criterion scales the computational cost of the approach to linear complexity in the number of observations. CGNN extensions, motivated by the redundancy of real-world variables, are under-going to achieve a causal model of the corporate- and human resource-related variables at the firm and economic sector levels.

**Generating Medical Data** This project, in collaboration with RPI (New York), aims to provide medical students with case studies, generated using CGNN . and fully preserving their confidentiality. We are exploring the benefits of using data generated by CGNNs in replacement for real data. Such data will preserve the structure of the original data, but the patient records will not represent real patients.

**Missing Data** Missing and corrupted data is a pervasive problem in data modeling. Our interest in this problem stems from 2 applications: epidemiology (in collaboration with Alain-Jacques Valleron, INSERM, and RPI New York) and computer vision (in collaboration with Aix-Marseille University and University of Barcelona). As it turns out, missing data is a causality problem [80]. In a paper under review, we outline the danger of imputing values in risk factor analysis in the presence of missing data. We are also preparing a challenge on the problem of “inpainting” to restore images with occlusions and to eliminate captions in movies.

**Power Networks** Berna Batu (post-doc Inria) explores causal modeling in time series to explain cascades of events. Other applications (e.g., in epidemiology) may develop from this approach.

#### 7.1.2. Explainability

**Explainable Machine Learning for Video Interviews** [21]. The challenge consisted in analyzing 15s videos, (human) annotated with the Big Five personality traits (Openness to experience, Conscientiousness, Extroversion, Agreeableness, and Neuroticism – sometimes referred to as OCEAN features). Human annotators also voted whether a given candidate should be invited for an interview. As organizers we provided a strong baseline system, which was based on deep learning methods having won part challenges. Only the winners outperformed quantitatively the baseline method.

The winner of the prediction challenge (BU-NKU) performed a very sophisticated analysis, combining face analysis (from the entire video) and scene analysis (from the first image), both analyses contributing to the final decision. Face analysis extracted spatio-temporal features from a pre-trained convolutional neural network (CNN) and using Gabor filters. Scene analysis features were also extracted with a pre-trained CNN. Acoustic features were extracted with the OpenSMILE tool. From the feature set, the personality traits are predicted with kernel ridge regression and from there on, the “invite for interview” is predicted using Random Forests.

For the explainability challenge, the BU-NKU team performed final predictions with a classifier based on binarized predicted OCEAN scores mapped to the binarized ground truth using a decision tree, a self-explanatory model that can be converted into an explicit recommender algorithm, using the trace of each decision from the root of the tree to the leaf. The verbal explanations are finally accompanied with the aligned image from the first face-detected frame and the bar graphs of corresponding mean normalized scores. Trained on the predicted OCEAN dimensions, this gave over 90% classification accuracy.

Note that another team (TUD), who did not enter the quantitative competition, nevertheless won first place ex-aequo with the BU-NKU team on the explainability challenge. Interestingly, they added facial features (using OpenFace) and text features (using published “Readability” features) in an effort to capture level of education from the sophistication of language, which was not captured by personality traits. They then used PCA to reduce dimension, and the coefficients of a linear regression model, fed back into the PCA model to generate explanations.

**Skin image classification** Also, the on-going collaboration with Roman Hossein Khonsari, surgeon at Necker hospital, is continuing, on the topic of skin disease image classification, with the goal of explaining how the trained neural networks produce their predictions, in order to be trusted by users. For this, we analyse the features that are learned, and show which ones are found in each image example.

### 7.1.3. Model systematic bias and reliability

A related problem is the reliability of models and their robustness to bias. We initiated research on this topic in the context of eliminating bias of High Energy Physics simulators. Discovering new particles relies on making accurate simulations of particle traces in detectors to diagnose collision events in high energy experiments. We are working on data from the ATLAS experiment at CERN, in collaboration with David Rousseau at the Laboratoire de l’Accélérateur Linéaire (LAL). We produced two preliminary studies on this topic: Adversarial learning to eliminate systematic errors: a case study in High Energy Physics [32] and Robust deep learning: A case study [43].

This line of research will extend to the calibration of other simulators, particularly energy transport and distribution simulators and medical data simulators, which we are working on in the context of other projects.

Beyond the calibration of simulators, we are also interested in using such approaches to foster fairness and de-bias data. For instance, in the “personality trait” data mentioned in the previous section, our analysis shows that labelers are biased favorably towards females (vs. males) and unfavorably towards African-American (vs. Caucasian or Asian).

## 7.2. Deep Learning and Information Theory

### 7.2.1. Convergence proofs for recurrent networks

Pierre-Yves Massé, in his PhD, defended Dec.2017 under the supervision of Yann Ollivier [3], obtained the very first rigorous results of convergence for online training of recurrent neural networks, by viewing them from the viewpoint of dynamical systems.

### 7.2.2. Fast algorithms for recurrent networks

Corentin Tallec (in his on-going PhD) and Yann Ollivier produced a new, faster algorithm for online training of recurrent networks, UORO, which is guaranteed to converge locally, and requires only linear time [49].

### 7.2.3. An explanation for LSTMs

The LSTM structure is currently the most popular recurrent network architecture. However, it is quite complex and very much ad hoc. Corentin Tallec (in his on-going PhD) and Yann Ollivier derived this architecture from first principles in a very simple axiomatic setting, simply by requiring that the model is invariant to arbitrary time deformations (such as accelerations, decelerations) in the data.



#### 7.2.4. *Bayesian neural networks*

The Bayesian approach to neural networks makes several suggestions. First, it suggests to artificially add a very specific amount of noise during training, as a protection against overfit. This has to be done carefully (Langevin dynamics) in relation with the Fisher information metric. Gaetan Marceau-Caron and Yann Ollivier demonstrated that this approach can be applied efficiently for neural networks [28] (Best paper award at GSI17).

Second, a Bayesian viewpoint can help select the right size for each layer in a neural network. A comparison to a theoretical model of an infinitely large network suggests ways to adapt learning rates and criteria to select or deselect neurons or even layers (Preliminary results in a preprint by Pierre Wolinski (PhD), Yann Ollivier and Guillaume Charpiat, in preparation.)

#### 7.2.5. *Kalman filtering and information geometry*

Filtering and optimization have been brought much closer by the following result [48]: the natural gradient in optimization is mathematically fully identical to the Kalman filter, for all probabilistic (machine learning) models. Even though both methods had been known for decades and were an important reference in their respective fields, they had not been brought together. The result extends to the non-iid setting (recurrent neural networks).

#### 7.2.6. *Computer vision*

The activity of computer vision is run jointly with the program of Looking at People (LaP) challenges [46]. We edited a book in Springer, which is a collection of tutorials and papers on gesture recognition [54], to which we contributed a survey chapter on deep-learning methods [34] a shorter version of which was published at the FG conference [17].

Several papers were published this year analyzing past LAP challenges. The “first impressions” challenge aimed at detecting personality traits from a few seconds of video. In [8], we demonstrate how deep residual networks attain state-of-the art performance on that task and lend themselves well to identifying which parts of the image is responsible for the final decision (interpretability). We also analyzed last years’ challenge on apparent age estimation from in still images and proposed improvements with deep residual networks [15]. A similar methodology based on deep-residual networks was applied to apparent personality trait analysis [24], [8].

#### 7.2.7. *Flexible deep learning architectures suitable to genetic data*

Genetic data is usually given in the form of matrices, one dimension standing for the different individuals studied and the other dimension standing for the DNA sites. These dimensions vary, depending on the individual sample size and on the DNA sequence length. On the other side, standard deep learning architectures require data of fixed size. We consequently search for suitable, flexible architectures, with as an application the prediction of the demographic history of a population given its genetic data (changes in the number of individuals through time). Théophile Sanchez, now PhD student, presented his work at the Junior Conference on Data Science and Engineering at Paris-Saclay [33]. To our knowledge this is the first attempt in the population genetics field to learn automatically from the raw data.

#### 7.2.8. *Image segmentation and classification*

Emmanuel Maggiori, PhD student in the Titane team, Inria Sophia-Antipolis, mainly supervised by Yuliya Tarabalka, and co-supervised by Guillaume Charpiat, defended his PhD thesis [73], on the topic of remote sensing image segmentation with neural networks. This year, an architecture for proposed to be able to deal with high resolution images; a benchmark was built and made public (as there is lack of those in the remote sensing community); and the output of segmentation predictions was turned into a vectorial representation by suitable automatic polygonization [9], [25], [26].

Through a collaboration with the company Armadillo within the ADAMme project, we have also worked on image classification with multiple tags. The database consists of 40 millions images, with thousands of different possible tags (each image is on averaged associated with 10 tags). We started from a ResNet pre-trained network and adapted it to our task. A demonstration of our results was performed at the annual review meeting of the project.

### 7.2.9. *Non-rigid image alignment*

Automatic image alignment was also studied. In remote sensing, the task consists in aligning satellite or aerial images with ground truth data such as OpenStreetMap's cadastral maps. This task is crucial in that such ground truth data is actually never well registered but is spatially deformed, preventing any further use by machine learning tools. Based on the analysis of multiple scale classical frameworks, a deep learning architecture was proposed to perform this task. This work is currently under submission to CVPR. On a related topic, in a collaboration with the start-up company Therapixel, we have been studying the registration of 3D medical images, but without any ground truth or template.

### 7.2.10. *Video analysis*

Time coherency is usually poorly handled in video analysis with neural networks. We have studied, on 3 different applications, different ways to take it better into account. First, in a collaboration with the Vision Institute, we studied different ways of incorporating neural networks in reinforcement learning approaches for the tracking of microbes with a motorized microscope. Second, in a collaboration with the SATIE team, we worked on the incorporation of optical flow for crowd density estimation, and, finally, in a collaboration with the Parietal team, we study how to link brain fMRI signals to the videos people are watching.

## 7.3. Algorithm Selection and Configuration

Automatic algorithm selection and configuration (hyper-parameter selection) depending on the problem instance at hand is a pervasive research topic in TAO, for both fundamental and practical reasons: in order to automatically deliver a peak performance on (nearly) every new problem instance, and to understand the specifics of a problem instance and the algorithm skills w.r.t. these specifics.

### 7.3.1. *Algorithm recommendation*

A collaborative filtering approach called Alors (Algorithm Recommender System) has been proposed to achieve algorithm selection [10], considering after [81] that a problem instance "likes better" algorithms with good performances on this instance. Alors, tackling a cold-start recommendation problem, enables to independently assess the quality of the benchmark data (representativity of the problem instances w.r.t. the algorithm portfolio) and the quality of the meta-features used to describe the problem instances. Experiments on SAT, CSP and ML benchmarks yield state-of-art performances in the former two domains; these good results contrast with the poor results obtained on the ML domain, blamed on the comparatively poor quality of the ML meta-features.

### 7.3.2. *AutoML and AutoDL*

Isabelle Guyon has organized [the AutoML challenge](#) (paper in preparation), proposing a series of algorithm selection and configuration problems of increasing difficulty. Following this successful challenge, a new challenge will be organized in collaboration with Google Zurich, specifically targeting the selection of deep network architectures (AutoDL: Automatic Deep learning) in five domains: Image; Video; Audio; Text; Customer demographic descriptors.

The expected result of the challenge is to alleviate the burden on data scientists to design a good architecture ("black art"), and to enforce the reproducibility of the results. In particular, this challenge will encourage advances regarding a few key research questions:

- How to make optimization algorithms more efficient without introducing more tunable parameters?
- How to efficiently automate the tuning of many hyper-parameters?
- How to automatically design or optimize a network architecture for a particular problem?
- How to further automate the learning process by directly learning how to learn?

### 7.3.3. *Per Instance Algorithm Configuration for Continuous Optimization*

Nacim Belkhir's PhD thesis (defended on Nov. 30., 2017) was centered on PIAC (Per Instance Algorithm Configuration) in the context of continuous optimization. After a detailed study of features that had been proposed in the literature, he studied the dependency of the PIAC results on the size of the sample on which they are computed. The rationale is that you must take into account the number of function evaluations that are used to compute the features when addressing a new target instance. He demonstrated that PIAC based on very small sample sets (down to 50 times the dimension) can nevertheless help improving the overall results of the optimization procedure [18], in particular by winning the single-objective track of the **GECCO 2017 Black Box Competition**.

### 7.3.4. *Feature-based Algorithm Selection in Combinatorial Optimization*

In the first part of his PhD (to be defended in Feb. 2018, see also Section 4.2), François Gonard designed ASAP, an Algorithm Selection algorithm that combines a global pre-scheduler and a per instance algorithm selector, to take advantage of the diversity of the problem instances on one hand and of the algorithms on the other hand. ASAP participated to two competitions: the 2016 ICON challenge [35], in which it obtained a *Special Mention* for its originality (and obtained excellent results on half of the problems); the 2017 OASC challenge where two versions of ASAP obtained the first overall best performances [23].

### 7.3.5. *Deep Learning calibration*

In a starting collaboration with Olivier Teytaud (who left TAO for Google Zurich in 2016), we proposed [40] an online scheme for Deep Learning hyper-parameter tuning that detects and early-stops unpromising runs using extrapolation of learning curves [64], taking advantage of the parallelism, and offering optimality guarantees within the multiple hypothesis testing framework.

### 7.3.6. *Learning Rate Adaptation in Stochastic Gradient Descent*

Based on an analogy with CMA-ES step-size adaptation (comparison with random walks), an original mechanism was proposed for adapting the learning rate of the stochastic gradient descent [52]. As increasing the learning rate can increase the number of catastrophic events (exploding gradients or loss values), a change detection test is used to detect such events and backtrack to safe regions. First experiments on small size problems (MNIST and CIFAR10) validate the approach. Interestingly, the same mechanism can be applied to the Adam optimizer and also improves on its basic version.

### 7.3.7. *Domain Adaptation*

The subject of V. Estrade's PhD is to advance domain adaptation methods in the specific context of uncertainty quantification and calibration in High Energy Physics analysis. The problem consists of learning a representation that is insensitive to perturbations induced by nuisance parameters. The need for the adversarial techniques, assuming a completely knowledge-free approach, has been questioned. Our results [32], [43] contrast the superior performance of incorporating a priori knowledge (Tangent Propagation approach) on a well separated classes problem (MNIST data) with a real case setting in HEP.

## 7.4. *Generative Models and Data-driven Design*

Learning generative models from observational data faces two critical issues: model selection (defining a loss criterion well suited to the considered distribution space) and tractable optimization.

### 7.4.1. *A Statistical Physics Perspective*

Restricted Boltzmann machines (RBM) define generative models, and advanced mean field methods of statistical physics can be leveraged to analyze the learning dynamics. Giancarlo Fissore's Master thesis (now in PhD), co-supervised by Aurélien Decelle and Cyril Furtlehner, has characterized the information content of an RBM from its spectral properties and derived a phenomenological equation of the learning process by means of the spectral dynamics of the weight matrix [5]. The learning dynamics has been analyzed in both linear and non-linear regimes, investigating the impact of the input data.

Secondly [37], the weight matrix ensemble which results from this spectral representation is used to analyze the thermodynamical properties of RBMs in terms of a phase diagram. The conditions for the RBM training, interpreted as a so-called ferromagnetic compositional phase, are given. Ferromagnetic order parameters are identified in the aforementioned phenomenological equation; a closed-form is obtained through explicit integration in simple cases, yielding a behavior of the learning spectral dynamics that matches the actual dynamics of standard RBM training (e.g. using contrastive divergence). After this model, a repulsive interaction takes place among the singular modes of the weight matrix, as some pressure of the lower modes is exerted on higher modes along training. Remarkably, this repulsive interaction is observed in algorithmic experiments for low learning rates.

#### 7.4.2. Functional Brain Dynamics

Generative models have also been used by Aurélien Decelle and Cyril Furtlehner to model the dynamics of the Functional connectome (FCD) in the context of the BRAINTIME exploratory project, along two lines.

On the one hand, Restricted Boltzmann Machines have been used to learn the statistics of the time-varying resting state BOLD activity of 49 human subjects in the age span of 18 to 80 years. RBM models trained on a *per* individual basis show at least two statistically distinct pure states for each subject, between which resting state activity is stochastically wandering. Through mean-field TAP approximations of free energy we have evaluated the energy barrier between these two states *per* individual. Interestingly young and old individuals have different switching statistics: more regular for young subjects *vs* bursty and temporally irregular for elderly subjects. Furthermore, the switching probability is correlated with the energy difference between the two pure RBM states, opening the way to a personalized “landscape” analysis of the resting state FCD.

On the other hand, extremely sparse precision matrices describing the co-activation statistics of different brain regions during resting state based on BOLD time-series have been derived using sparse Gaussian copula models. Such extremely sparse models support direct inter-subject comparisons, in contrast with usually dense FC descriptions. A further step is to characterize the brain activity dynamics, e.g. through considering multi-temporal slice models.

#### 7.4.3. Power systems Design and Optimization

Last work within the POST project, Vincent Berthier’s PhD [2] addressed issues in global continuous optimization, and proposed to use unit commitment problems to go beyond classical benchmarks of analytical functions.

Benjamin Donnot (RTE Cifre PhD, now under Isabelle Guyon’s supervision), successfully started to disseminate his work in the power system community [20]. His main results regard the design of an original alternative to the one-hot encoding for the topology of the French power grid, termed *Guided Dropout*. Taking advantage of the high redundancy of network connections, the idea is to learn a random mapping between all possible “n-1” topologies and the connections of the neurons [65], [42].

#### 7.4.4. Multi-Objective Optimization

**Dynamic Objectives:** Within the E-Lucid project, coordinated by Thales Communications & Security, the on-going work about anomaly detection in network flow [74] led to an original approach to many-objective problem, where the objectives are gradually introduced, preventing the population to be abruptly driven toward satisficing only the easy objectives at the beginning of the evolution [27] (runner-up for the Best Paper Award of the Evolutionary Multi-Objective track at GECCO 2017).

**Dynamic Fitness Cases:** In [22], we propose to gradually introduce the fitness cases in the case of symbolic regression with Genetic Programming, so as to guide the search more smoothly. Experimental results demonstrate a better success rate in the case of both static and dynamic problems.

#### **7.4.5. Space Weather Forecasting**

In the context of the MDG-TAU joint team project, focusing on space weather forecasting, Mhamed Hajaiej's Master thesis (under Aurélien Decelle, Cyril Furtlehner and Michèle Sebag's supervision) has tackled the prediction of magnetic storms from solar magnetograms, more specifically considering the representation of solar magnetograms based on auto-encoders. Besides finding a well-suited NN architecture, the difficulty was to find a loss function well suited to the data distribution. A next step (Mandar Chandorkar's PhD at CWI under Enrico Camporeale supervision) is to estimate from the solar images the speed of the solar wind, and the time needed for solar storms to reach the first Lagrange point; this estimation is meant to build a well-defined supervised learning problem, associating a solar image at  $t$  to its effect measured at  $t + \delta$  on the first Lagrange point.

## TROPICAL Team

## 7. New Results

### 7.1. Optimal control and zero-sum games

#### 7.1.1. Fixed points of order preserving homogeneous maps and zero-sum games

**Participants:** Marianne Akian, Stéphane Gaubert.

The PhD work of Antoine Hochart [88] was dealing with the applications of methods of non-linear fixed point theory to zero-sum games.

A highlight of his PhD is the characterization of the property of ergodicity for zero-sum games. In the special “zero-player” case, i.e., for a Markov chain equipped with an additive functional (payment) of the trajectory, the ergodicity condition entails that the mean payoff is independent of the initial state, for any choice of the payment. In the case of finite Markov chains, ergodicity admits several characterizations, including a combinatorial one (the uniqueness of the final class). This carries over to the two player case: ergodicity is now characterized by the absence of certain pairs of conjugate invariant sets (dominions), and it can be checked using directed hypergraphs algorithms. This leads to an explicit combinatorial sufficient condition for the solvability of the “ergodic equation”, which is the main tool in the numerical approach of the mean payoff problem. These results appeared in [52] for the case of bounded paiements. A more general approach was developed in [87], in which zero-sum games are now studied abstractly in terms of accretive operators. This allows one to show that the bias vector (the solution of the ergodic equation) is unique for a generic perturbation of the payments. A more recent work include the introduction of an abstract game allowing us to deal with general monotone additively homogeneous operators and thus to unbounded paiements.

Another series of results of the thesis concern the finite action space, showing that the set of payments for which the bias vector is not unique coincides with the union of lower dimensional cells of a polyhedral complex, which an application to perturbation schemes in policy iteration [12].

A last result of the thesis is a representation theorem for “payment free” Shapley operators, showing that these are characterized by monotonicity and homogeneity axioms [13]. This extends to the two-player case known representation theorems for risk measures.

#### 7.1.2. The operator approach to entropy games

**Participants:** Marianne Akian, Stéphane Gaubert.

Entropy games were recently introduced by Asarin et al. A player (Despot) wishes to minimize a measure of “freedom” given by a topological entropy, whereas the other player (Tribune) wishes to maximize it. In [25], we developed an operator approach for entropy games. We showed that they reduce to risk sensitive type game problems, and deduced that entropy games in Despot has a few positions with non-trivial actions can be solved in polynomial time.

#### 7.1.3. Probabilistic and max-plus approximation of Hamilton-Jacobi-Bellman equations

**Participants:** Marianne Akian, Eric Fodjo.

The PhD thesis of Eric Fodjo concerns stochastic control problems obtained in particular in the modelisation of portfolio selection with transaction costs. The dynamic programming method leads to a Hamilton-Jacobi-Bellman partial differential equation, on a space with a dimension at least equal to the number of risky assets. The curse of dimensionality does not allow one to solve numerically these equations for a large dimension (greater to 5). We propose to tackle these problems with numerical methods combining policy iterations, probabilistic discretisations, max-plus discretisations, in order to increase the possible dimension.

We consider fully nonlinear Hamilton-Jacobi-Bellman equations associated to diffusion control problems with finite horizon involving a finite set-valued (or switching) control and possibly a continuum-valued control. In [47], we constructed a lower complexity probabilistic numerical algorithm by combining the idempotent expansion properties obtained by McEneaney, Kaise and Han [91], [97] for solving such problems with a numerical probabilistic method such as the one proposed by Fahim, Touzi and Warin [74] for solving some fully nonlinear parabolic partial differential equations, when the volatility does not oscillate too much. In [38], [39] (also presented in [24]), we improve the method of Fahim, Touzi and Warin by introducing probabilistic schemes which are monotone without any restrictive condition, allowing one to solve fully nonlinear parabolic partial differential equations with general volatilities. We study the convergence and obtain error estimates when the parameters and the value function are bounded. We are now studying the more general quadratic growth case.

#### 7.1.4. Tropical-SDDP algorithms for stochastic control problems involving a switching control

**Participants:** Marianne Akian, Duy Nghi, Benoît Tran.

The PhD thesis of Benoît Tran, supervised by Jean-Philippe Chancelier (ENPC) and Marianne Akian concerns the numerical solution of the dynamic programming equation of discrete time stochastic control problems.

Several methods have been proposed in the literature to bypass the curse of dimensionality difficulty of such an equation, by assuming a certain structure of the problem. Examples are the max-plus based method of McEneaney [98], [99], the stochastic dual dynamic programming (SDDP) algorithm of Pereira and Pinto [104], the mixed integer dynamic approximation scheme of Philpott, Faisal and Bonnans [60], the probabilistic numerical method of Fahim, Touzi and Warin [74]. We propose to associate and compare these methods in order to solve more general structures, in particular problems involving a finite set-valued (or switching) control and a continuum-valued control, with the property that the value function associated to a fixed switching strategy is convex.

## 7.2. Non-linear Perron-Frobenius theory, nonexpansive mappings and metric geometry

### 7.2.1. Order reversing maps on cones

**Participant:** Cormac Walsh.

We have been studying non-linear operators on open cones, particularly ones that preserve or reverse the order structure associated to the cone. A bijective map that preserves the order in both directions is called an order isomorphism. Those that reverse the order in both directions are order antimorphisms. These are closely related to the isometries of the Hilbert and Thompson metrics on the cone.

Previously, we have shown [118] that if there exists an antimorphism on an open cone that is homogeneous of degree  $-1$ , then the cone must be a symmetric cone, that is, have a transitive group of linear automorphisms and be self-dual.

The technique was to consider the Funk metric on the cone, which is a non-symmetric metric defined using the order and homogeneity structures. Each antimorphism on a cone that is homogeneous of degree  $-1$  reverses this metric, and so interchanges the two horofunction boundaries of the metric, the one in the forward direction and the one in the backward direction. By studying these boundaries we obtained the result.

More recently, we have shown [45] that the homogeneity assumption is not actually necessary: every antimorphism on a cone is automatically homogeneous of degree  $-1$ .

Without the homogeneity assumption, the metric techniques do not work. Instead, it was necessary to study how the map acts on line segments parallel to extreme rays of the cone. This is similar to the what was done by Rothaus, Noll and Schäffer, and Artstein-Avidan and Slomka in their work on order isomorphisms. This means that our proof is essentially finite dimensional. Indeed, there are many interesting cones in infinite dimension that have few or no extreme rays.



In infinite dimension, it is natural to consider order unit spaces as a generalisation of cones, and JB-algebras as a generalisation of symmetric cones. Lemmens, Roelands, and Wortel have asked whether the existence of an order antimorphism that is homogeneous of degree  $-1$  on the cone of an order-unit space implies that the space is a JB-algebra? The result above suggests further that one might even be able to drop the homogeneity assumption.

### 7.2.2. *The set of minimal upper bounds of two matrices in the Loewner order*

**Participant:** Nikolas Stott.

A classical theorem of Kadison shows that the space of symmetric matrices equipped with the Loewner order is an anti-lattice, meaning that two matrices have a least upper bound if and only if they are comparable. In [115], we refined this theorem by characterizing the set of minimal upper bounds: we showed that it is homeomorphic to the quotient space  $O(p) \setminus O(p, q)/O(q)$ , where  $O(p, q)$  denotes the orthogonal group associated to the quadratic form with signature  $(p, q)$ , and  $O(p)$  denotes the standard  $p$ th orthogonal group.

### 7.2.3. *Checking the strict positivity of Kraus maps is NP-hard*

**Participant:** Stéphane Gaubert.

In collaboration with Zheng Qu (now with HKU, Hong Kong), I studied several decision problems arising from the spectral theory of Kraus maps (trace preserving completely positive maps), acting on the cone of positive semidefinite matrices. The latter appear in quantum information. We showed that checking the irreducibility (absence of non-trivial invariant face of the cone) and primitivity properties (requiring the iterates of the map to send the cone to its interior) can be checked in polynomial time, whereas checking positivity (whether the map sends the cone to its interior) is NP-hard. In [20], we studied complexity issues related to Kraus maps, and showed in particular that checking whether a Kraus map sends the cone to its interior is NP-hard.

## 7.3. Tropical algebra and convex geometry

### 7.3.1. *Formalizing convex polyhedra in Coq*

**Participants:** Xavier Allamigeon, Ricardo Katz [Conicet, Argentine].

In [27], we have made the first steps of a formalization of the theory of convex polyhedra in the proof assistant Coq. The originality of our approach lies in the fact that our formalization is carried out in an effective way, in the sense that the basic predicates over polyhedra (emptiness, boundedness, membership, etc) are defined by means of Coq programs. All these predicates are then proven to correspond to the usual logical statements. The latter take the form of the existence of certificates: for instance, the emptiness of a polyhedron is shown to be equivalent to the existence of a certificate *a la* Farkas. This equivalence between Boolean predicates and formulas living in the kind Prop is implemented by using the boolean reflection methodology, and the supporting tools provided by the Mathematical Components library and its tactic language. The benefit of the effective nature of our approach is demonstrated by the fact that we easily arrive at the proof of important results on polyhedra, such as several versions of Farkas Lemma, duality theorem of linear programming, separation from convex hulls, Minkowski Theorem, etc.

Our effective approach is made possible by implementing the simplex method inside Coq, and proving its correctness and termination. Two difficulties need to be overcome to formalize it. On the one hand, we need to deal with its termination. More precisely, the simplex method iterates over the so-called bases. Its termination depends on the specification of a pivoting rule, whose aim is to determine, at each iteration, the next basis. In this work, we have focused on proving that the lexicographic rule ensures termination. On the other hand, the simplex method is actually composed of two parts. The part that we previously described, called Phase II, requires an initial basis to start with. Finding such a basis is the purpose of Phase I. It consists in building an extended problem (having a trivial initial basis), and applying to it Phase II. Both phases need to be formalized to obtain a fully functional algorithm. a

### 7.3.2. *Tropical totally positive matrices*

**Participant:** Stéphane Gaubert.



In [81] (joint work with Adi Niv) we investigate the tropical analogues of totally positive and totally non-negative matrices, i.e, the images by the valuation of the corresponding classes of matrices over a non-archimedean field. We show in particular that tropical totally positive matrices essentially coincide with the Monge matrices (defined by the positivity of  $2 \times 2$  tropical minors), arising in optimal transport. More recent developments include relations between tropical total positivity and planar networks.

### 7.3.3. Tropical compound matrix identities

**Participants:** Marianne Akian, Stéphane Gaubert.

A number of polynomial identities in tropical semirings can be derived from their classical analogues by application of a transfer principle [49], [51]. In the present work [40], joint with Adi Niv, we prove identities on compound matrices in extended tropical semirings, which cannot be obtained by transfer principles, but are rather obtained by combinatorial methods. Such identities include analogues to properties of conjugate matrices, powers of matrices and  $\text{adj}(A) \det(A)^{-1}$ , all of which have implications on the eigenvalues of the corresponding matrices. A tropical Sylvester-Franke identity is provided as well.

### 7.3.4. Group algebra in characteristic one and invariant distances over finite groups

**Participant:** Stéphane Gaubert.

In [19] (joint work with Dominique Castella), we investigated a tropical analogue of group algebras. We studied tropical characters and related them to invariant distances over groups.

### 7.3.5. Volume and integer points of tropical polytopes

**Participants:** Marie Maccaig, Stéphane Gaubert.

We investigate in [43] the volume of tropical polytopes, as well as the number of integer points contained in integer polytopes. We proved that even approximating these values for a tropical polytope given by its vertices is hard, with no approximation algorithm with factor  $2^{\text{poly}(m,n)}$  existing unless  $P = NP$ . We further proved the  $\sharp P$ -hardness for the analogous problems for tropical polytopes instead defined by inequalities.

## 7.4. Tropical methods applied to optimization, perturbation theory and matrix analysis

### 7.4.1. Majorization inequalities for valuations of eigenvalues using tropical algebra

**Participants:** Marianne Akian, Stéphane Gaubert.

In [14], with Meisam Sharify (IPM, Tehran, Iran), we establish log-majorization inequalities of the eigenvalues of matrix polynomials using the tropical roots of some scalar polynomials depending only on the norms of the matrix coefficients. This extends to the case of matrix polynomials some bounds obtained by Hadamard, Ostrowski and Pólya for the roots of scalar polynomials.

These works have been presented in [46].

### 7.4.2. Tropicalization of the central path and application to the complexity of interior point methods

**Participants:** Xavier Allamigeon, Stéphane Gaubert.

This work is in collaboration with Pascal Benchimol (EDF Labs) and Michael Joswig (TU Berlin).

In optimization, path-following interior point methods are driven to an optimal solution along a trajectory called the central path. The *central path* of a linear program  $\text{LP}(A, b, c) \equiv \min\{c \cdot x \mid Ax \leq b, x \geq 0\}$  is defined as the set of the optimal solutions  $(x^\mu, w^\mu)$  of the barrier problems:

$$\begin{aligned} & \text{minimize} && c \cdot x - \mu \left( \sum_{j=1}^n \log x_j + \sum_{i=1}^m \log w_i \right) \\ & \text{subject to} && Ax + w = b, \quad x > 0, \quad w > 0 \end{aligned}$$

While the complexity of interior point methods is known to be polynomial, an important question is to study the number of iterations which are performed by interior point methods, in particular whether it can be bounded by a polynomial in the dimension ( $mn$ ) of the problem. This is motivated by Smale 9th problem [113], on the existence of a strongly polynomial complexity algorithm for linear programming. So far, this question has been essentially addressed through the study of the curvature of the central path, which measures how far a path differs from a straight line, see [71], [70], [73], [72]. In particular, by analogy with the classical Hirsch conjecture, Deza, Terlaky and Zinchenko [72] proposed the “continuous analogue of the Hirsch conjecture”, which says that the total curvature of the central path is linearly bounded in the number  $m$  of constraints.

In a work of X. Allamigeon, P. Benchimol, S. Gaubert, and M. Joswig [41], we prove that primal-dual log-barrier interior point methods are not strongly polynomial, by constructing a family of linear programs with  $3r + 1$  inequalities in dimension  $2r$  for which the number of iterations performed is in  $\Omega(2^r)$ . The total curvature of the central path of these linear programs is also exponential in  $r$ , disproving the continuous analogue of the Hirsch conjecture.

Our method is to tropicalize the central path in linear programming. The tropical central path is the piecewise-linear limit of the central paths of parameterized families of classical linear programs viewed through logarithmic glasses. We give an explicit geometric characterization of the tropical central path, as a tropical analogue of the barycenter of a sublevel set of the feasible set induced by the duality gap. We study the convergence properties of the classical central path to the tropical one. This allows us to show that the number of iterations performed by interior point methods is bounded from below by the number of tropical segments constituting the tropical central path.

#### 7.4.3. Tropical approach to semidefinite programming

**Participants:** Xavier Allamigeon, Stéphane Gaubert, Mateusz Skomra.

Semidefinite programming consists in optimizing a linear function over a spectrahedron. The latter is a subset of  $\mathbb{R}^n$  defined by linear matrix inequalities, i.e., a set of the form

$$\left\{x \in \mathbb{R}^n : Q^{(0)} + x_1 Q^{(1)} + \cdots + x_n Q^{(n)} \succeq 0\right\}$$

where the  $Q^{(k)}$  are symmetric matrices of order  $m$ , and  $\succeq$  denotes the Loewner order on the space of symmetric matrices. By definition,  $X \succeq Y$  if and only if  $X - Y$  is positive semidefinite.

Semidefinite programming is a fundamental tool in convex optimization. It is used to solve various applications from engineering sciences, and also to obtain approximate solutions or bounds for hard problems arising in combinatorial optimization and semialgebraic optimization.

A general issue in computational optimization is to develop combinatorial algorithms for semidefinite programming. Indeed, semidefinite programs are usually solved via interior point methods. However, the latter provide an approximate solution in a polynomial number of iterations, provided that a strictly feasible initial solution. Semidefinite programming becomes a much harder matter if one requires an exact solution. The feasibility problem belongs to  $\text{NP}_{\mathbb{R}} \cap \text{coNP}_{\mathbb{R}}$ , where the subscript  $\mathbb{R}$  refers to the BSS model of computation. It is not known to be in NP in the bit model.

We address semidefinite programming in the case where the field  $\mathbb{R}$  is replaced by a nonarchimedean field, like the field of Puiseux series. In this case, methods from tropical geometry can be applied and are expected to allow one, in generic situations, to reduce semialgebraic problems to combinatorial problems, involving only the nonarchimedean valuations (leading exponents) of the coefficients of the input.

To this purpose, we first study tropical spectrahedra, which are defined as the images by the valuation of nonarchimedean spectrahedra. We establish that they are closed semilinear sets, and that, under a genericity condition, they are described by explicit inequalities expressing the nonnegativity of tropical minors of order 1 and 2. These results are gathered in the preprint [59].

Then, we show in [17] that the feasibility problem for a generic tropical spectrahedron is equivalent to solving a stochastic mean payoff game (with perfect information). The complexity of these games is a long-standing open problem. They are not known to be polynomial, however they belong to the class  $NP \cap coNP$ , and they can be solved efficiently in practice. This allows to apply stochastic game algorithms to solve nonarchimedean semidefinite feasibility problems. We obtain in this way both theoretical bounds and a practicable method which solves some large scale instances.

A long-standing problem is to characterize the convex semialgebraic sets that are SDP representable, meaning that they can be represented as the image of a spectrahedron by a (linear) projector. Helton and Nie conjectured that every convex semialgebraic set over the field of real numbers are SDP representable. Recently, [110] disproved this conjecture. In [26], we show, however, that the following result, which may be thought of as a tropical analogue of this conjecture, is true: over a real closed nonarchimedean field of Puiseux series, the convex semialgebraic sets and the projections of spectrahedra have precisely the same images by the nonarchimedean valuation. The proof relies on game theory methods applied to our previous results [59] and [17].

## 7.5. Applications

### 7.5.1. Geometry of the Loewner order and application to the synthesis of quadratic invariants in static analysis of program

**Participants:** Xavier Allamigeon, Stéphane Gaubert, Nikolas Stott.

This section presents the PhD work of Nikolas Stott. An essential part of the present work is in collaboration with Éric Goubault and Sylvie Putot (from LIX).

We develop a numerical abstract domain based on ellipsoids designed for the formal verification of switched linear systems. The novelty of this domain does not consist in the use of ellipsoids as abstractions, but rather in the fact that we overcome two key difficulties which so far have limited the use of ellipsoids in abstract interpretation. The first issue is that the ordered set of ellipsoids does not constitute a lattice. This implies that there is a priori no canonical choice of the abstraction of the union of two sets, making the analysis less predictable as it relies on the selection of good upper bounds. The second issue is that most recent works using on ellipsoids rely on LMI methods. The latter are efficient on moderate size examples but they are inherently limited by the complexity of interior point algorithms, which, in the case of matrix inequality problems, do not scale as well as for linear programming or second order cone programming problems.

We developed a new approach, in which we reduce the computation of an invariant to the determination of a fixed point, or eigenvector, of a non-linear map that provides a safe upper-approximation of the action induced by the program on the space of quadratic forms. This allows one to obtain invariants of systems of sized inaccessible by LMI methods, at the price of a limited loss of precision. A key ingredient here is the fast computation of least upper bounds in Löwner ordering, by an algebraic algorithm. This relies on the study of the geometry of the space of quadratic forms (Section 7.2.2).

The initial part of this work was described in the article [57], in which we obtained a single ellipsoidal invariant. In [16], we showed that finer disjunctive invariants, expressed as union of ellipsoids, can still be obtained by nonlinear fixed point methods in a scalable way. In [30], we developed a dual approach, which we applied to the problem of computing the joint spectral radius. We showed that an approximation of a Barabanov norm by a supremum of quadratic forms can be obtained by solving a nonlinear eigenvalue problem involving “tropical Kraus maps”. The latter can be thought of as the tropical analogues of the completely positive maps appearing in quantum information. The fixed point methods in [30] allow one to solve large scale instances, inaccessible by earlier (LMI based) methods.

### 7.5.2. Performance evaluation of an emergency call center

**Participants:** Xavier Allamigeon, Vianney Boeuf, Stéphane Gaubert.

This work arose from a question raised by Régis Reboul from Préfecture de Police de Paris (PP), regarding the analysis of the projected evolution of the treatment of emergency calls (17-18-112). This work benefited from the help of LtL Stéphane Raclot, from Brigade de Sapeurs de Pompiers de Paris (BSPP), now with PP. It is part of the PhD work of Vianney Bœuf, carried out in collaboration with BSPP.

We introduced an algebraic approach which allows to analyze the performance of systems involving priorities and modeled by timed Petri nets. Our results apply to the class of Petri nets in which the places can be partitioned in two categories: the routing in certain places is subject to priority rules, whereas the routing at the other places is free choice.

We initially introduced a discrete model in [54], showing that the counter variables, which determine the number of firings of the different transitions as a function of time, are the solutions of a piecewise linear dynamical system. We showed the stationary regimes are precisely the solutions of a set of lexicographic piecewise linear equations, which constitutes a polynomial system over a tropical (min-plus) semifield of germs. However, the convergence to a stationary regime may not occur in the discrete model. We developed in [15] a continuous time analogue of this model, involving a piecewise linear dynamical systems, and showed that it has the same stationary regimes, avoiding some pathologies of the discrete model.

In essence, this result shows that computing stationary regimes reduces to solving tropical polynomial systems. Solving tropical polynomial systems is one of the most basic problems of tropical geometry. The latter provides insights on the nature of solutions, as well as algorithmic tools. In particular, the tropical approach allows one to determine the different congestion phases of the system. This analysis has been recovered by a probabilistic model in [42].

We applied this approach to a case study relative to the project led by Préfecture de Police de Paris, involving BSPP, of a new organization to handle emergency calls to Police (number 17), Firemen (number 18), and untyped emergency calls (number 112), in the Paris area. We combined explicit analytic computations of the different congestion phases of a simplified model and extensive simulations of a realistic and detailed model, to evaluate the performance of the center as a function of the number of operators. This analysis also suggested some ways to monitor early signs of potential congestions as well as possible correcting measures to avoid congestion.

### 7.5.3. Tropical models of fire propagation in urban areas

**Participants:** Stéphane Gaubert, Daniel Jones.

As part of the team work in the ANR project Democrite, we developed a model of fire propagation in urban areas, involving a discrete analogue of a Hamilton-Jacobi PDE. This model indicates that the fire propagates according to polyhedral ball, which is in accordance from data from historical fires (London, Chicago, or more recently Kobe).

### 7.5.4. Smart Data Pricing

**Participants:** Marianne Akian, Jean-Bernard Eytard.

This work is in collaboration with Mustapha Bouhtou (Orange Labs).

The PhD work of Jean-Bernard Eytard concerns the optimal pricing of data traffic in mobile networks. We developed a bilevel programming approach, allowing to an operator to balance the load in the network through price incentives. We showed that a subclass of bilevel programs can be solved in polynomial time, by combining methods of tropical geometry and of discrete convexity. This work is presented in [28]. In a followup work (collaboration with Gleb Koshevoy), we managed to extend these results to wider classes of bilevel problems, and to relate them to competitive equilibria problems.

### 7.5.5. Game theory models of decentralized mechanisms of pricing of the smart grid

**Participants:** Stéphane Gaubert, Paulin Jacquot.

This work is in collaboration with Nadia Oudjane and Olivier Beaude (EDF).

The PhD work of Paulin Jacquot concerns the application of game theory techniques to pricing of energy. We are developing a game theory framework for demand side management in the smart grid, in which users have movable demands (like charging an electric vehicle). We compared in particular the daily and hourly billing mechanisms. The latter, albeit more complex to analyse, has a merit in terms of incitatives, as it leads the user to move his or her consumption at off peak hours. We showed the Nash equilibrium is unique, under some assumptions, and gave theoretical bounds of the price of anarchy of the game with a hourly billing, showing this mechanism remains efficient while being more “fair” than the daily billing. We proposed and tested decentralized algorithms to compute the Nash equilibrium. These contriutions are presented In [31], [32], [44].

## AMIBIO Team

# 5. New Results

## 5.1. New circular RNAs identified in *Pyrococcus abyssi*

We contributed a new method for the detection of circRNAs, which we validated on simulated data, and used to analyze the transcriptome of *Pyrococcus abyssi*, an archae living at high depth and temperature [1]. Using this method, which was shown to produce less false positives than previous computational approaches, we analyzed data produced in collaboration with LOB (Ecole Polytechnique), and detected roughly a hundred of novel candidates circular RNAs. Moreover, we provided evidence, on a large scale, that the protein *Pab1020* acts as a ligase, and interacts with some of these circular RNAs, shedding new light on the mechanisms underlying the circularization process.

## 5.2. Minimal absent words

Minimal absent words are words that do not occur but whose proper factors all occur in the sequence. In a collaboration with King's College, several algorithms, we have designed algorithms to search for minimal absent words in external memory [8], and *in-line*, using a sliding window [13] (parallelization, external memory,...) that outperform previous solutions and achieve near-optimal speed up. This opens new scenarios in the applications of minimal absent words in computational biology, including phylogeny or evolution. For instance, it was shown that there exist three minimal words in Ebola virus genomes which are absent from human genome. As two strings coincide iff they have the same set of minimal absent words, an interesting side result is to solve in optimal time the pattern matching problem using *negative information*.

## 5.3. Kinematics-inspired algorithms for macromolecular modeling

At a geometric level, RNA is much more flexible than protein, and undergoes smooth transitions between its various conformations. Such transitions are difficult to observe, but can be predicted using algorithms inspired by kinematics and motion-planning. With our partners at Stanford, we designed and implemented such an algorithm within the KGS library [8] to morph between two RNA conformations while keeping distance constraints induced by base pairs and, more importantly, avoiding clashes. In a more preliminary work, we also used similar approaches to automagically fit multi-conformer ligand models into electron density maps [16].

## 5.4. RNA design

In a paper published in *Algorithmica* [6], we have shown that our previous results [30] hold for more sophisticated energy models where base-pairs are associated with arbitrary energy contributions. This result, which required a complete overhaul of our previous proofs (e.g. using arguments based on graph coloring), allows us to foresee an extension of (at least some of) our results to state-of-the-art models, such as the Turner energy model.

In collaboration with Danny Barash's group at Ben-Gurion university (Israel), we contributed a review of existing tools and techniques for RNA design, which was published in *Briefings in Bioinformatics* series [3].

Finally, in a paper [14] recently accepted for a presentation at the prestigious RECOMB'18 conference, we revisited the problem of generating at random an RNA sequence which is simultaneously compatible with a set of target secondary structures. This problem was previously addressed by our collaborators at the TBI Vienna/Univ. Leipzig, using an exponential-time algorithm. We established the  $\#P$ -hardness of the problem, and its inapproximability in general. However, the problem is still amenable to an efficient parametrization, and we proposes an FTP algorithm named *RNARedPrint* based on the tree decomposition for the random generation, to which we adapted a multidimensionnal Boltzmann sampling technique in order to gain (probabilistic) control over secondary features such as the *GC%*, the relative free-energy of the various structures...

## 5.5. Game theory and macromolecular modeling

Initially based on a very coarse representation of RNA, we refined our model of RNA folding as a game, using on-lattice coordinates and statistical potentials for the utility function. The resulting algorithm was implemented in the subsequent version of the GARN [2] software.

The final year of Amélie Héliou's PhD led to theoretical developments in game theory, mainly obtained in collaboration with J. Cohen (LRI, Univ. Paris-Sud). First, the quasi-exponential convergence, under reasonable assumptions, of the HEDGE algorithm was demonstrated in collaboration with the POLARIS team in Grenoble [11]. Moreover, in a paper accepted at NIPS'17 [12], we addressed the learning of Nash equilibria. In this context, we established the convergence with high probability of no-regret learning in the bandit and semi-bandit settings.

## 5.6. RNA kinetics using non-redundant sampling

RNA kinetics is arguably the next frontier in RNA 2D bioinformatics. In particular, computational methods for studying the kinetics of RNA beyond 150nts are hindered by the combinatorial explosion of the conformation space. In an effort to circumvent such an effect, we have proposed a sampling approach that explicitly target local minima of the energy function. Our sampling algorithm, jointly proposed with H. Touzet (Bonsai, Inria Lille & CrisTaL, Univ. Lille I) and accepted for a presentation at the ISMB/ECCB'17 conference in Prague [15], uses non-redundant sampling principles to avoid an excessive concentration of samples within low local minima.

## 5.7. New insight from SHAPE probing data

Existing computational methods for structure prediction are typically hindered by their assumption of a single structure, and their assumption of orthogonal signals stemming from different reagents. To overcome these limitations, we contributed an integrative approach combining stochastic sampling and structural clustering [17] (journal version pending). In collaboration with ENS Lyon/Univ. Lyon I and Univ. Paris-Descartes, we used this method to model the structure of the HIV-1 gag open-reading frame [4].

We also addressed the problem of binning sets of NGS reads arising from the simultaneous probing, using the SHAPEmap protocol, of variants produced by a error-prone PCR. We proposed a variant of the Expectation-Maximization algorithm [10] to jointly infer maximum-likelihood origins for reads and mutational profiles for each variant.



## GALEN Project-Team

# 7. New Results

## 7.1. Graph Based Slice-to-Volume Deformable Registration

**Participants:** Enzo Ferrante, Nikos Paragios

Deformable image registration is a fundamental problem in computer vision and medical image computing. In this contribution [9], we investigate the use of graphical models in the context of a particular type of image registration problem, known as slice-to-volume registration, while we introduced the first comprehensive survey [10] of the literature about slice-to-volume registration, presenting a categorical study of the algorithms according to an ad-hoc taxonomy and analyzing advantages and disadvantages of every category. We introduce a scalable, modular and flexible formulation that can accommodate low-rank and high order terms, that simultaneously selects the plane and estimates the in-plane deformation through a single shot optimization approach. The proposed framework is instantiated into different variants seeking either a compromise between computational efficiency (soft plane selection constraints and approximate definition of the data similarity terms through pair-wise components) or exact definition of the data terms and the constraints on the plane selection. Simulated and real-data in the context of ultrasound and magnetic resonance registration (where both framework instantiations as well as different optimization strategies are considered) demonstrate the potentials of our method.

## 7.2. Deformable Registration Through Learning of Context-Specific Metric Aggregation

**Participants:** Enzo Ferrante, Rafael Marini, Punnet K. Dokania, Nikos Paragios

We propose a novel weakly supervised discriminative algorithm [21] for learning context specific registration metrics as a linear combination of conventional similarity measures. Conventional metrics have been extensively used over the past two decades and therefore both their strengths and limitations are known. The challenge is to find the optimal relative weighting (or parameters) of different metrics forming the similarity measure of the registration algorithm. Hand-tuning these parameters would result in sub optimal solutions and quickly become infeasible as the number of metrics increases. Furthermore, such hand-crafted combination can only happen at global scale (entire volume) and therefore will not be able to account for the different tissue properties. We propose a learning algorithm for estimating these parameters locally, conditioned to the data semantic classes. The objective function of our formulation is a special case of non-convex function, difference of convex function, which we optimize using the concave convex procedure. As a proof of concept, we show the impact of our approach on three challenging datasets for different anatomical structures and modalities.

## 7.3. Promises and challenges for the implementation of computational medical imaging (radiomics) in oncology

**Participants:** Roger Sun, Evangelia I. Zacharaki, Nikos Paragios (in collaboration with Gustave Roussy and Paris Sud University)

Computational medical imaging (also known as radiomics) is a promising and rapidly growing discipline that consists in the analysis of high-dimensional data extracted from medical imaging, to further describe tumour phenotypes. The end goal of radiomics is to determine imaging biomarkers as decision support tools for clinical practice and to facilitate better understanding of cancer biology, allowing the assessment of the changes throughout the evolution of the disease and the therapeutic sequence. We have reviewed [12], [17] the critical issues necessary for proper development of radiomics as a biomarker and for its implementation in clinical practice.



## 7.4. Multi-atlas segmentation in medical imagery

**Participants:** Stavros Alchatzidis, Evangelia I. Zacharaki, Nikos Paragios (in collaboration with University of Pennsylvania)

Multi-atlas segmentation has emerged in recent years as a simple yet powerful approach in medical image segmentation. It commonly comprises two steps: (1) a series of pairwise registrations that establish correspondences between a query image and a number of atlases, and (2) the fusion of the available segmentation hypotheses towards labeling objects of interest. In [5], we introduce a novel approach that solves simultaneously for the underlying segmentation labels and the multi-atlas registration. We propose a pairwise Markov Random Field approach, where registration and segmentation nodes are coupled towards simultaneously recovering all atlas deformations and labeling the query image.

## 7.5. Protein function prediction

**Participants:** Evangelia I. Zacharaki, Nikos Paragios (in collaboration with University of Patras)

The massive expansion of the worldwide Protein Data Bank (PDB) provides new opportunities for computational approaches which can learn from available data and extrapolate the knowledge into new coming instances. The aim of our work in [6], [18] was to exploit experimentally acquired structural information of enzymes through machine learning techniques in order to produce models that predict enzymatic function.

## 7.6. Deformable group-wise registration using a physiological model: Application to diffusion-weighted MRI

**Participants:** Evgenios Kornaropoulos, Evangelia I. Zacharaki, Nikos Paragios (in collaboration with Centre Hospitalier Universitaire Henri-Mondor and Chang Gung Memorial Hospital)

In this contribution [2] we develop a novel group-wise deformable registration method for motion correction in Diffusion-Weighted MRI towards computing a more accurate Apparent Diffusion Coefficient parametric map (ADC map). Calculation of the ADC has been performed without motion correction in the previous studies. It is reported though that ADC is a parameter susceptible to artifacts, the most frequent of all being patient's motion and breathing, resulting in misregistration of the images obtained with different b-values. Being group-wise designed, the image registration method we propose has no need of choosing a reference template while in the same time it is computationally efficient. We aim at finding the optimal deformation fields of the diffusion-weighted (DW) images using a temporal constraint, related to the diffusion process, as well as a smoothness penalty on the deformations. To this end, we address the deformation fields estimation problem with an Markov Random Fields formulation, in which the latent variables are the deformations (B-spline polynomials) of the images. The latent variables are connected with the observations towards ensuring meaningful temporal correspondence among the DW images. They are also inter-connected in order to decrease the cost of pairwise comparisons between individual images. Linear programming and duality are used to determine the optimal solution of the problem. Finally, as an image similarity criterion in the MRF framework, we used a metric that was based on a physiological model describing the image acquisition process. Quantitative evaluation of the method was performed, in which it was compared against two state-of-the-art methods that use other modelling criteria. It outperformed both of them, while the ADC map derived by our method appeared to preserve structure, that was not observable by the other methods.

## 7.7. Variational Bayesian Approach for Image Restoration

**Participants:** Emilie Chouzenoux and Jean-Christophe Pesquet (in collaboration with Y. Marnissi, SAFRAN TECH and Y. Zheng, IBM Research China)

In the work [13], a methodology is investigated for signal recovery in the presence of non-Gaussian noise. In contrast with regularized minimization approaches often adopted in the literature, in our algorithm the regularization parameter is reliably estimated from the observations. As the posterior density of the unknown parameters is analytically intractable, the estimation problem is derived in a variational Bayesian framework where the goal is to provide a good approximation to the posterior distribution in order to compute posterior mean estimates. Moreover, a majorization technique is employed to circumvent the difficulties raised by the intricate forms of the non-Gaussian likelihood and of the prior density. We demonstrate the potential of the proposed approach through comparisons with state-of-the-art techniques that are specifically tailored to signal recovery in the presence of mixed Poisson-Gaussian noise. Results show that the proposed approach is efficient and achieves performance comparable with other methods where the regularization parameter is manually tuned from an available ground truth.

## 7.8. Non-Modular Loss Functions

**Participant:** Jiaqian Yu

Defining Non-modular loss functions and their optimization procedure present an interesting direction for many classes of problems. Jiaqian Yu has completed her PhD Thesis on Non-Modular Loss Functions this year. The PhD Thesis has included several yet unpublished results regarding approximate losses for Jaccard index and DICE coefficients commonly used in evaluating segmentation algorithms.

## 7.9. Graph Structure Discovery

**Participant:** Eugene Belilovsky

Discovering the interaction structure amongst variables, particularly from few observations, has important implications in many fields including neuroimaging, genetics and finance. Eugene Belilovsky in collaboration with Gael Varoquaux (Inria Parietal), Kyle Kastner (University of Montreal) and Matthew Blaschko has published a new approach for graph structure discovery in high dimensional gaussian markov random fields. The work has been presented in [19].

## 7.10. Structured and Efficient Convolutional Networks

**Participant:** Eugene Belilovsky

Convolutional Neural Networks have revolutionized the computer vision field. Yet, they are not well understood and do not well leverage basic geometric structures known by the computer vision community. In recent work in collaboration with the Ecole Normale Supérieure and the École des Ponts ParisTech we have tried to address some of these issues. We use as a starting point the recently introduced Scattering Transform and show that we can use this to build Convolutional Networks that are more interpretable and can generalize faster in the few sample regime. This work has been presented in [25].

## 7.11. Stochastic Majorize-Minimize Subspace Algorithm

**Participants:** Emilie Chouzenoux and Jean-Christophe Pesquet

Stochastic optimization plays an important role in solving many problems encountered in machine learning or adaptive processing. In this context, the second-order statistics of the data are often unknown a priori or their direct computation is too intensive, and they have to be estimated on-line from the related signals. In the context of batch optimization of an objective function being the sum of a data fidelity term and a penalization (e.g. a sparsity promoting function), Majorize-Minimize (MM) subspace methods have recently attracted much interest since they are fast, highly flexible and effective in ensuring convergence. The goal of the work [8] is to show how these methods can be successfully extended to the case when the cost function is replaced by a sequence of stochastic approximations of it. Simulation results illustrate the good practical performance of the proposed MM Memory Gradient (3MG) algorithm when applied to 2D filter identification

## 7.12. Deconvolution and Deinterlacing of Video Sequences

**Participants:** Emilie Chouzenoux and Jean-Christophe Pesquet (in collaboration with F. Abboud, PhD student, J.-H. Chenot and L. Laborelli, research engineers, Institut National de l'Audiovisuel)

Optimization methods play a central role in the solution of a wide array of problems encountered in various application fields, such as signal and image processing. Especially when the problems are highly dimensional, proximal methods have shown their efficiency through their capability to deal with composite, possibly non smooth objective functions. The cornerstone of these approaches is the proximity operator, which has become a quite popular tool in optimization. In the work [31], we propose new dual forward-backward formulations for computing the proximity operator of a sum of convex functions involving linear operators. The proposed algorithms are accelerated thanks to the introduction of a block coordinate strategy combined with a preconditioning technique. Numerical simulations emphasize the good performance of our approach for the problem of jointly deconvoluting and deinterlacing video sequences.

## 7.13. PALMA, an improved algorithm for DOSY signal processing

**Participants:** Emilie Chouzenoux (in collaboration with M.-A. Delsuc, IGBMC, Strasbourg, and A. Cherni, PhD student, Univ. Strasbourg)

NMR is a tool of choice for the measure of diffusion coefficients of species in solution. The DOSY experiment, a 2D implementation of this measure, has proven to be particularly useful for the study of complex mixtures, molecular interactions, polymers, etc. However, DOSY data analysis requires to resort to inverse Laplace transform, in particular for polydisperse samples. This is a known difficult numerical task, for which we present here a novel approach. A new algorithm based on a splitting scheme and on the use of proximity operators is introduced in [7]. Used in conjunction with a Maximum Entropy and  $\ell_1$  hybrid regularisation, this algorithm converges rapidly and produces results robust against experimental noise. This method has been called PALMA. It is able to reproduce faithfully monodisperse as well as polydisperse systems, and numerous simulated and experimental examples are presented. It has been implemented on the server <http://palma.labo.igbmc.fr> where users can have their datasets processed automatically.

## 7.14. Proximal Approaches for Solving Matrix Optimization Problems

**Participants:** Emilie Chouzenoux and Jean-Christophe Pesquet (in collaboration with A. Benfenati, Univ. Paris Est)

In recent years, there has been a growing interest in problems where the underlining mathematical model involves the minimization in a matrix space of a Bregman divergence function coupled with a regularization term. We consider a general framework where the regularization term is decoupled in two parts, one acting only on the eigenvalues of the matrix and the other on the whole matrix. We propose in [26], [32] a new minimization approach to address problem of this type, by providing a list of proximity operators allowing us to consider various choices for the fit-to-data functional and for the regularization term. The numerical experience show that this approach gives better results in term of computational time with respect to some state of the arts algorithms.

## 7.15. Fast Algorithm for Least-Squares Regression with GMRF Prior

**Participants:** Emilie Chouzenoux and Jean-Christophe Pesquet (in collaboration with J.Y. Tourneret, IRIT, Toulouse, and Q. Wei, Duke Univ.)

The paper [29] presents a fast approach for penalized least squares (LS) regression problems using a 2D Gaussian Markov random field (GMRF) prior. More precisely, the computation of the proximity operator of the LS criterion regularized by different GMRF potentials is formulated as solving a Sylvester-like matrix equation. By exploiting the structural properties of GMRFs, this matrix equation is solved column-wise in an analytical way. The proposed algorithm can be embedded into a wide range of proximal algorithms to solve LS regression problems including a convex penalty. Experiments carried out in the case of a constrained

LS regression problem arising in a multichannel image processing application, provide evidence that an alternating direction method of multipliers performs quite efficiently in this context.

## 7.16. Optimization Approach for Deep Neural Network Training

**Participants:** Emilie Chouzenoux, Jean-Christophe Pesquet, Vyacheslav Dudar (in collaboration with G. Chierchia, Univ. Paris Est and V. Semenov, Univ. of Kiev)

In paper [28], we develop a novel second-order method for training feed-forward neural nets. At each iteration, we construct a quadratic approximation to the cost function in a low-dimensional subspace. We minimize this approximation inside a trust region through a two-stage procedure: first inside the embedded positive curvature subspace, followed by a gradient descent step. This approach leads to a fast objective function decay, prevents convergence to saddle points, and alleviates the need for manually tuning parameters. We show the good performance of the proposed algorithm on benchmark datasets.

## 7.17. Auxiliary Variable Method for MCMC Algorithms in High Dimension

**Participants:** Emilie Chouzenoux and Jean-Christophe Pesquet (in collaboration with Y. Marnissi, SAFRAN TECH and A. Benazza-Benhayia, SUP'COM, COSIM, Tunis)

When the parameter space is high dimensional, the performance of stochastic sampling algorithms is very sensitive to existing dependencies between parameters. For instance, this problem arises when one aims to sample from a high dimensional Gaussian distribution whose covariance matrix does not present a simple structure. Then, one often resorts to sampling algorithms based on a perturbation-optimization technique that requires to minimize a cost function using an iterative algorithm. This makes the sampling process time consuming, especially when used within a Gibbs sampler. Another challenge is the design of Metropolis-Hastings proposals that make use of information about the local geometry of the target density in order to speed up the convergence and improve mixing properties in the parameter space, while being not too computationally expensive. These two contexts are mainly related to the presence of two heterogeneous sources of dependencies stemming either from the prior or the likelihood in the sense that the related covariances matrices cannot be diagonalized in the same basis. In paper [34], we are interested in inverse problems where either the data fidelity term or the prior distribution is Gaussian or driven from a hierarchical Gaussian model. We propose to add auxiliary variables to the model in order to dissociate the two sources of dependencies. In the new augmented space, only one source of correlation remains directly related to the target parameters, the other sources of correlations being captured by the auxiliary variables. Experiments conducted on two image restoration problems show the good performance of the proposed strategy.

## 7.18. Block Coordinate Approach for Sparse Logistic Regression

**Participants:** Emilie Chouzenoux and Jean-Christophe Pesquet (in collaboration with G. Chierchia, Univ. Paris Est, L. M. Briceno-Arias, CMM - Univ. Chile, and A. Cherni, PhD student, Univ. Strasbourg)

We propose in [20], [33] stochastic optimization algorithms for logistic regression based on a randomized version of Douglas-Rachford splitting method. Our approach sweeps the training set by randomly selecting a mini-batch of data at each iteration, and it performs the update step by leveraging the proximity operator of the logistic loss, for which a closed-form expression is derived. Experiments carried out on standard datasets compare the efficiency of our algorithm to stochastic gradient-like methods.

## 7.19. An Alternating Proximal Approach for Blind Video Deconvolution

**Participants:** Emilie Chouzenoux and Jean-Christophe Pesquet (in collaboration with Feriel Abboud, WITBE, Jean-Hugues Chenot, Louis Laborelli, INA)

Blurring occurs frequently in video sequences captured by consumer devices, as a result of various factors such as lens aberrations, defocus, relative camera scene motion, and camera shake. When it comes to the contents of archive documents such as old films and television shows, the degradations are even more serious due to several physical phenomena happening during the sensing, transmission, recording, and storing processes. We propose in [31] a versatile formulation of blind video deconvolution problems that seeks to estimate both the sharp unknown video sequence and the underlying blur kernel from an observed video. This inverse problem is severely ill-posed, and an appropriate solution can be obtained by modeling it as a nonconvex minimization problem. We provide a novel iterative algorithm to solve it, grounded on the use of recent advances in convex and nonconvex optimization techniques, and having the ability of including numerous well-known regularization strategies

## 7.20. BRANE Clust: Cluster-Assisted Gene Regulatory Network Inference Refinement

**Participants:** Jean-Christophe Pesquet (in collaboration with Aurélie Pirayre, IFP Energies nouvelles, Camille Couprie, Facebook Research, Laurent Duval, IFP Energies nouvelles)

Discovering meaningful gene interactions is crucial for the identification of novel regulatory processes in cells. Building accurately the related graphs remains challenging due to the large number of possible solutions from available data. Nonetheless, enforcing *a priori* on the graph structure, such as modularity, may reduce network indeterminacy issues. BRANE Clust (Biologically-Related *A priori* Network Enhancement with Clustering) refines gene regulatory network (GRN) inference thanks to cluster information. It works as a post-processing tool for inference methods (i.e. CLR, GENIE3). In BRANE Clust, the clustering is based on the inversion of a system of linear equations involving a graph-Laplacian matrix promoting a modular structure. Our approach [16] is validated on DREAM4 and DREAM5 datasets with objective measures, showing significant comparative improvements. We provide additional insights on the discovery of novel regulatory or co-expressed links in the inferred *Escherichia coli* network evaluated using the STRING database. The comparative pertinence of clustering is discussed computationally (SIMoNe, WGCNA, X-means) and biologically (RegulonDB).

## 7.21. Proximity Operators of Discrete Information Divergences

**Participants:** Jean-Christophe Pesquet (in collaboration with Mireille El Gheche, EPFL, Giovanni Chierchia, ESIEE Paris)

Information divergences allow one to assess how close two distributions are from each other. Among the large panel of available measures, a special attention has been paid to convex  $\phi$ -divergences, such as Kullback-Leibler, Jeffreys-Kullback, Hellinger, Chi-Square, Renyi, and  $I_\alpha$  divergences. While  $\phi$ -divergences have been extensively studied in convex analysis, their use in optimization problems often remains challenging. In this regard, one of the main shortcomings of existing methods is that the minimization of  $\phi$ -divergences is usually performed with respect to one of their arguments, possibly within alternating optimization techniques. In this paper, we overcome this limitation by deriving new closed-form expressions for the proximity operator of such two-variable functions. This makes it possible to employ standard proximal methods for efficiently solving a wide range of convex optimization problems involving  $\phi$ -divergences. In addition, we show that these proximity operators are useful to compute the epigraphical projection of several functions of practical interest. The proposed proximal tools are numerically validated in the context of optimal query execution within database management systems, where the problem of selectivity estimation plays a central role. Experiments are carried out on small to large scale scenarios.

## 7.22. Stochastic Quasi-Fejér Block-Coordinate Fixed Point Iterations With Random Sweeping: Mean-Square and Linear Convergence

**Participants:** Jean-Christophe Pesquet (in collaboration with Patrick L. Combettes, North Carolina State University)

In one of our previous works, we investigated the almost sure weak convergence of a block-coordinate fixed point algorithm and discussed its application to nonlinear analysis and optimization. This algorithm features random sweeping rules to select arbitrarily the blocks of variables that are activated over the course of the iterations and it allows for stochastic errors in the evaluation of the operators. The present paper establishes results on the mean-square and linear convergence of the iterates. Applications to monotone operator splitting and proximal optimization algorithms are presented.

### 7.23. Human Joint Angle Estimation and Gesture Recognition for Assistive Robotic Vision

**Participants:** Riza Alp Guler, Siddhartha Chandra, Iasonas Kokkinos (in collaboration with National Technical University of Athens)

In this work, we explore new directions for automatic human gesture recognition and human joint angle estimation as applied for human-robot interaction in the context of an actual challenging task of assistive living for real-life elderly subjects. Our contributions include state-of-the-art approaches for both low- and mid-level vision, as well as for higher level action and gesture recognition. The first direction investigates a deep learning based framework for the challenging task of human joint angle estimation on noisy real world RGB-D images. The second direction includes the employment of dense trajectory features for online processing of videos for automatic gesture recognition with real-time performance. Our approaches are evaluated both qualitatively and quantitatively on a newly acquired dataset that is constructed on a challenging real-life scenario on assistive living for elderly subjects.

### 7.24. Fast, Exact and Multi-Scale Inference for Semantic Image Segmentation with Deep Gaussian CRFs

**Participants:** Siddhartha Chandra, Iasonas Kokkinos

In this work we propose a structured prediction technique that combines the virtues of Gaussian Conditional Random Fields (G-CRF) with Deep Learning: (a) our structured prediction task has a unique global optimum that is obtained exactly from the solution of a linear system (b) the gradients of our model parameters are analytically computed using closed form expressions, in contrast to the memory-demanding contemporary deep structured prediction approaches that rely on back-propagation-through-time, (c) our pairwise terms do not have to be simple hand-crafted expressions, as in the line of works building on the DenseCRF, but can rather be ‘discovered’ from data through deep architectures, and (d) our system can be trained in an end-to-end manner. Building on standard tools from numerical analysis we develop very efficient algorithms for inference and learning, as well as a customized technique adapted to the semantic segmentation task. This efficiency allows us to explore more sophisticated architectures for structured prediction in deep learning: we introduce multi-resolution architectures to couple information across scales in a joint optimization framework, yielding systematic improvements. We demonstrate the utility of our approach on the challenging VOC PASCAL 2012 image segmentation benchmark, showing substantial improvements over strong baselines.

### 7.25. Dense and Low-Rank Gaussian CRFs Using Deep Embeddings

**Participants:** Siddhartha Chandra, Iasonas Kokkinos

In this work we introduce a structured prediction model that endows the Deep Gaussian Conditional Random Field (G-CRF) with a densely connected graph structure. We keep memory and computational complexity under control by expressing the pairwise interactions as inner products of low-dimensional, learnable embeddings. The G-CRF system matrix is therefore low-rank, allowing us to solve the resulting system in a few milliseconds on the GPU by using conjugate gradient. As in G-CRF, inference is exact, the unary and pairwise terms are jointly trained end-to-end by using analytic expressions for the gradients, while we also develop even faster, Potts-type variants of our embeddings. We show that the learned embeddings capture pixel-to-pixel affinities in a task-specific manner, while our approach achieves state of the art results on three challenging benchmarks, namely semantic segmentation, human part segmentation, and saliency estimation. This work was published in [30].



## 7.26. DenseReg: Fully Convolutional Dense Shape Regression In-the-Wild

**Participants:** Riza Alp Guler, Iasonas Kokkinos (in collaboration with Imperial College London)

In this work we propose to learn a mapping from image pixels into a dense template grid through a fully convolutional network. We formulate this task as a regression problem and train our network by leveraging upon manually annotated facial landmarks “in-the-wild”. We use such landmarks to establish a dense correspondence field between a three-dimensional object template and the input image, which then serves as the ground-truth for training our regression system. We show that we can combine ideas from semantic segmentation with regression networks, yielding a highly-accurate ‘quantized regression’ architecture.

Our system, called DenseReg allows us to estimate dense image-to-template correspondences in a fully convolutional manner. As such our network can provide useful correspondence information as a stand-alone system, while when used as an initialization for Statistical Deformable Models we obtain landmark localization results that largely outperform the current state-of-the-art on the challenging 300W benchmark. We thoroughly evaluate our method on a host of facial analysis tasks, and also demonstrate its use for other correspondence estimation tasks, such as modelling of the human ear. This work was published in [22].

## 7.27. Structured Output Prediction and Learning for Deep Monocular 3D Human Pose Estimation

**Participants:** Stefan Kinauer, Riza Alp Guler, Siddhartha Chandra, Iasonas Kokkinos

In this work we address the problem of estimating 3D human pose from a single RGB image by blending a feed-forward Convolutional Neural Network (CNN) with a graphical model that couples the 3D positions of parts. The CNN populates a volumetric output space that represents the possible positions of 3D human joints, and also regresses the estimated displacements between pairs of parts. These constitute the ‘unary’ and ‘pairwise’ terms of the energy of a graphical model that resides in a 3D label space and delivers an optimal 3D pose configuration at its output. The CNN is trained on the 3D human pose dataset 3.6M, the graphical model is trained jointly with the CNN in an end-to-end manner, allowing us to exploit both the discriminative power of CNNs and the top-down information pertaining to human pose. We introduce (a) memory efficient methods for getting accurate voxel estimates for parts by blending quantization with regression (b) employ efficient structured prediction algorithms for 3D pose estimation using branch-and-bound and (c) develop a framework for qualitative and quantitative comparison of competing graphical models. We evaluate our work on the Human 3.6M dataset, demonstrating that exploiting the structure of the human pose in 3D yields systematic gains.

## 7.28. Newton-type Methods for Inference in Higher-Order Markov Random Fields

**Participants:** Hariprasad Kannan, Nikos Paragios

Linear programming relaxations are central to MAP inference in discrete Markov Random Fields. The ability to properly solve the Lagrangian dual is a critical component of such methods. In this paper, we study the benefit of using Newton-type methods to solve the Lagrangian dual of a smooth version of the problem. We investigate their ability to achieve superior convergence behavior and to better handle the ill-conditioned nature of the formulation, as compared to first order methods. We show that it is indeed possible to efficiently apply a trust region Newton method for a broad range of MAP inference problems. In this paper we propose a provably convergent and efficient framework that includes (i) excellent compromise between computational complexity and precision concerning the Hessian matrix construction, (ii) a damping strategy that aids efficient optimization, (iii) a truncation strategy coupled with a generic pre-conditioner for Conjugate Gradients, (iv) efficient sum-product computation for sparse clique potentials. Results for higher-order Markov Random Fields demonstrate the potential of this approach. This work was published in [23].

## 7.29. Alternating Direction Graph Matching

**Participants:** D. Khuê Lê-Huu, Nikos Paragios

In this work, we introduce a graph matching method that can account for constraints of arbitrary order, with arbitrary potential functions. Unlike previous decomposition approaches that rely on the graph structures, we introduce a decomposition of the matching constraints. Graph matching is then reformulated as a non-convex non-separable optimization problem that can be split into smaller and much-easier-to-solve subproblems, by means of the alternating direction method of multipliers. The proposed framework is modular, scalable, and can be instantiated into different variants. Two instantiations are studied exploring pairwise and higher-order constraints. Experimental results on widely adopted benchmarks involving synthetic and real examples demonstrate that the proposed solutions outperform existing pairwise graph matching methods, and competitive with the state of the art in higher-order settings. This work was published in [24].

### 7.30. Prediction and classification in biological and information networks

**Participants:** Fragkiskos Malliaros (in collaboration with Duong Nguyen, UC San Diego)

We investigate how network representation learning algorithms can be applied to deal with the problem of link prediction and classification in protein-protein interaction networks as well as in social and information networks. In particular, we have proposed BiasedWalk, a scalable, unsupervised feature learning algorithm that is based on biased random walks to sample context information about each node in the network.



## LIFEWARE Project-Team

# 7. New Results

## 7.1. Strong Turing completeness of continuous CRNs

**Participants:** François Fages, Guillaume Le Guludec (former Member), Sylvain Soliman.

When seeking to understand how computation is carried out in the cell to maintain itself in its environment, process signals and make decisions, the continuous nature of protein interaction processes forces us to consider also analog computation models and mixed analog-digital computation programs. However, recent results in the theory of analog computability and complexity obtained by Pouly and Bournez, establish fundamental links between analog and digital computing. In [8] and [10], we derive from these results the strong (uniform computability) Turing completeness of chemical reaction networks over a finite set of molecular species under the differential semantics, solving a long standing open problem. Furthermore we derive from the proof a compiler of mathematical functions into elementary chemical reactions. We illustrate the reaction code generated by our compiler on trigonometric functions, and on various sigmoid functions which can serve as markers of presence or absence for implementing program control instructions in the cell and imperative programs. This makes it possible to start comparing our compiler-generated circuits to the natural circuit of the MAPK signaling network, which plays the role of an analog-digital converter in the cell with a Hill type sigmoid input/output functions.

## 7.2. Influence networks compared with reaction networks

**Participants:** François Fages, Thierry Martinez (former Member), David Rosenblueth (former Member), Sylvain Soliman, Denis Thieffry.

Biochemical reaction networks are one of the most widely used formalism in systems biology to describe the molecular mechanisms of high-level cell processes. However modellers also reason with influence diagrams to represent the positive and negative influences between molecular species and may find an influence network useful in the process of building a reaction network. In [11], we introduce a formalism of influence networks with forces, and equip it with a hierarchy of Boolean, Petri net, stochastic and differential semantics, similarly to reaction networks with rates. We show that the expressive power of influence networks is the same as that of reaction networks under the differential semantics, but weaker under the discrete semantics. Furthermore, the hierarchy of semantics leads us to consider a (positive) Boolean semantics without test for absence, that we compare with the (negative) Boolean semantics with test for absence of gene regulatory networks à la Thomas. We study the monotonicity properties of the positive semantics and derive from them an algorithm to compute attractors in both the positive and negative Boolean semantics. We illustrate our results on models of the literature about the p53/Mdm2 DNA damage repair system, the circadian clock, and the influence of MAPK signaling on cell-fate decision in urinary bladder cancer.

## 7.3. Machine learning influence networks from data

**Participants:** Arthur Carcano, François Fages, Jérémy Grignard, Sylvain Soliman.

Automating the process of model building from experimental data is a very desirable goal to palliate the lack of modellers for many applications. However, despite the spectacular progress of machine learning techniques in data analytics, classification, clustering and prediction making, learning dynamical models from data time-series is still challenging. In [7], we investigate the use of the Probably Approximately Correct (PAC) learning framework of Leslie Valiant as a method for the automated discovery of influence models of biochemical processes from Boolean and stochastic traces. We show that Thomas' Boolean influence systems can be naturally represented by k-CNF formulae, and learned from time-series data with a number of Boolean activation samples per species quasi-linear in the precision of the learned model, and that positive Boolean influence systems can be represented by monotone DNF formulae and learned actively with both activation samples and oracle calls. We consider Boolean traces and Boolean abstractions of stochastic simulation traces, and show the space-time tradeoff there is between the diversity of initial states and the length of the time horizon, together with its impact on the error bounds provided by the PAC learning algorithms. We evaluate the performance of this approach on a model of T-lymphocyte differentiation, with and without prior knowledge, and discuss its merits as well as its limitations with respect to realistic experiments.

#### **7.4. Shaping bacterial population behavior through computer-interfaced control of individual cells**

**Participant:** Jakob Ruess.

Bacteria in groups vary individually, and interact with other bacteria and the environment to produce population-level patterns of gene expression. Investigating such behavior in detail requires measuring and controlling populations at the single-cell level alongside precisely specified interactions and environmental characteristics. In [1], we present an automated, programmable platform that combines image-based gene expression and growth measurements with on-line optogenetic expression control for hundreds of individual *Escherichia coli* cells over days, in a dynamically adjustable environment. This integrated platform broadly enables experiments that bridge individual and population behaviors. We demonstrate: (i) population structuring by independent closed-loop control of gene expression in many individual cells, (ii) cell-cell variation control during antibiotic perturbation, (iii) hybrid bio-digital circuits in single cells, and freely specifiable digital communication between individual bacteria. These examples showcase the potential for real-time integration of theoretical models with measurement and control of many individual cells to investigate and engineer microbial population behavior.

#### **7.5. Balancing a genetic toggle switch by real-time feedback control and periodic forcing**

**Participants:** Gregory Batt, Jean-Baptiste Lugagne, Melanie Kirch (former Member), Agnes Köhler (former Member), Sebastian Sosa Carrillo.

Cybergenetics is a novel field of research aiming at remotely pilot cellular processes in real-time with to leverage the biotechnological potential of synthetic biology. Yet, the control of only a small number of genetic circuits has been tested so far. Here we investigate the control of multistable gene regulatory networks, which are ubiquitously found in nature and play critical roles in cell differentiation and decision-making. Using an in silico feedback control loop, we demonstrate that a bistable genetic toggle switch can be dynamically maintained near its unstable equilibrium position for extended periods of time [2]. Importantly, we show that a direct method based on dual periodic forcing is sufficient to simultaneously maintain many cells in this undecided state. These findings pave the way for the control of more complex cell decision-making systems at both the single cell and the population levels, with vast fundamental and biotechnological applications.

#### **7.6. Abstracting the dynamics of biological pathways using information theory: a case study of apoptosis pathway**

**Participants:** Gregory Batt, François Bertaux (former Member), Sucheendra Palaniappan (former Member).

Quantitative models are increasingly used in systems biology. Usually, these quantitative models involve many molecular species and their associated reactions. When simulating a tissue with thousands of cells, using these large models becomes computationally and time limiting. In our paper, we propose to construct abstractions using information theory notions [3]. Entropy is used to discretize the state space and mutual information is used to select a subset of all original variables and their mutual dependencies. We apply our method to an hybrid model of TRAIL-induced apoptosis in HeLa cell. Our abstraction, represented as a Dynamic Bayesian Network (DBN), reduces the number of variables from 92 to 10, and accelerates numerical simulation by an order of magnitude, yet preserving essential features of cell death time distributions.

## **7.7. Long-term tracking of budding yeast cells in brightfield microscopy: CellStar and the Evaluation Platform**

**Participants:** Gregory Batt, Art  mis Llamosi (former Member).

With the continuous expansion of single cell biology, the observation of the behaviour of individual cells over extended durations and with high accuracy has become a problem of central importance. Surprisingly, even for yeast cells that have relatively regular shapes, no solution has been proposed that reaches the high quality required for long-term experiments for segmentation and tracking (S&T) based on brightfield images. In this contribution, we present CellStar, a tool chain designed to achieve good performance in long-term experiments [5]. The key features are the use of a new variant of parametrized active rays for segmentation, a neighbourhood-preserving criterion for tracking, and the use of an iterative approach that incrementally improves S&T quality. A graphical user interface enables manual corrections of S&T errors and their use for the automated correction of other, related errors and for parameter learning. We created a benchmark dataset with manually analysed images and compared CellStar with six other tools, showing its high performance, notably in long-term tracking. As a community effort, we set up a website, the Yeast Image Toolkit, with the benchmark and the Evaluation Platform to gather this and additional information provided by others.

## **7.8. Sensitivity estimation for stochastic models of biochemical reaction networks in the presence of extrinsic variability**

**Participant:** Jakob Ruess.

Determining the sensitivity of certain system states or outputs to variations in parameters facilitates our understanding of the inner working of that system and is an essential design tool for the de novo construction of robust systems. In cell biology, the output of interest is often the response of a certain reaction network to some input (e.g., stressors or nutrients) and one aims to quantify the sensitivity of this response in the presence of parameter heterogeneity. We argue that for such applications, parametric sensitivities in their standard form do not paint a complete picture of a system's robustness since one assumes that all cells in the population have the same parameters and are perturbed in the same way. In the published contribution, we consider stochastic reaction networks in which the parameters are randomly distributed over the population and propose a new sensitivity index that captures the robustness of system outputs upon changes in the characteristics of the parameter distribution, rather than the parameters themselves [4]. Subsequently, we make use of Girsanov's likelihood ratio method to construct a Monte Carlo estimator of this sensitivity index. However, it turns out that this estimator has an exceedingly large variance. To overcome this problem, we propose a novel estimation algorithm that makes use of a marginalization of the path distribution of stochastic reaction networks and leads to Rao-Blackwellized estimators with reduced variance.

## **7.9. Recombinase-based genetic circuit optimization by integer linear programming**

**Participant:** Fran  ois Fages.

The rapid advancements of synthetic biology show promising potential in biomedical and other applications. Recently, recombinases were proposed as a tool to engineer genetic logic circuits with long-term memory in living and even mammalian cells. The technology is under active development, and the complexity of engineered genetic circuits grows continuously. However, how to minimize a genetic circuit composed of recombinase-based logic gates remain largely open. In [12], we formulate the problem as a cubic-time assignment problem and solved by a 0/1-ILP solver to minimize DNA sequence length of genetic circuits. Experimental results show effective reduction of our optimization method, which may be crucial to enable practical realization of complex genetic circuits.

## 7.10. Coupled models of the cell cycle and circadian clock

**Participants:** François Fages, Sylvain Soliman, Pauline Traynard (former Member).

Experimental observations have put in evidence autonomous self-sustained circadian oscillators in most mammalian cells, and proved the existence of molecular links between the circadian clock and the cell cycle. Some mathematical models have also been built to assess conditions of control of the cell cycle by the circadian clock, with applications to cancer chronotherapy optimization. However, recent studies in individual NIH3T3 fibroblasts have shown an unexpected acceleration of the circadian clock together with the cell cycle when the culture medium is enriched with growth factors, and the absence of such acceleration in confluent cells. In order to explain these observations, we have studied a possible entrainment of the circadian clock by the cell cycle through a regulation of clock genes around the mitosis phase. We developed a computational model in Biocham with a formal specification of the observed behavior in quantitative temporal logic to investigate the conditions of entrainment in period and phase. We showed that either the selective activation of RevErb- $\alpha$  or the selective inhibition of Bmal1 transcription during the mitosis phase, allowed us to fit the experimental data on both period and phase, while a uniform inhibition of transcription during mitosis seems incompatible with the phase data. In [6], we presented those results and some further predictions of the bidirectional model with a coupling in both directions.

## M3DISIM Project-Team

## 7. New Results

### 7.1. Mathematical and Mechanical Modeling

#### 7.1.1. *Modelling of collagen fibers elastic properties*

**Participants:** Peter Baumgartner, Florent Wijanto, Jean-Marc Allain [correspondant], Matthieu Caruel [Univ. Paris-Est].

Our studies on collagen tissues have shown that the collagen fibers are able to elongate inelastically under stretch. In tendons, this effect has been attributed to the non-permanent cross-bridges that connect the different collagen fibrils (to assemble a fiber). This sliding effect appears experimentally to be reversible (at least partially) if the tissue is left long enough at its initial resting length. However, this sliding is classically included as an irreversible plastic response, or as a damage of the tissue. We are building a model based on a stochastic description of the binding and unbinding of the cross-bridges. This approach will enable us to have a microscopically based picture of the sliding, which will be able to explain some alterations in case of aging or pathologies of the tissue. At the moment, we have shown the importance of the density of cross-bridges in the cooperative response of the system. A publication is in preparation on the topic.

#### 7.1.2. *Multi-scale modeling of cardiac contraction*

**Participants:** François Kimmig, Matthieu Caruel [Univ. Paris-Est], Dominique Chapelle [correspondant], Philippe Moireau.

This work aims at proposing a set of models of the muscular contraction targeting different scales in time and space and that can be used in the context of heart simulation. To this end, we developed so far two models using different approaches for the modeling of the force generating process at the molecular level called power stroke. First, we revised the standard chemo-mechanical models, which see the power stroke as a series of chemical states. Following the idea introduced by Truskinovsky and collaborators describing the power stroke as a continuum of mechanical states with the dynamics of the myosin head in the prescribed energy landscape governed by Langevin equations, we incorporated the attachment and detachment dynamics in the form of jump processes. In a second step, noting that the power stroke time scale is much shorter than that of heart contraction, we eliminated the power strokes dynamics and derived a two state – attached and detached – simplified model, each state being in fact associated with a statistical distribution of myosin head configurations. Both models have been integrated into our simulation framework CardiacLab, in order to benefit from the other modeling compartments available in the code, such as the geometrically reduced model of the heart left ventricle also developed in the team. These modeling elements will be confronted with experiments performed on cardiac muscle cells by collaborators in the team of Professor Lombardi at the University of Florence.

#### 7.1.3. *Mathematical and numerical modeling of shear waves propagation in the heart*

**Participants:** Federica Caforio, Sébastien Imperiale [correspondant], Dominique Chapelle.

Shear acoustic waves remotely induced by the acoustic radiation force (ARF) of a focused ultrasound beam generated by piezoelectric sensors have been recently used in biomedical applications, e.g. in transient elastography techniques. By measuring the propagation velocity of generated shear waves in biological tissues, it is possible to locally assess biomechanical properties highly sensitive to structural changes corresponding to physiological and pathological processes. Recent experimental studies show the feasibility of applying transient elastography to the cardiac setting. In this context, the wave propagation induced by the ARF is superposed with the nonlinear mechanics associated with the heart deformation during the cardiac cycle. The aim of this work is to mathematically justify an original expression of the excitation induced by the ARF in nonlinear solids, based on energy considerations and asymptotic analysis. In soft media the propagation

velocity of shear waves ( $1 - 10 \text{ m.s}^{-1}$ ) is much smaller than the velocity of pressure waves ( $1500 \text{ m.s}^{-1}$ ). The approach we propose consists in considering a family of problems parametrised by a small parameter  $\varepsilon$  related to the velocity ratio between the two wave propagation phenomena, the high frequency of the piezoelectric source term and the viscosity. In order to derive a simplified model for the expression of ARF, we investigate the limit behavior of the solution for  $\varepsilon \rightarrow 0$ . We show that the leading term of the expansion is related to the underlying nonlinear mechanics of the heart deformation, and the first two correction terms correspond to a fast-oscillating pressure wave excited by the probe, and an elastic field having as source term a nonlinear function of the first corrector. This field corresponds to the shear acoustic wave induced by the ARF.

#### 7.1.4. Analysis and 2-scale convergence of a heterogeneous microscopic bidomain model

**Participants:** Sébastien Imperiale [correspondant], Annabelle Collin [Monc].

The aim of this work is to provide a complete mathematical analysis of the periodic homogenization procedure that leads to the macroscopic bidomain model in cardiac electrophysiology. We consider space-dependent and tensorial electric conductivities as well as space-dependent physiological and phenomenological non-linear ionic models. We provide the nondimensionalization of the bidomain equations and derive uniform estimates of the solutions. The homogenization procedure is done using 2-scale convergence theory which enables us to study the behavior of the non-linear ionic models in the homogenization process.

#### 7.1.5. A reduced thoracic model for inverse problem solving in seismocardiography

**Participants:** Alexandre Laurin, Sébastien Imperiale [correspondant], Dominique Chapelle, Philippe Moireau.

Seismocardiography (SCG) is the study of low-frequency ( $< 60 \text{ Hz}$ ) vibrations of the thorax caused by the beating heart. Although it is assumed that SCG signals are caused by forces applied on the interior of the thorax by the heart, no comprehensive model exists to describe the parameters and relationships that govern the system. The main goal of this study is to describe in some detail the filter applied by the thorax on cardiac forces, taking into account its zone of contact with the heart as well as the zone of measurement, i.e. the location of the accelerometer on a participant's chest. A secondary goal is to identify the smallest set of parameters capable of reproducing the filter, reducing the model while retaining its capacity to lend itself to physiological interpretation. Finally, we described a method to use the reduced model to estimate cardiac forces from measured thoracic accelerations. The overall aim of the study is to develop numerical methods that can augment the existing SCG interpretations to include mechanical indices of the heart muscle, and do so in real time.

## 7.2. Numerical Methods

### 7.2.1. Numerical methods for computing cyclic steady states

**Participants:** Ustim Khristenko, Patrick Le Tallec [correspondant].

This work is focused on two techniques for fast computing of the steady cyclic states of evolution problems in non-linear mechanics with space-time periodicity conditions. This kind of problems can be faced in various applications, for instance in the rolling of a tyre with periodic sculptures as well as in a beating heart. Direct solvers for such problems are not very convenient, since they require the inversion of very large matrices. In order to avoid this, a cyclic solution is usually computed as an asymptotic limit of the associated initial value problem with prescribed initial data. However, when the relaxation time is high, convergence to the limit cycle can be very slow. The first technique considered is the Newton-Krylov method, looking for the unknown initial state that provides the space-time periodic solution. This initial state is defined by the space-time periodicity condition, solved with the Newton-Raphson technique. Since the associated Jacobian cannot be expressed explicitly, the method uses one of the matrix-free Krylov iterative solvers. Using information stored while computing the residual to solve the linear system makes its calculation time negligible with respect to the residual calculation time. The second method is the delayed feedback control: an observer-controller type modification of the standard evolution to the limit cycle by introducing a feedback control term, based on

the periodicity error. The main result is the optimal form of the control term for a very general class of linear evolution problems, providing the fastest convergence to the cyclic solution. This control has also been adapted and tested for nonlinear problems. The methods discussed have been assessed using academic applications and they have also been implemented into the Michelin industrial code – applied to the rolling tyre model – as well as into the M3DISIM code for the cardiac contraction problem.

### 7.2.2. *Solving isotropic elastodynamics using potentials*

**Participants:** Sébastien Imperiale [correspondant], Jorge Albella.

This work has the potential to provide an original efficient method for the computations of elastic waves propagation in soft media (such as biological tissues), based on the property that pressure and shear waves decouple in isotropic media. Towards this direction, we considered the numerical solution of 2D elastodynamics isotropic equations using the decomposition of the displacement fields into potentials. This appears as a challenge for finite element methods, and we have addressed here the particular question of free boundary conditions. A stable (mixed) variational formulation of the evolution problem is proposed.

### 7.2.3. *The Arlequin method for transient wave scattering by small obstacles*

**Participants:** Sébastien Imperiale [correspondant], Jorge Albella.

In this work we extend the Arlequin method to overlapping domain decomposition technique for transient wave equation scattering by small obstacles. The main contribution of this work is to construct and analyze some variants of the Arlequin method from the continuous level to the fully discrete level. The constructed discretizations allow to solve wave propagation problems while using non-conforming and overlapping meshes for the background propagating medium and the surrounding of the obstacle, respectively. Hence we obtain a flexible and stable method in terms of the space discretization – an inf-sup condition is proven – while the stability of the time discretization is ensured by energy identities.

### 7.2.4. *Construction of a fourth-order time scheme for dissipative wave equations*

**Participants:** Sébastien Imperiale [correspondant], Juliette Chabassier [Magique-3d], Julien Diaz [Magique-3d].

This work deals with the construction of a fourth-order, energy preserving, explicit time discretization for dissipative linear wave equations. This discretization is obtained by replacing the inversion of a matrix – that comes naturally after using the technique of the Modified Equation on the second order Leap Frog scheme applied to dissipative linear wave equations – by an explicit approximation of its inverse. The stability of the scheme is studied first using an energy analysis, then an eigenvalue analysis. Numerical results in 1D illustrate the good behavior regarding space/time convergence and the efficiency of the newly derived scheme compared to more classical time discretizations. A loss of accuracy is observed for non-smooth profiles of dissipation, and we propose an extension of the method that fixes this issue. Finally, we assess the good performance of the scheme for a realistic dissipation phenomenon in Lorentz materials.

### 7.2.5. *Coupled variational formulations of linear elasticity and the DPG methodology*

**Participant:** Patrick Le Tallec [correspondant].

In this work, we develop a general approach akin to domain-decomposition methods to solve a single linear PDE, but where each subdomain of a partitioned domain is associated with a distinct variational formulation coming from a mutually well-posed family of so-called broken variational formulations of the original PDE. It can be exploited to solve challenging problems in a variety of physical scenarios where stability or a particular mode of convergence is desired in some part of the domain. The linear elasticity equations are solved in this work, but the approach can be applied to other equations as well. The broken variational formulations, which are essentially extensions of more standard formulations, are characterized by the presence of mesh-dependent broken test spaces and interface trial variables at the boundaries of the elements of the mesh. This allows necessary information to be naturally transmitted between adjacent subdomains, resulting in coupled variational formulations which are then proved to be globally well-posed. They are solved numerically using the DPG methodology, which is especially crafted to produce stable discretizations of broken formulations. Finally, expected convergence rates are verified in two different illustrative examples. This work has resulted in the publication [19].



### 7.2.6. *A discontinuous Galerkin approach for cardiac electrophysiology*

**Participant:** Radomir Chabiniok [correspondant].

Cardiac electrophysiology simulations are numerically challenging due to the propagation of a steep electrochemical wave front, and thus require discretizations with small mesh sizes to obtain accurate results. In this work – in collaboration with the Institute for Computational Mechanics, Technical University Munich and published in [21] – we present an approach based on the Hybridizable Discontinuous Galerkin method (HDG), which allows an efficient implementation of high-order discretizations into a computational framework. In particular using the advantage of the discontinuous function space, we present an efficient p-adaptive strategy for accurately tracking the wave front. HDG allows to reduce the overall degrees of freedom in the final linear system to those only on the element interfaces. Additionally, we propose a rule for a suitable integration accuracy for the ionic current term depending on the polynomial order and the cell model to handle high-order polynomials. Our results show that for the same number of degrees of freedom coarse high-order elements provide more accurate results than fine low-order elements. Introducing p-adaptivity further reduces computational costs while maintaining accuracy by restricting the use of high-order elements to resolve the wave front. For a patient-specific simulation of a cardiac cycle, p-adaptivity reduces the average number of degrees of freedom by 95% compared to the non-adaptive model. In addition to reducing computational costs, using coarse meshes with our p-adaptive high-order HDG method also simplifies practical aspects of mesh generation and postprocessing.

## 7.3. Inverse Problems

### 7.3.1. *Discrete-time optimal filtering or Mortensen observer discretization*

**Participant:** Philippe Moireau [correspondant].

In this work, we seek exact formulations of the optimal estimator and filter for a non-linear framework, as the Kalman filter is for a linear framework. The solution is well established with the Mortensen filter in a continuous-time setting, but we seek here its counterpart in a discrete-time context. We demonstrate that it is possible to pursue at the discrete-time level an exact dynamic programming strategy and we find an optimal estimator combining a prediction step using the model and a correction step using the data. This optimal estimator reduces to the discrete-time Kalman estimator when the operators are in fact linear. Furthermore, the strategy that consists of discretizing the least square criterion and then finding the exact estimator at the discrete level allows to determine a new time-scheme for the Mortensen filter which is proven to be consistent and unconditionally stable, with also a consistent and stable discretization of the underlying Hamilton-Jacobi-Bellman equation. This work has resulted in the publication [30].

### 7.3.2. *An iterative method for identifying a stress-free state in image-based biomechanics*

**Participant:** Martin Genet [correspondant].

Continued advances in computational power and methods have enabled image-based biomechanical modeling to become an important tool in basic science, diagnostic and therapeutic medicine, and medical device design. One of the many challenges of this approach, however, is identification of a stress-free reference configuration based on in vivo images of loaded and often prestrained or residually stressed soft tissues and organs. Fortunately, iterative methods have been proposed to solve this inverse problem, among them Sellier's method. This method is particularly appealing because it is easy to implement, converges reasonably fast, and can be coupled to nearly any finite element package. By means of several practical examples, however, we demonstrate that in its original formulation Sellier's method is not optimally fast and may not converge for problems with large deformations. Nevertheless, we can also show that a simple, inexpensive augmentation of Sellier's method based on Aitken's delta-squared process can not only ensure convergence but also significantly accelerate the method. This work has resulted in the publication [31].

### 7.3.3. *A continuum finite strain formulation for finite element image correlation*

**Participant:** Martin Genet [correspondant].



We propose a novel continuum finite strain formulation of the equilibrium gap principle – originally introduced in [Claire, Hild and Roux, 2004, Int. J. Num. Meth. Eng.] at the discrete level for linearized elasticity – used as a regularizer for finite element-based image correlation problems. Consistent linearization and finite element discretization is provided. The method is implemented using FEniCS & VTK, in a freely available Python library. The equilibrium gap constraint regularizes the image correlation problem, even in the presence of noise, and without affecting strain measurements.

### 7.3.4. *Front shape similarity measure for Eikonal PDE data assimilation*

**Participants:** Annabelle Collin [Monc], Philippe Moireau [correspondant].

We present a shape-oriented data assimilation strategy suitable for front-tracking problems through the example of wildfire. The concept of “front” is used to model, at regional scales, the burning area delimitation that moves and undergoes shape and topological changes under heterogeneous orography, biomass fuel and micrometeorology. The simulation-observation discrepancies are represented using a front shape similarity measure inspired from image processing and based on the Chan-Vese contour fitting functional. We show that consistent corrections of the front location and uncertain physical parameters can be obtained using this measure applied on a level-set fire growth model solving for an eikonal equation. This study involves a Luenberger observer for state estimation, including a topological gradient term to track multiple fronts, and a reduced-order Kalman filter for joint parameter estimation. We also highlight the need – prior to parameter estimation – for sensitivity analysis based on the same discrepancy measure, and for instance using polynomial chaos metamodels, to ensure that a meaningful inverse solution is achieved. The performance of the shape-oriented data assimilation strategy is assessed on a synthetic configuration subject to uncertainties in front initial position, near-surface wind magnitude and direction. The use of a robust front shape similarity measure paves the way toward the direct assimilation of infrared images and is a valuable asset in the perspective of data-driven wildfire modeling. This work has resulted in the publication [32].

### 7.3.5. *The mechanism of monomer transfer between two distinct PrP oligomers*

**Participants:** Aurora Armiento, Marie Doumic [Mamba], Philippe Moireau [correspondant].

In mammals, Prion pathology refers to a class of infectious neuropathologies whose mechanism is based on the self-perpetuation of structural information stored in the pathological conformer. The characterisation of the PrP folding landscape has revealed the existence of a plethora of pathways conducing to the formation of structurally different assemblies with different biological properties. However, the biochemical interconnection between these diverse assemblies remains unclear. The PrP oligomerisation process leads to the formation of neurotoxic and soluble assemblies called O1 oligomers with a high size heterodispersity. By combining the measurements in time of size distribution and average size with kinetic models and data assimilation, we revealed the existence of at least two structurally distinct sets of assemblies, termed Oa and Ob, forming O1 assemblies. We propose a kinetic model representing the main processes in prion aggregation pathway: polymerisation, depolymerisation, and disintegration. The two groups interact by exchanging monomers through a disintegration process that increases the size of Oa. Our observations suggest that PrP oligomers constitute a highly dynamic population. This work has resulted in the publication [14].

### 7.3.6. *Joint-state and parameters estimation using ROUKF for HIV mechanistic models*

**Participants:** Annabelle Collin [Monc], Philippe Moireau [correspondant], Mélanie Prague [Sism].

Various methods have been used in the statistical field to estimate parameters in mechanistic models. In particular, an approach based on penalised likelihood for the estimation of parameters in ordinary differential equations with non linear models on parameters (ODE-NLME) has proven successful. For instance, we consider the NIMROD program as a benchmark for estimation in these models. However, such an approach is time consuming. To circumvent this problem, we consider data assimilation approaches that historically arose in the context of geophysics. Here, we propose a Luenberger (also called nudging) state observer coupled with a parameter Kalman-based observer (RoUKF filter, also called SEIK filter) to perform a joint state and parameter estimation on a dataset composed of longitudinal observations of biomarkers for multiple patients. We compare these methods in terms of performances and computation time. We discuss how the concept of

random effect can be modeled using Kalman-based filter and its limitations. We illustrate both methods in simulation and on two datasets (the ALBI ANRS 070 trial and the Aquitaine cohort observational data) using an HIV mechanistic model.

## 7.4. Experimental Assessments

### 7.4.1. *Microstructural interpretation of mouse skin mechanics from multiscale characterization*

**Participant:** Jean-Marc Allain [correspondant].

Skin is a complex, multi-layered organ, with important functions in the protection of the body. The dermis provides structural support to the epidermal barrier, and thus has attracted a large number of mechanical studies. As the dermis is made of a mixture of stiff fibres embedded in a soft non-fibrillar matrix, it is classically considered that its mechanical response is based on an initial alignment of the fibres, followed by the stretching of the aligned fibres. Using a recently developed set-up combining multiphoton microscopy with mechanical assay, we imaged the fibres network evolution during dermis stretching. These observations, combined with a wide set of mechanical tests, allowed us to challenge the classical microstructural interpretation of the mechanical properties of the dermis: we observed a continuous alignment of the collagen fibres along the stretching. All our results can be explained if each fibre contributes by a given stress to the global response. This plastic response is likely due to inner sliding inside each fibre. The non-linear mechanical response is due to structural effects of the fibres network in interaction with the surrounding non-linear matrix. This multiscale interpretation explains our results on genetically-modified mice with a simple alteration of the dermis microstructure. This work has resulted in the publication [27].

### 7.4.2. *Affine kinematics in planar fibrous connective tissues: an experimental investigation*

**Participants:** Jean-Sébastien Affagard, Jean-Marc Allain [correspondant].

The affine transformation hypothesis is usually adopted in order to link the tissue scale with the fibers scale in structural constitutive models of fibrous tissues. Thanks to the recent advances in imaging techniques, such as multiphoton microscopy, the microstructural behavior and kinematics of fibrous tissues can now be monitored at different stretching within the same sample. Therefore, the validity of the affine hypothesis can be investigated. In this study, the fiber reorientation predicted by the affine assumption is compared with experimental data obtained during mechanical tests on skin and liver capsule coupled with microstructural imaging using multiphoton microscopy. The values of local strains and the collagen fibers orientation measured at increasing loading levels are used to compute a theoretical estimation of the affine reorientation of collagen fibers. The experimentally measured reorientation of collagen fibers during loading could not be successfully reproduced with this simple affine model. It suggests that other phenomena occur in the stretching process of planar fibrous connective tissues, which should be included in structural constitutive modeling approaches. This work has resulted in the publication [22].

### 7.4.3. *Improving the experimental protocol for the identification of skin mechanical behavior*

**Participants:** Jean-Sébastien Affagard, Florent Wijanto, Jean-Marc Allain [correspondant].

Mechanical properties of the skin, the external organ of the human body, are important for many applications such as surgery or cosmetics. Due to the highly hierarchical structure of the tissue, it is interesting to develop microstructural models that have better predictability and should reduce the consequences of sample variability. However, these models generally include a quite large number of mechanical parameters. Therefore, complex assays are required to achieve a proper identification of the microstructural models. We investigated in this study the best experimental protocol to identify a nonlinear, anisotropic, model of skin behavior, namely, the Holzapfel law, using displacement field and force measurements. This was done through a sensitivity analysis of the different parameters. We determined first the optimal assay, which appears to be a biaxial test with an alternated loading: first a stretch in one direction, then in the perpendicular one, and so on. To further improve the quality of the assay, we also determined the optimal geometry. Interestingly, slightly asymmetric geometries are more adequate than symmetric ones, while being easier to realise. This work has resulted in the publication [13].

#### **7.4.4. *How aging impacts skin biomechanics: a multiscale study in mice***

**Participants:** Jean-Sébastien Affagard, Jean-Marc Allain [correspondant].

Skin aging is a complex process that strongly affects the mechanical behavior of skin. This study aims at deciphering the relationship between age-related changes in dermis mechanical behavior and the underlying changes in dermis microstructure. To that end, we use multiphoton microscopy to monitor the reorganization of dermal collagen during mechanical traction assays in ex vivo skin from young and old mice. The simultaneous variations of a full set of mechanical and microstructural parameters are analyzed in the framework of a multiscale mechanical interpretation. They show consistent results for wild-type mice as well as for genetically-modified mice with modified collagen V synthesis. We mainly observe an increase of the tangent modulus and a lengthening of the heel region in old murine skin from all strains, which is attributed to two different origins that may act together: (i) increased cross-linking of collagen fibers and (ii) loss of water due to proteoglycans deterioration, which impedes inner sliding within these fibers. In contrast, the microstructure reorganization upon stretching shows no age-related difference, which can be attributed to opposite effects of the decrease of collagen content and of the increase of collagen cross-linking in old mice. This work has resulted in the publication [28].

#### **7.4.5. *Recent advances in studying single bacteria and biofilm mechanics***

**Participant:** Jean-Marc Allain [correspondant].

Bacterial biofilms correspond to surface-associated bacterial communities embedded in hydrogel-like matrix, in which high cell density, reduced diffusion and physico-chemical heterogeneity play a protective role and induce novel behaviors. We made a summary of the recent advances on the understanding of how bacterial mechanical properties, from single cell to high-cell density community, determine biofilm three-dimensional growth and eventual dispersion, and we attempt to draw a parallel between these properties and the mechanical properties of other well-studied hydrogels and living systems. This work has resulted in the publication [18].

### **7.5. Clinical Applications**

#### **7.5.1. *Assessment of atrioventricular valve regurgitation using cardiac modeling***

**Participants:** Radomir Chabiniok [correspondant], Philippe Moireau, Dominique Chapelle.

In this work, we introduce the modeling of atrioventricular valve regurgitation in a spatially reduced-order biomechanical heart model. The model can be fast calibrated using non-invasive data of cardiac magnetic resonance imaging and provides an objective measure of contractile properties of the myocardium in the volume overloaded ventricle, for which the real systolic function may be masked by the significant level of the atrioventricular valve regurgitation. After demonstrating such diagnostic capabilities, we show the potential of modeling to address some clinical questions concerning possible therapeutic interventions for specific patients. The fast running of the model allows targeting specific questions of referring clinicians in a clinically acceptable time. The work was presented at the “Functional Imaging and Modeling of the Heart” conference (FIMH 2017, Toronto, Canada) and is included in the conference proceedings [35].

#### **7.5.2. *Model for the dobutamine response in exercise-induced failure of the Fontan circulation***

**Participants:** Radomir Chabiniok [correspondant], Philippe Moireau, Dominique Chapelle.

Understanding physiological phenomena and mechanisms of failure in congenital heart diseases is often challenging due to the complex hemodynamics and high inter-patient variations in anatomy and function. Computational modeling techniques have the potential to greatly improve the understanding of these complex diseases and provide patient-specific clues on mechanisms of deterioration and impact of treatments. This work employs a reduced 0D biomechanical heart model coupled with venous return to capture various key pathophysiological phenomena observed in patients with completed Fontan circulation – a complex surgically established circulation used to palliate patients in whom only one of the two ventricles is functionally able to support the vascular system – with exercise-induced heart failure during dobutamine stress. The framework we propose is fast, efficient and well-suited to the type of pathology and available clinical data obtained by a

combined cardiac catheterization and magnetic resonance imaging exam. We demonstrate that the outcomes of modeling are a valuable addition to the current clinical diagnostic investigations and explain patient-specific exercise hemodynamics, identify potential mechanisms of Fontan failure, and enable evaluation of a potential new therapy – selective heart rate modulation – in the treatment of patients with Fontan circulation. The paper is currently in preparation.

### **7.5.3. Heart and vessels modeling with data interaction for monitoring anesthetized patients**

**Participants:** Arthur Le Gall, Radomir Chabiniok [correspondant], Fabrice Vallée, Dominique Chapelle.

By using mathematical models of heart and vessels developed in the team, we aim at improving intra-operative cardio-vascular safety of anesthetized patients. The patient-specific models, calibrated by echocardiography images and fed by continuous monitoring of aortic arterial pressure and aortic cardiac outflow would allow us to: 1) diagnose pathophysiological modifications associated with changes in the cardio-vascular state; 2) predict the drug response of the patient before the administration of the vaso-active treatment.

### **7.5.4. Intra-operative monitoring of cardiac afterload**

**Participants:** Arthur Le Gall, Fabrice Vallée [correspondant].

General anesthesia leads to alterations of the cardiovascular system. Intra-operative arterial hypotension is linked to post-operative complications, but using vasopressors to treat arterial hypotension has shown conflicting results. Vasopressors act mainly by elevating cardiac afterload, which could be deleterious in fragile patients, in case of excessive response. Moreover, differences among the most used vasopressors have been observed in vivo [34]. The choice of vasopressor could be important to improve our patients' care. Consequently, we proposed a tool (Velocity-Pressure Loops) to continuously quantify changes in cardiac afterload [33]. Although the first work involves invasive measurement of aortic blood pressure and cardiac outflow, consistent results have been observed when Velocity-Pressure Loops were obtained by a radial arterial catheter with a mathematical transform function [23]. Those findings allow the usage of the Velocity-Pressure Loop without addition of any invasive device.

### **7.5.5. Review on extra-corporeal circulation**

**Participant:** Arthur Le Gall [correspondant].

This clinical review [26] aims at describing the issues of the management of extra-corporeal membrane oxygenation (ECMO) in the Intensive Care Unit (ICU). From pathophysiology to the description of the impact on mortality, this document shows a global picture of current clinical practices.

### **7.5.6. On the importance of consistency in cardiac timings measurements**

**Participants:** Arthur Le Gall, Alexandre Laurin, Fabrice Vallee [correspondant].

With the contribution of Denis Chemla, professor of Cardiology at Bicêtre Hospital, we presented this work at the CinC conference in Rennes [36]. In this work, we emphasize the need for a consistent method to measure systolic period duration, which is related to cardiac afterload and could be used to quantify arterial pressure amplification phenomenon.

## PARIETAL Project-Team

## 7. New Results

### 7.1. Joint prediction of multiple scores captures better individual traits from brain images

To probe individual variations in brain organization, population imaging relates features of brain images to rich descriptions of the subjects such as genetic information or behavioral and clinical assessments. Capturing common trends across these measurements is important: they jointly characterize the disease status of patient groups. In particular, mapping imaging features to behavioral scores with predictive models opens the way toward more precise diagnosis. Here we propose to jointly predict all the dimensions (behavioral scores) that make up the individual profiles, using so-called multi-output models. This approach often boosts prediction accuracy by capturing latent shared information across scores. We demonstrate the efficiency of multi-output models on two independent resting-state fMRI datasets targeting different brain disorders (Alzheimer's Disease and schizophrenia). Furthermore, the model with joint prediction generalizes much better to a new cohort: a model learned on one study is more accurately transferred to an independent one. Finally, we show how multi-output models can easily be extended to multi-modal settings, combining heterogeneous data sources for a better overall accuracy.

More information can be found in Fig. 3 in [46].

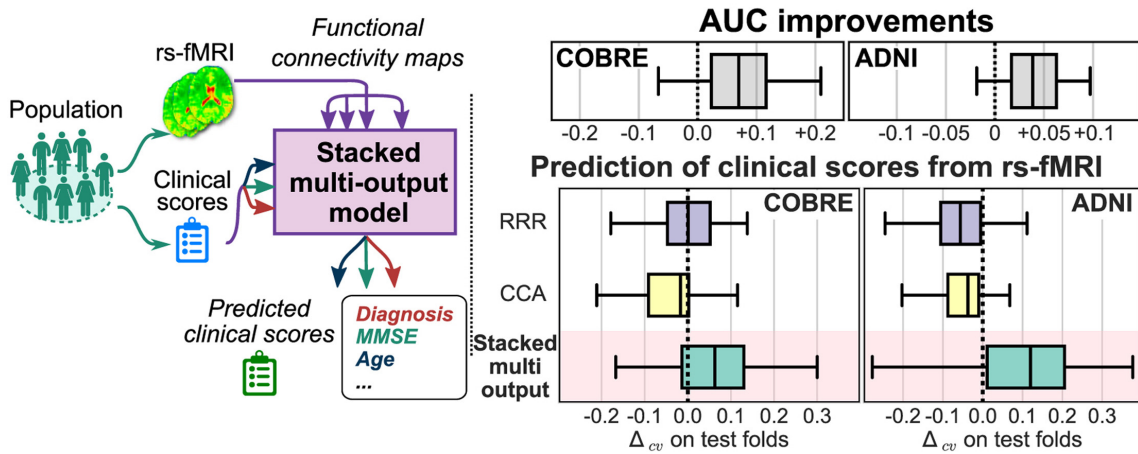


Figure 3. Joint prediction of multiple scores captures better individual traits from brain images

### 7.2. Population-shrinkage of covariance to estimate better brain functional connectivity

Brain functional connectivity, obtained from functional Magnetic Resonance Imaging at rest (r-fMRI), reflects inter-subject variations in behavior and characterizes neuropathologies. It is captured by the covariance matrix between time series of remote brain regions. With noisy and short time series as in r-fMRI, covariance estimation calls for penalization, and shrinkage approaches are popular. Here we introduce a new covariance

estimator based on a non-isotropic shrinkage that integrates prior knowledge of the covariance distribution over a large population. The estimator performs shrinkage tailored to the Riemannian geometry of symmetric positive definite matrices, coupled with a probabilistic modeling of the subject and population covariance distributions. Experiments on a large-scale dataset show that such estimators resolve better intra-and inter-subject functional connectivities compared existing co-variance estimates. We also demonstrate that the estimator improves the relationship across subjects between their functional-connectivity measures and their behavioral assessments. More information can be found in Fig. 4 in [47].

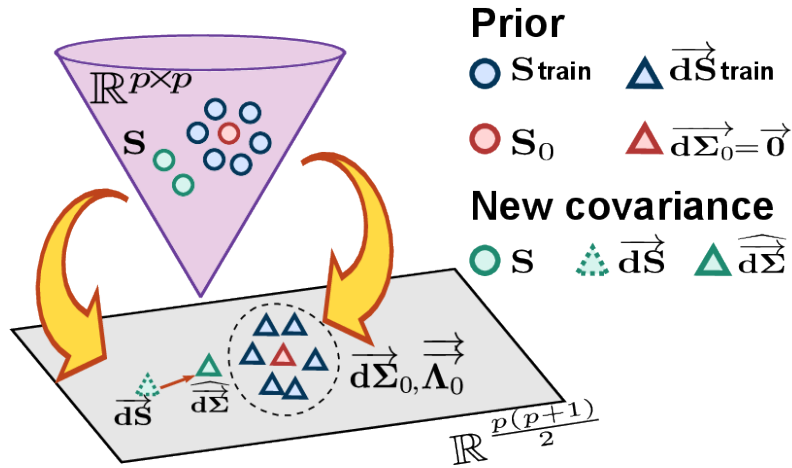


Figure 4. (a) Shrunk embedding estimation workflow: the empirical covariance is estimated from r-fMRI time-series; it is projected onto a tangent space built from a prior population; the embedding is then shrunk towards the prior  $(\vec{d\Sigma}_0, \vec{\Lambda}_0)$ . (b) Principle of tangent embedding shrinkage towards population distribution.

### 7.3. Fast Regularized Ensembles of Models

Brain decoding relates behavior to brain activity through predictive models. These are also used to identify brain regions involved in the cognitive operations related to the observed behavior. Training such multivariate models is a high-dimensional statistical problem that calls for suitable priors. State of the art priors –eg small total-variation– enforce spatial structure on the maps to stabilize them and improve prediction. However, they come with a hefty computational cost. We build upon very fast dimension reduction with spatial structure and model ensembling to achieve decoders that are fast on large datasets and increase the stability of the predictions and the maps. Our approach, fast regularized ensemble of models (FReM), includes an implicit spatial regularization by using a voxel grouping with a fast clustering algorithm. In addition, it aggregates different estimators obtained across splits of a cross-validation loop, each time keeping the best possible model. Experiments on a large number of brain imaging datasets show that our combination of voxel clustering and model ensembling improves decoding maps stability and reduces the variance of prediction accuracy. Importantly, our method requires less samples than state-of-the-art methods to achieve a given level of prediction accuracy. Finally, FReM is highly parallelizable, and has lower computation cost than other spatially-regularized methods.

More information can be found in Fig. 5 in [23].

### 7.4. time decoding



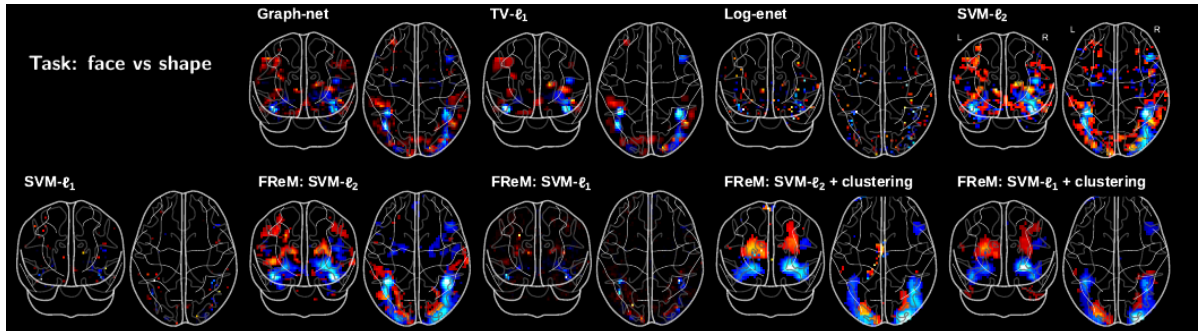


Figure 5. Qualitative comparison of decoder weight maps: Weight maps for different discriminative tasks on the HCP dataset. The maps are thresholded at the 99 percentile for visualization purposes. These correspond to a face-recognition task. The weight maps obtained with TV-L1 and FReM methods with clustering outline the organization of the functional areas of the visual mosaic, such as: primary visual areas, lateral occipital complex, the face and place specific regions in the fusiform gyrus.

Most current functional Magnetic Resonance Imaging (fMRI) decoding analyses rely on statistical summaries of the data resulting from a deconvolution approach: each stimulation event is associated with a brain response. This standard approach leads to simple learning procedures, yet it is ill-suited for decoding events with short inter-stimulus intervals. In order to overcome this issue, we propose a novel framework that separates the spatial and temporal components of the prediction by decoding the fMRI time-series continuously, i.e. scan-by-scan. The stimulation events can then be identified through a deconvolution of the reconstructed time series. We show that this model performs as well as or better than standard approaches across several datasets, most notably in regimes with small inter-stimuli intervals (3 to 5s), while also offering predictions that are highly interpretable in the time domain. This opens the way toward analyzing datasets not normally thought of as suitable for decoding and makes it possible to run decoding on studies with reduced scan time.

More information can be found in Fig. 6 in [28].

## 7.5. Hierarchical Region-Network Sparsity for High-Dimensional Inference in Brain Imaging

Structured sparsity penalization has recently improved statistical models applied to high-dimensional data in various domains. As an extension to medical imaging, the present work incorporates priors on network hierarchies of brain regions into logistic-regression to distinguish neural activity effects. These priors bridge two separately studied levels of brain architecture: functional segregation into regions and functional integration by networks. Hierarchical region-network priors are shown to better classify and recover 18 psychological tasks than other sparse estimators. Varying the relative importance of region and network structure within the hierarchical tree penalty captured complementary aspects of the neural activity patterns. Local and global priors of neurobiological knowledge are thus demonstrated to offer advantages in generalization performance, sample complexity, and domain interpretability.

More information can be found in Fig. 7 in [48].

## 7.6. Cross-validation failure: small sample sizes lead to large error bars

Predictive models ground many state-of-the-art developments in statistical brain image analysis: decoding, MVPA, searchlight, or extraction of biomarkers. The principled approach to establish their validity and

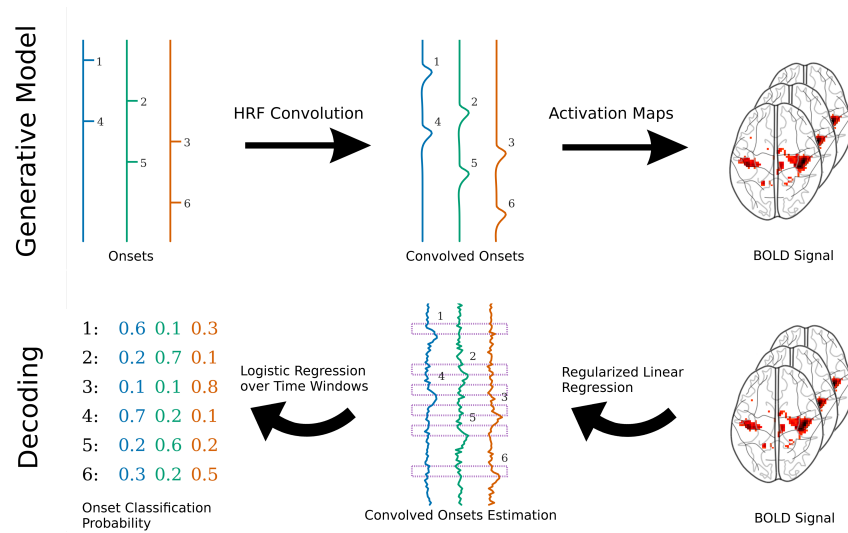


Figure 6. Schema of the time-domain decoding model. Straight arrows represent generative steps, while curved ones represent estimation steps.

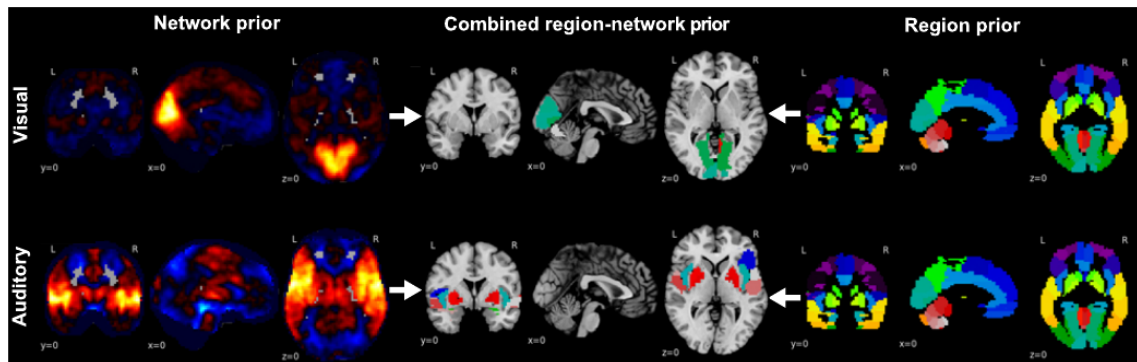


Figure 7. Building blocks of the hierarchical region-network tree. Displays the a-priori neurobiological knowledge introduced into the classification problem by hierarchical structured sparsity. Left: Continuous, partially overlapping brain network priors (hot-colored) accommodate the functional integration perspective of brain organization. Right: Discrete, non-overlapping brain region priors (single-colored) accommodate the functional segregation perspective. Middle: These two types of predefined voxel groups are incorporated into a joint hierarchical prior of parent networks with their descending region child nodes. Top to bottom: Two exemplary region-network priors are shown, including the early cortices that process visual and sound information from the environment.



usefulness is cross-validation, testing prediction on unseen data. Here, we raise awareness on error bars of cross-validation, which are often underestimated. Simple experiments show that sample sizes of many neuroimaging studies inherently lead to large error bars, eg  $\pm 10\%$  for 100 samples. The standard error across folds strongly underestimates them. These large error bars compromise the reliability of conclusions drawn with predictive models, such as biomarkers or methods developments where, unlike with cognitive neuroimaging MVPA approaches, more samples cannot be acquired by repeating the experiment across many subjects. Solutions to increase sample size must be investigated, tackling possible increases in heterogeneity of the data.

More information can be found in Fig. 8 in [33].

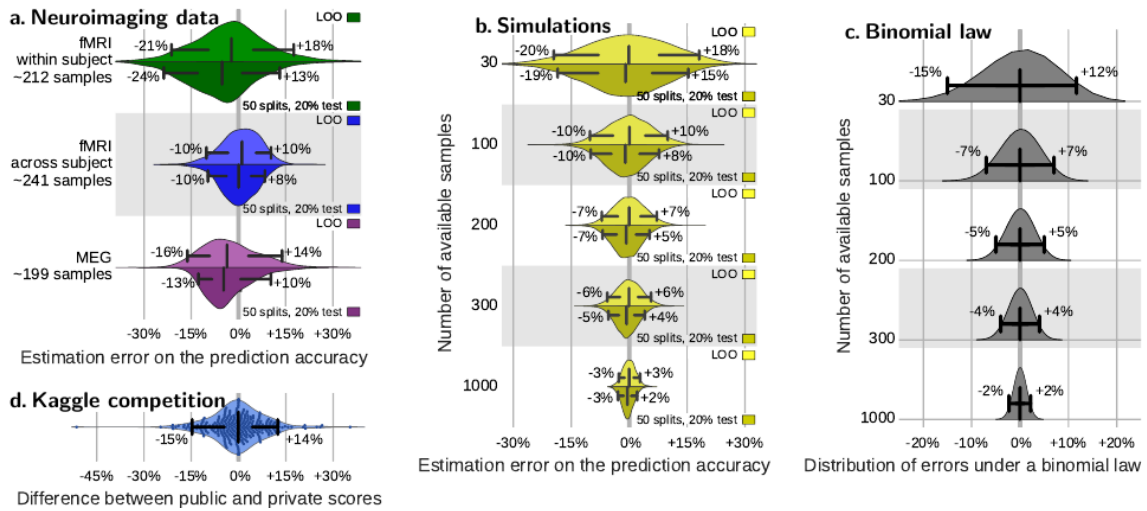


Figure 8. Cross-validation errors. *a* – Distribution of errors between the prediction accuracy as assessed via cross-validation (average across folds) and as measured on a large independent test set for different types of neuroimaging data. *b* – Distribution of errors between the prediction accuracy as assessed via cross-validation on data of various sample sizes and as measured on 10 000 new data points for simple simulations. *c* – Distribution of errors as given by a binomial law: difference between the observed prediction error and the population value of the error;  $p = 75\%$ , for different sample sizes. *d* – Discrepancies between private and public score. Each dot represents the difference between the accuracy of a method on the public test data and the private one. The scores are retrieved from <http://www.kaggle.com/c/mlsp-2014-mri>, in which 144 subjects were used total, 86 for training predictive model, 30 for the public test set, and 28 for the private test set. The bar and whiskers indicate the median and the 5th and 95th percentile. Measures on cross-validation (*a* and *b*) are reported for two reasonable choices of cross-validation strategy: leave one out (leave one run out or leave one subject out in data with multiple runs or subjects), or 50-times repeated splitting of 20% of the data.

## 7.7. Autoreject: Automated artifact rejection for MEG and EEG data

We present an automated algorithm for unified rejection and repair of bad trials in magnetoencephalography (MEG) and electroencephalography (EEG) signals. Our method capitalizes on cross-validation in conjunction with a robust evaluation metric to estimate the optimal peak-to-peak threshold – a quantity commonly used for identifying bad trials in M/EEG. This approach is then extended to a more sophisticated algorithm which estimates this threshold for each sensor yielding trial-wise bad sensors. Depending on the number of bad sensors, the trial is then repaired by interpolation or by excluding it from subsequent analysis. All

steps of the algorithm are fully automated thus lending itself to the name Autoreject. In order to assess the practical significance of the algorithm, we conducted extensive validation and comparisons with state-of-the-art methods on four public datasets containing MEG and EEG recordings from more than 200 subjects. The comparisons include purely qualitative efforts as well as quantitatively benchmarking against human supervised and semi-automated preprocessing pipelines. The algorithm allowed us to automate the preprocessing of MEG data from the Human Connectome Project (HCP) going up to the computation of the evoked responses. The automated nature of our method minimizes the burden of human inspection, hence supporting scalability and reliability demanded by data analysis in modern neuroscience.

More information can be found in Fig. 9 and in [24].

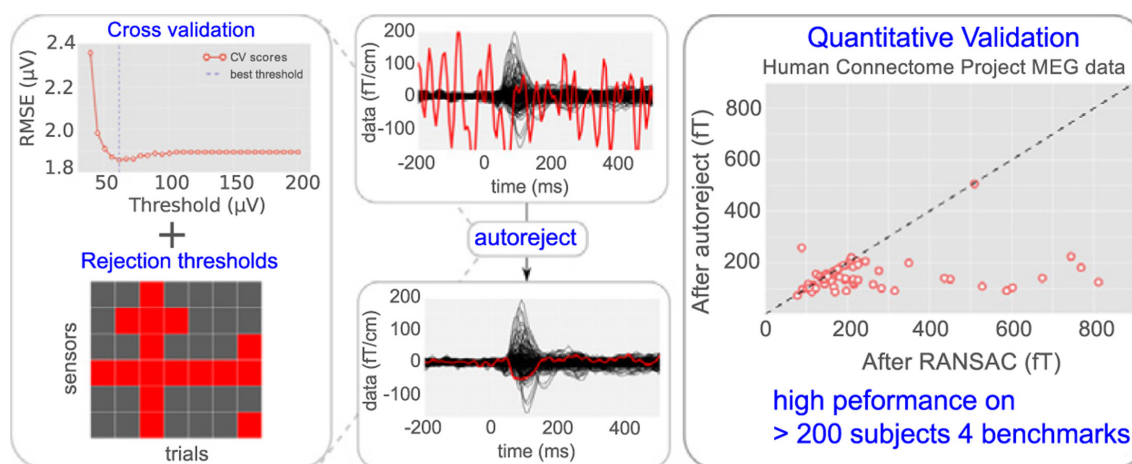


Figure 9. Autoreject: Automated artifact rejection for MEG and EEG data.

## 7.8. Learning Neural Representations of Human Cognition across Many fMRI Studies

Cognitive neuroscience is enjoying rapid increase in extensive public brain-imaging datasets. It opens the door to large-scale statistical models. Finding a unified perspective for all available data calls for scalable and automated solutions to an old challenge: how to aggregate heterogeneous information on brain function into a universal cognitive system that relates mental operations/cognitive processes/psychological tasks to brain networks? We cast this challenge in a machine-learning approach to predict conditions from statistical brain maps across different studies. For this, we leverage multi-task learning and multi-scale dimension reduction to learn low-dimensional representations of brain images that carry cognitive information and can be robustly associated with psychological stimuli. Our multi-dataset classification model achieves the best prediction performance on several large reference datasets, compared to models without cognitive-aware low-dimension representations; it brings a substantial performance boost to the analysis of small datasets, and can be introspected to identify universal template cognitive concepts.

More information can be found in Fig. 10 in [45].

## 7.9. SPARKLING: Novel Non-Cartesian Sampling Schemes for Accelerated 2D Anatomical Imaging at 7T Using Compressed Sensing

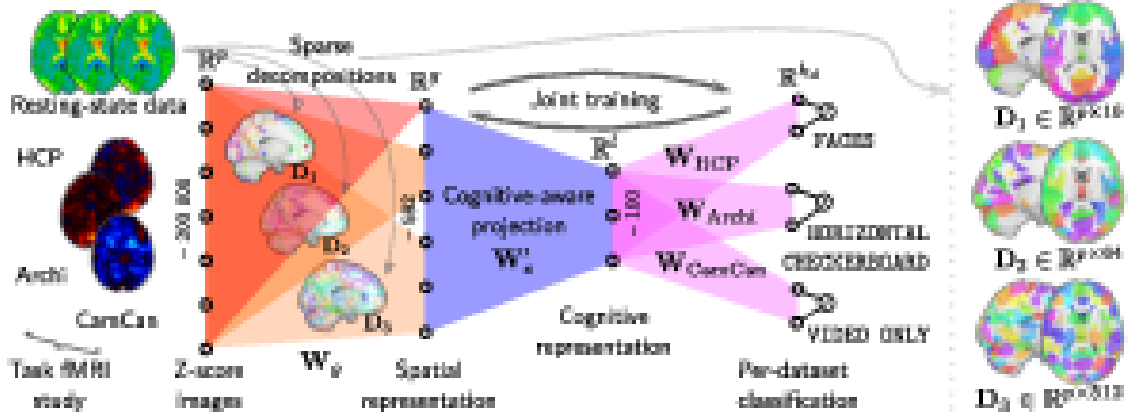


Figure 10. **Model architecture: Three-layer multi-dataset classification.** The first layer (orange) is learned from data acquired outside of cognitive experiments and captures a spatially coherent signal at multiple scales, the second layer (blue) embeds these representations in a space common to all datasets, from which the conditions are predicted (pink) from multinomial models.

We have presented for the first time the implementation of non-Cartesian trajectories on a 7T scanner for 2D anatomical imaging. The proposed SPARKLING curves (Segmented Projection Algorithm for Random K-space samPLING) are a new type of non-Cartesian segmented sampling trajectories which allow fast and efficient coverage of the k-space according to a chosen variable density. To demonstrate their potential, a high-resolution ( $0.4 \times 0.4 \times 3.0\text{mm}$ ) T2\*-weighted image was acquired with an 8-fold undersampled SPARKLING trajectory. Images were reconstructed using non-linear iterative reconstructions derived from the Compressed Sensing theory.

More information can be found in Fig. 11 in [43], [42].

## 7.10. A Projection Method on Measures Sets

We consider the problem of projecting a probability measure  $\pi$  on a set  $\mathcal{M}_N$  of Radon measures. The projection is defined as a solution of the following variational problem:

$$\inf_{\mu \in \mathcal{M}_N} \|h * (\mu - \pi)\|_2^2,$$

where  $h \in L^2(\Omega)$  is a kernel,  $\Omega \subset \mathbb{R}^d$  and denotes the convolution operator. To motivate and illustrate our study, we show that this problem arises naturally in various practical image rendering problems such as stippling (representing an image with  $N$  dots) or continuous line drawing (representing an image with a continuous line). We provide a necessary and sufficient condition on the sequence  $(\mathcal{M}_N)_{N \in \mathbb{N}}$  that ensures weak convergence of the projections  $(\mu_N^*)_{N \in \mathbb{N}}$  to  $\pi$ . We then provide a numerical algorithm to solve a discretized version of the problem and show several illustrations related to computer-assisted synthesis of artistic paintings/drawings.

More information can be found in [19].

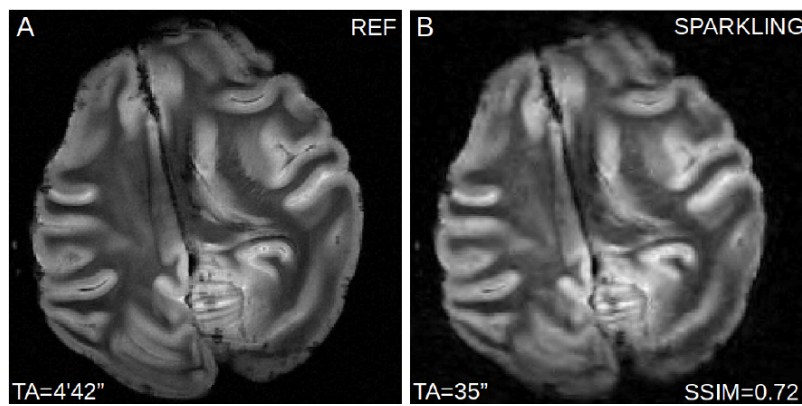


Figure 11. T2\*-weighted Gradient-Echo transversal slice of the ex vivo baboon brain is displayed for A) the full Cartesian reference sampling lasting 4 minutes and 42 seconds and B) the presented 8-fold undersampled SPARKLING trajectories lasting only 35 seconds. A good visual quality of the subsampled reconstruction was observed with the preservation of major folded patterns. The structural similarity score between the SPARKLING reconstructions and the reference was also very satisfactory.

## XPOP Project-Team

## 7. New Results

### 7.1. Sampling from a log-concave distribution with compact support with proximal Langevin Monte Carlo

A detailed theoretical analysis of the Langevin Monte Carlo sampling algorithm was conducted when applied to log-concave probability distributions that are restricted to a convex body  $K$ . This method relies on a regularisation procedure involving the Moreau-Yosida envelope of the indicator function associated with  $K$ . Explicit convergence bounds in total variation norm and in Wasserstein distance of order 1 are established. In particular, we show that the complexity of this algorithm given a first order oracle is polynomial in the dimension of the state space.

### 7.2. Clustering and Model Selection via Penalized Likelihood for Different-sized Categorical Data Vectors

In this study, we consider unsupervised clustering of categorical vectors that can be of different size using mixture. We use likelihood maximization to estimate the parameters of the underlying mixture model and a penalization technique to select the number of mixture components. Regardless of the true distribution that generated the data, we show that an explicit penalty, known up to a multiplicative constant, leads to a non-asymptotic oracle inequality with the Kullback-Leibler divergence on the two sides of the inequality. This theoretical result is illustrated by a document clustering application. To this aim a novel robust expectation-maximization algorithm is proposed to estimate the mixture parameters that best represent the different topics. Slope heuristics are used to calibrate the penalty and to select a number of clusters.

### 7.3. Low-rank Interaction Contingency Tables

Contingency tables are collected in many scientific and engineering tasks including image processing, single-cell RNA sequencing and ecological studies. Low-rank methods have proved useful to analyze them, by facilitating visualization and interpretation. However, common methods do not take advantage of extra information which is often available, such as row and column covariates. We propose a method to denoise and visualize high-dimensional count data which directly incorporates the covariates at hand. Estimation is done by minimizing a Poisson log-likelihood and enforcing a low-rank structure on the interaction matrix with a nuclear norm penalty. We also derive theoretical upper and lower bounds on the Frobenius estimation risk. A complete methodology is proposed, including an algorithm based on the alternating direction method of multipliers, and automatic selection of the regularization parameter. The simulation study reveals that our estimator compares favorably to competitors. Then, analyzing environmental science data, we show the interpretability of the model using a biplot visualization. The method is available as an R package.

### 7.4. Online EM for functional data

A novel approach to perform unsupervised sequential learning for functional data is proposed. The goal is to extract reference shapes (referred to as templates) from noisy, deformed and censored realizations of curves and images. The proposed model generalizes the Bayesian dense deformable template model, a hierarchical model in which the template is the function to be estimated and the deformation is a nuisance, assumed to be random with a known prior distribution. The templates are estimated using a Monte Carlo version of the online Expectation-Maximization (EM) algorithm. The designed sequential inference framework is significantly more computationally efficient than equivalent batch learning algorithms, especially when the missing data is high-dimensional. Some numerical illustrations on curve registration problem and templates extraction from images are provided to support the methodology.

## INFINE Project-Team

## 6. New Results

### 6.1. Online Social Networks (OSN)

#### 6.1.1. Capacity of Information Processing Systems

- Participants: Laurent Massoulié and Kuang Xu

We propose and analyze a family of information processing systems, where a finite set of experts or servers are employed to extract information about a stream of incoming jobs. Each job is associated with a hidden label drawn from some prior distribution. An inspection by an expert produces a noisy outcome that depends both on the job's hidden label and the type of the expert, and occupies the expert for a finite time duration. A decision maker's task is to dynamically assign inspections so that the resulting outcomes can be used to accurately recover the labels of all jobs, while keeping the system stable. Among our chief motivations are applications in crowd-sourcing, diagnostics, and experiment designs, where one wishes to efficiently learn the nature of a large number of items, using a finite pool of computational resources or human agents. We focus on the capacity of such an information processing system. Given a level of accuracy guarantee, we ask how many experts are needed in order to stabilize the system, and through what inspection architecture. Our main result provides an adaptive inspection policy that is asymptotically optimal in the following sense: the ratio between the required number of experts under our policy and the theoretical optimal converges to one, as the probability of error in label recovery tends to zero. This work was firstly accepted and presented at the COLT conference.

### 6.2. Spontaneous Wireless Networks (SWN)

#### 6.2.1. Spatio-Temporal Prediction of Cellular Data Traffic

- Participants: Guangshuo Chen, Aline Carneiro Viana, Marco Fiore, Carlos Sarraute

The understanding of human behaviors is a central question in multi-disciplinary research and has contributed to a wide range of applications. The ability to foresee human activities has essential implications in many aspects of cellular networks. In particular, the high availability of mobility prediction can enable various application scenarios such as location-based recommendation, home automation, and location-related data dissemination; the better understanding of future mobile data traffic demand can help to improve the design of solutions for network load balancing, aiming at improving the quality of Internet-based mobile services. Although a large and growing body of literature has investigated the topic of predicting human mobility, there has been little discussion in anticipating mobile data traffic in cellular networks, especially in spatiotemporal view of individuals. We address the problem of understanding spatiotemporal mobile data traffic demand for individuals and perform an theoretical and empirical analysis of jointly predicting human whereabouts and mobile data traffic, by collaboratively mining human mobility dataset and mobile data traffic dataset. Our contributions are summarized as follows:

- We investigate the limits of predictability by measuring the maximum predictability that any algorithm has potential to achieve based on tools of information theory. Our theoretical analysis shows that it is theoretically possible to anticipate the individual demand with a typical accuracy of 75% despite the heterogeneity of users and with an improved accuracy of 80% using joint prediction with mobility information. This work was published at the IEEE LCN 2017 international conference and the Technical report RT-0483 brings a full description of the work, which is being prepared for a journal submission.

- We evaluate the state-of-the-art predictors and propose novel solutions for predicting mobile data traffic via machine learning algorithms. Our data-driven test on the performance of these predictors show that the 2nd order Markov predictor outperforms all the legacy time series predictors. It can achieve a mean accuracy of 62% but can hardly have an enhancement from knowing human mobility information. Besides, based on machine learning techniques, our proposed solutions can achieve a typical accuracy of 70% and have a 1% 5% degree of improvement by learning individual whereabouts (what confirms the predictability theoretical results). Finally, our analysis show that knowing mobile data traffic of a user can significantly help the prediction of his whereabouts for 50% of the users, leading to an improvement up to 10% regarding accuracy. The Technical Report hal-01675573 brings more details on this work. A conference paper is also in preparation.

All those works were performed in the context of the Guangshuo Chen's PhD thesis, who will defend in March 2018.

### 6.2.2. *Human Mobility completion of Sparse Call Detail Records for Mobility Analysis*

- Participants: Guangshuo Chen, Aline Carneiro Viana, Marco Fiore, Sahar Hoteit

Call Detail Records (CDR) are an important source of information in the study of diverse aspects of human mobility. The accuracy of mobility information granted by CDR strongly depends on the radio access infrastructure deployment and the frequency of interactions between mobile users and the network. As cellular network deployment is highly irregular and interaction frequencies are typically low, CDR are often characterized by spatial and temporal sparsity, which, in turn, can bias mobility analyses based on such data. In this paper, we precisely address this subject. First, we evaluate the spatial error in CDR, caused by approximating user positions with cell tower locations. Second, we assess the impact of the limited spatial and temporal granularity of CDR on the estimation of standard mobility metrics. Third, we propose novel and effective techniques to reduce temporal sparsity in CDR, by leveraging regularity in human movement patterns.

These works have been published as invited papers at the ACM CHANTS 2016 workshop (in conjunction with ACM MobiCom 2016) and at the IEEE DAWM workshop (in conjunction with IEEE Percom 2017). A journal version (also registered as TR: hal-01646608) is in revision at the Computer Communication Elsevier Journal, and got the first notification asking for minor revisions. Finally, a new completion methodology improving the previously described that leverages tensor factorization was designed and will be submitted to a journal: the technical report hal-01675570 describes this work.

### 6.2.3. *Sampling frequency of human mobility*

- Participants: Panagiota Katsikouli, Aline Carneiro Viana, Marco Fiore, Alberto Tarable

Recent studies have leveraged tracking techniques based on positioning technologies to discover new knowledge about human mobility. These investigations have revealed, among others, a high spatiotemporal regularity of individual movement patterns. Building on these findings, we aim at answering the question “*at what frequency should one sample individual human movements so that they can be reconstructed from the collected samples with minimum loss of information?*”. Our quest for a response leads to the discovery of (i) seemingly universal spectral properties of human mobility, and (ii) a linear scaling law of the localization error with respect to the sampling interval. Our findings are based on the analysis of fine-grained GPS trajectories of 119 users worldwide. The applications of our findings are related to a number of fields relevant to ubiquitous computing, such as energy-efficient mobile computing, location-based service operations, active probing of subscribers' positions in mobile networks and trajectory data compression. to an international conference in the next months. This work was published at the IEEE Globecom 2017 international conference.

We are improving the currently published sampling approach by incorporating human behavioral features at the sampling decisions to make it more adaptive. This is an on-going work with Panagiota Katsikouli, who spent 5 months in our team working as an internship and is currently doing a Post-Doc at the AGORA Inria team.



#### 6.2.4. *Inference of human personality from mobile phones datasets*

- Participants: Adriano di Luzio, Aline Carneiro Viana, Julinda Stefa, Katia Jaffres

Personality research has enjoyed a strong resurgence over the past decade. Trait-based personality theories define personality as the traits that predict a person's behavior through learning and habits. Personality traits are relatively stable over time, differ across individuals, and most importantly, influence behavior. In psychology, the human personality has been modeled into a set of independent factors that, together, accurately describe any individual: The Five Factors Personality Model. This personality model presents the Big Five personality traits, often represented by the OCEAN acronym: Openness: appreciation for a variety of experiences; Conscientiousness: planning ahead rather than being spontaneous; Extraversion: being sociable, energetic and talkative; Agreeableness: being kind, sympathetic and happy to help; Neuroticism: inclined to worry or be vulnerable or temperamental.

This is a very recently started work, where we are firstly analysing the relationship between smartphone usages (i.e., social interactions, content interest, mobility, and communication) and personality traits in the Big Five Model. Most of the studies on personality traits were performed by social scientists and in particular, by psychologists. Studies reveal that one of the most distal influences shaping personality lie in the environment where development occurs. Nevertheless, the identification of precise environmental sources impacting personality is still an open research. More recently, computer science researchers have tried to extract personality from datasets collected through smartphones. Although laying the ground work to understand human personality from smartphones usage, much still remain to be investigated. Thus, we are performing analysis to study the correlation between traits and technological features. We plan then to establish a methodology to infer traits from features and consequently, to investigate how different traits influence different features.

This is an on-going work with Adriano di Luzio, who spent 4 months in our team working as an internship, and Julinda Stefa, an invited research visitor at Infine.

#### 6.2.5. *Predicting new places to visit in human mobility decision*

- Participants: Maria Astefanoaei, Aline Carneiro Viana, Rik Sarkar

Most location prediction methods need a large user mobility history to accurately predict the next location of a user (markov chains, rnn). These methods are particularly good for predicting locations that are frequently visited by users, but not as good for predicting new places or how a user's trajectories change in case of random events. We amend this by using contextual information to manage new places and random events and the movement patterns of users who exhibit similar behaviours. In this context, we plan to use the user's profile and social ties to identify the most probable next category of locations (type of actions: entertainment, social, food etc.). Then, use subtrajectory similarity to predict the route taken to the identified area. This is an on-going work with the intern Maria Astefanoaei and her advisor, who spent 5 months in our team.

#### 6.2.6. *Data offloading decision via mobile crowdsensing*

- Participants: Emanuel Lima, Aline Carneiro Viana, Ana Aguiar

With the steady growth of smart-phones sales [1], the demand for services that generate mobile data traffic has grown tremendously. WiFi offloading has been considered as a promising solution to the recent boost up of mobile data consumption that is making excessive demands on cellular networks in metropolitan areas. The idea consists in shifting the traffic off of cellular networks to WiFi networks. Characterizing the capacity and availability of a chaotic deployed dense WiFi network is crucial to understand and decide where and when to offload data. This is the first goal of this work, where the MACACO dataset was considered in the characterization. Our final goal is the design of a decision strategy allowing a mobile phone of a user to decide if offload or not her traffic, i.e., when, where (using what Access Point in her usual mobility) and how (if the traffic will be offloaded to one or more Access Points). This is an on-going work with the intern emanuel Lima and his advisor, who spent 4 months in our team.



### 6.2.7. *Inferring friends in the crowd in Device-to-Device communication*

- Participants: Rafael Costa, Aline Carneiro Viana, Leobino Sampaio, Artur Ziviani

The next generation of mobile phone networks (5G) will have to deal with spectrum bottleneck and other major challenges to serve more users with high-demanding requirements. Among those are higher scalability and data rates, lower latencies and energy consumption plus reliable ubiquitous connectivity. Thus, there is a need for a better spectrum reuse and data offloading in cellular networks while meeting user expectations. According to literature, one of the 10 key enabling technologies for 5G is device-to-device (D2D) communications, an approach based on direct user involvement. Nowadays, mobile devices are attached to human daily life activities, and therefore communication architectures using context and human behavior information are promising for the future. User-centric communication arose as an alternative to increase capillarity and to offload data traffic in cellular networks through opportunistic connections among users. Although having the user as main concern, solutions in the user-centric communication/networking area still do not see the user as an individual, but as a network active element. Hence, these solutions tend to only consider user features that can be measured from the network point of view, ignoring the ones that are intrinsic from human activity (e.g., daily routines, personality traits, etc). In this work, we plan to investigate how human-aspects and behavior can be useful to leverage future device-to-device communication. This is a recently started PhD thesis subject, aiming the design of a methodology to select next-hops in a D2D communication that will be human-aware: i.e., that will consider not only available physical resources at the mobile device of a wireless neighbor, her mobility features and restrictions but also any information allowing to infer how much sharing willing she is.

## 6.3. Internet of Things (IoT) and Information Centric Networking (ICN)

### 6.3.1. *Low-power Internet of Things with NDN and Cooperative Caching*

- Participants: Oliver Hahm, Emmanuel Baccelli, Thomas C. Schmidt, Matthias Wählisch, Cédric Adjih, and Laurent Massoulié

Energy efficiency is a major driving factor in the Internet of Things (IoT). In this context, an IoT approach based on Information-Centric Networking (ICN) offers prospects for low energy consumption. Indeed, ICN can provide local in-network content caching so that relevant IoT content remains available at any time while devices are in deep-sleep mode most of the time. In our paper on the subject, we evaluated NDN enhanced with CoCa, a simple side protocol we designed to exploit content names together with smart interplay between cooperative caching and power-save sleep capabilities on IoT devices. We performed extensive, large scale experiments on real hardware with IoT networks comprising of up to 240 nodes, and on an emulator with up to 1000 nodes. We have shown in practice that, with NDN+CoCa, devices can reduce energy consumption by an order of magnitude while maintaining recent IoT content availability above 90 %. We furthermore provided auto-configuration mechanisms enabling practical ICN deployments on IoT networks of arbitrary size with NDN+CoCa. With such mechanisms, each device could autonomously configure names and auto-tune parameters to reduce energy consumption as demonstrated in our paper.

### 6.3.2. *Information Centric Networking for the IoT Robotics*

- Participants: Loic Dauphin, Emmanuel Baccelli, Cédric Adjih

In the near-future, humans will interact with swarms of low-cost, interconnected robots. Such robots will hence integrate the Internet of Things, and coin the term IoT robotics. Using ROS (Robot Operating System) is currently the dominant approach to implement distributed robotic software modules communicating with one another. ROS nodes can publish or subscribe to topics, which are named and typed data streams sent over the network. In our work on the subject, we presented preliminary work exploring the potential of using NDN as network primitive for ROS2 nodes (the newest version of ROS).

### 6.3.3. *Data Synchronization through Information Centric Networking*

- Participants: Ayat Zaki Hindi, Cédric Adjih, Michel Kieffer, Claudio Weidmann

The use of Named Data Networking (NDN) for distributed multiuser applications, e.g. group messaging and file sharing, requires NDN synchronization protocols to maintain the same shared dataset (and its updates) among all nodes. ChronoSync, RoundSync, and PartialSync are some proposals to address this issue.

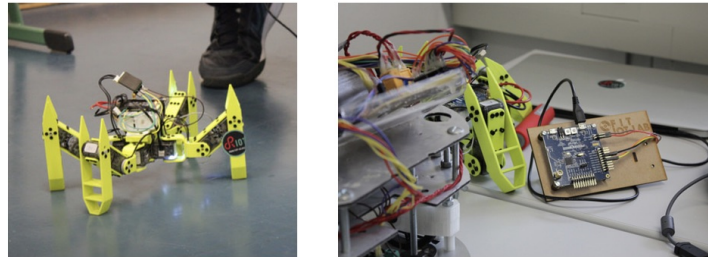


Figure 1. Demonstration of the use of NDN in IoT Robotics

In our work on the subject, we focused on the state-of-the-art protocol RoundSync: we study its core features, that permit participating nodes to detect, propagate, and reconcile all changes. Particular attention is given to the case of multiple changes per round. We then proposed an improved variant, iRoundSync, that exchanges fewer messages in the multiple-change case and is more resilient to packet losses. We have quantified the performance gain of iRoundSync on a simple topology.

## 6.4. Internet of Things (IoT) and 5G

### 6.4.1. Efficient Random Access for 5G Systems: Coded Slotted Aloha

- Participants: Ehsan Ebrahimi Khaleghi, Cédric Adjih, Amira Alloum, Paul Mützlethaler, Vinod Kumar

Motivated by scenario requirements for 5G cellular networks, we have studied one of the candidate protocols for massive random access: the family of random access methods known as Coded Slotted ALOHA (CSA). A recent trend in research has explored aspects of such methods in various contexts, but one aspect has not been fully taken into account: the impact of pathloss, which is a major design constraint in long-range wireless networks. In one article, we explored the behavior of CSA, by focusing on the path loss component correlated to the distance to the base station. Path loss provides opportunities for capture, improving the performance of CSA. We revised methods for estimating CSA behavior, provide bounds of performance, and then, focusing on the achievable throughput, we extensively explored the key parameters, and their associated gain (experimentally). Our results shed light on the behavior of the optimal distribution of repetitions in actual wireless networks.

### 6.4.2. Real Implementation of Coded Slotted Aloha

- Participants: Cédric Adjih, Vinod Kumar

In 2017, we implemented Coded Slotted Aloha (CSA) as a proof of concept on our FIT IoT-LAB testbed (with 20+ nodes), with 802.15.4 transmissions and using a real SDR software.

This was presented in the seminar of the GT task 2 Future Access Networks of Digicosme. It was also presented as part of the tutorial "IoT in practice" in the ANTS 2017 conference.

## 6.5. Resource and Traffic Management

### 6.5.1. Utility Optimization Approach to Network Cache Design

**Participants:** Mostafa Dehghan, Laurent Massoulié, Don Towsley, Daniel Menasche, Y.c. Tay.

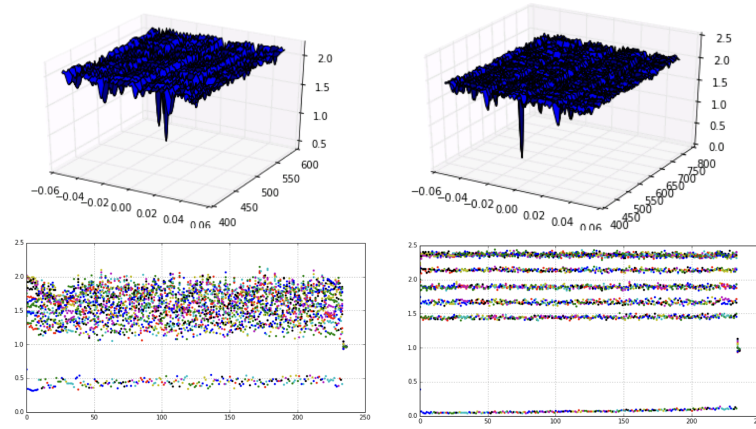


Figure 2. Example of demodulation steps in Coded Slotted Aloha

In any caching system, the admission and eviction policies determine which contents are added and removed from a cache when a miss occurs. Usually, these policies are devised so as to mitigate staleness and increase the hit probability. Nonetheless, the utility of having a high hit probability can vary across contents. This occurs, for instance, when service level agreements must be met, or if certain contents are more difficult to obtain than others. In this paper, we propose utility-driven caching, where we associate with each content a utility, which is a function of the corresponding content hit probability. We formulate optimization problems where the objectives are to maximize the sum of utilities over all contents. These problems differ according to the stringency of the cache capacity constraint. Our framework enables us to reverse engineer classical replacement policies such as LRU and FIFO, by computing the utility functions that they maximize. We also develop online algorithms that can be used by service providers to implement various caching policies based on arbitrary utility functions.

This work was published and presented at the IEEE Infocom 2016 conference as "A Utility Optimization Approach to Network Cache Design".

## AVIZ Project-Team

## 6. New Results

### 6.1. HCI Requirements for Progressive Data Analysis

**Participants:** Jean-Daniel Fekete [correspondant], Sriram Karthik Badam, Niklas Elmqvist.

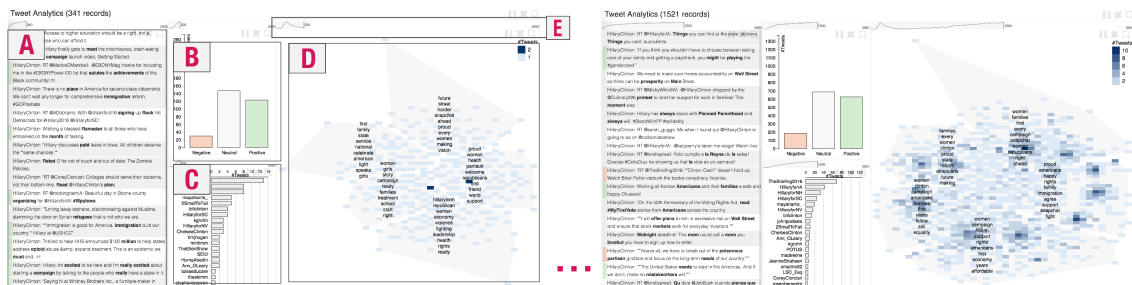


Figure 3. The InsightsFeed tool for progressive visual analytics of Twitter (left): (A) a list of tweets, (B) a sentiment chart, (C) user popularity chart, (D) a map from a 2D projection of tweets with important keywords highlighted in each region, and (E) feedback and controls over the progression and computations. (Right) The interface is progressively updated when more data is processed.

Progressive visual analytics (PVA) has emerged in recent years to manage the latency of data analysis systems. When analysis is performed progressively, rough estimates of the results are generated quickly and are then improved over time. Analysts can therefore monitor the progression of the results, steer the analysis algorithms, and make early decisions if the estimates provide a convincing picture. In this article, we describe interface design guidelines for helping users understand progressively updating results and make early decisions based on progressive estimates. To illustrate our ideas, we present a prototype PVA tool called INSIGHTSFEED for exploring Twitter data at scale. As validation, we investigate the tradeoffs of our tool when exploring a Twitter dataset in a user study. We report the usage patterns in making early decisions using the user interface, guiding computational methods, and exploring different subsets of the dataset, compared to sequential analysis without progression.

More on the project Web page: [ProgressiveDataAnalysis](#).

### 6.2. Embedded Data Representations

**Participants:** Wesley Willett, Yvonne Jansen, Pierre Dragicevic [correspondant].

We introduced *embedded data representations*, the use of visual and physical representations of data that are deeply integrated with the physical spaces, objects, and entities to which the data refers. Technologies like lightweight wireless displays, mixed reality hardware, and autonomous vehicles are making it increasingly easier to display data in-context. While researchers and artists have already begun to create embedded data representations, the benefits, trade-offs, and even the language necessary to describe and compare these approaches remain unexplored. In our paper [17], we formalized the notion of physical data referents – the real-world entities and spaces to which data corresponds – and examined the relationship between referents and the visual and physical representations of their data. We differentiated situated representations, which display data in proximity to data referents, and embedded representations, which display data so that it spatially

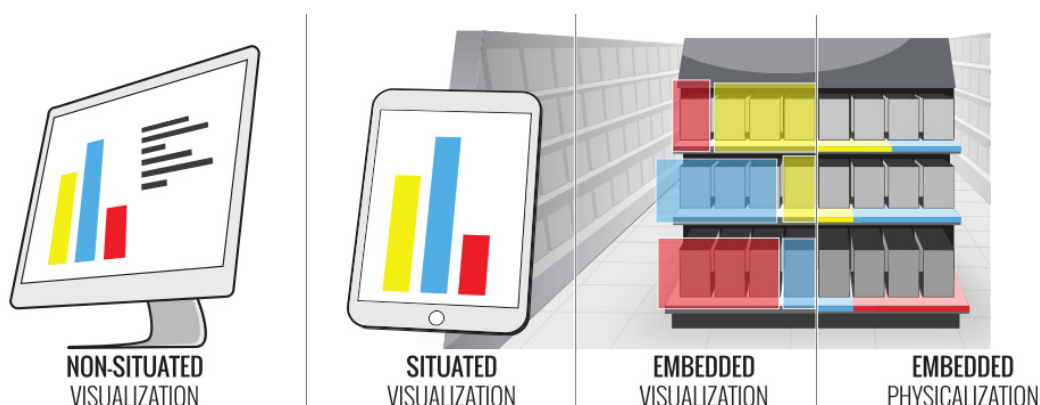


Figure 4. From left to right: A desktop setting with non-situated visualization. A situated visualization of the same data on a tablet in the store itself. An embedded visualization overlays the data on top of individual products as a heat map. An embedded physicalization displays data by changing properties of the shelves themselves.

coincides with data referents. Drawing on examples from visualization, ubiquitous computing, and art, we explored the role of spatial indirection, scale, and interaction for embedded representations. We also examined the tradeoffs between non-situated, situated, and embedded data displays, including both visualizations and physicalizations. Based on our observations, we identified a variety of design challenges for embedded data representation, and suggested opportunities for future research and applications.

More on the project Web page: [yvonnejansen.me/embedded](http://yvonnejansen.me/embedded).

### 6.3. Blinded with Science or Informed by Charts? A Replication Study

**Participants:** Pierre Dragicevic [correspondant], Yvonne Jansen.

We provided a reappraisal of Tal and Wansink's study "Blinded with Science", where seemingly trivial charts were shown to increase belief in drug efficacy, presumably because charts are associated with science. Through a series of four replications conducted on two crowdsourcing platforms, we investigated an alternative explanation, namely, that the charts allowed participants to better assess the drug's efficacy. Considered together, our experiments suggested that the chart seems to have indeed promoted understanding, although the effect is likely very small. Meanwhile, we were unable to replicate the original study's findings, as text with chart appeared to be no more persuasive – and sometimes less persuasive – than text alone. This suggested that the effect may not be as robust as claimed and may need specific conditions to be reproduced. Regardless, within our experimental settings and considering our study as a whole ( $N = 623$ ), the chart's contribution to understanding was clearly larger than its contribution to persuasion.

The main lesson from our study is that with charts, the peripheral route of persuasion cannot be studied independently from the central route: in order to establish that a chart biases judgment, it is necessary to also rigorously establish that it does not aid comprehension. Our replication also opens many relevant questions for infovis. Are charts really associated with science? More generally, what associations do charts or visualizations trigger depending on their visual design? When exactly is a chart trivial? Two arguments against minimalistic charts is that they take up space and they break the flow of the text. How do word-scale visualizations change these trade-offs?

Experimental material can be downloaded here: [www.aviz.fr/blinded](http://www.aviz.fr/blinded).

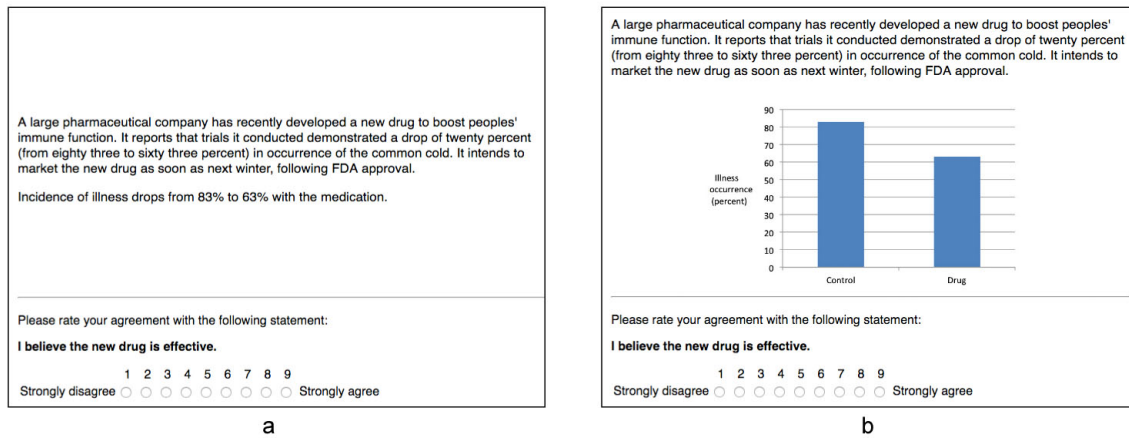


Figure 5. First page of our second experiment, replicating experiment 2 from Tal and Wansink. (a) no-chart condition, with an extra sentence repeating the two quantities with numerals; (b) chart condition: the extra sentence is replaced with a bar chart.

## 6.4. Vispubdata

**Participants:** Petra Isenberg [correspondant], Florian Heimerl, Steffen Koch, Tobias Isenberg, Panpan Xu, Charles Stolper, Michael Sedlmair, Torsten Möller, John Stasko.

We have created and keep maintaining a dataset with information about every paper that has appeared at the IEEE Visualization (VIS) set of conferences: InfoVis, SciVis, VAST, and Vis. The information about each paper includes its title, abstract, authors, and citations to other papers in the conference series, among many other attributes. This data is meant to be useful to the broad data visualization community to help understand the evolution of the field and as an example document collection for text data visualization research.

## 6.5. An Exploratory Study of Word-Scale Graphics in Data-Rich Text Documents

**Participants:** Pascal Goffin, Jeremy Boy, Wesley Willett, Petra Isenberg [correspondant].

We contribute an investigation of the design and function of word-scale graphics and visualizations embedded in text documents. Word-scale graphics include both data-driven representations such as word-scale visualizations and sparklines, and non-data-driven visual marks. Their design, function, and use has so far received little research attention. We conducted an open ended exploratory study with 9 graphic designers. The study resulted in a rich collection of different types of graphics, data provenance, and relationships between text, graphics, and data. Based on this corpus, we derived a systematic overview of word-scale graphic designs, and examine how designers used them. We also discussed the designers' goals in creating their graphics, and characterized how they used word-scale graphics to visualize data, add emphasis, and create alternative narratives. Building on these examples, we discuss implications for the design of authoring tools for word-scale graphics and visualizations, and explore how new authoring environments could make it easier for designers to integrate them into documents.

## 6.6. Hybrid Tactile/Tangible Interaction for 3D Data Exploration

**Participants:** Lonni Besançon [correspondant], Paul Issartel, Mehdi Ammi, Tobias Isenberg.

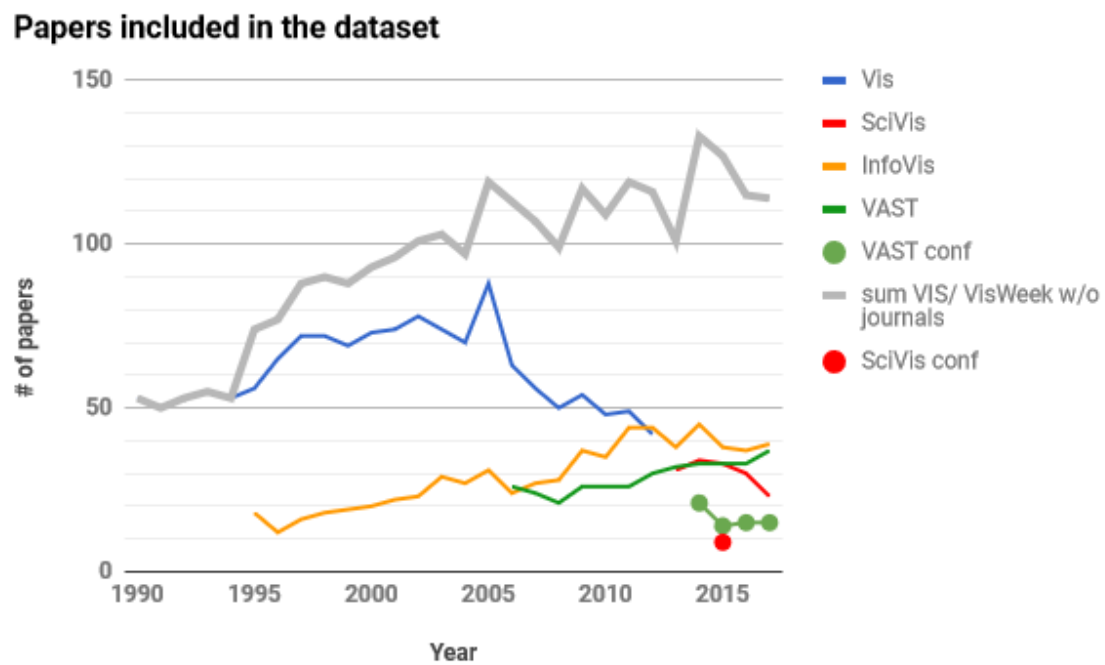


Figure 6. Overview of the files included in the dataset.



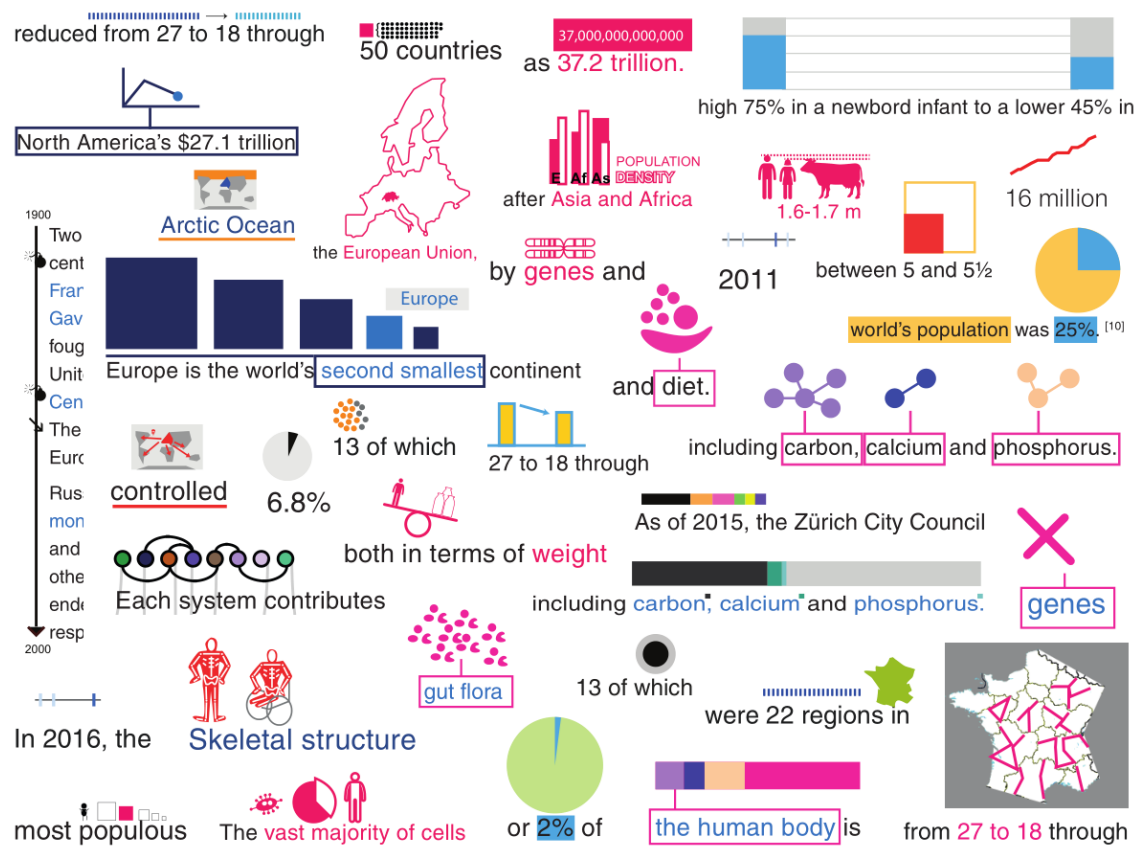


Figure 7. Overview of the word-scale visualizations created in our study.



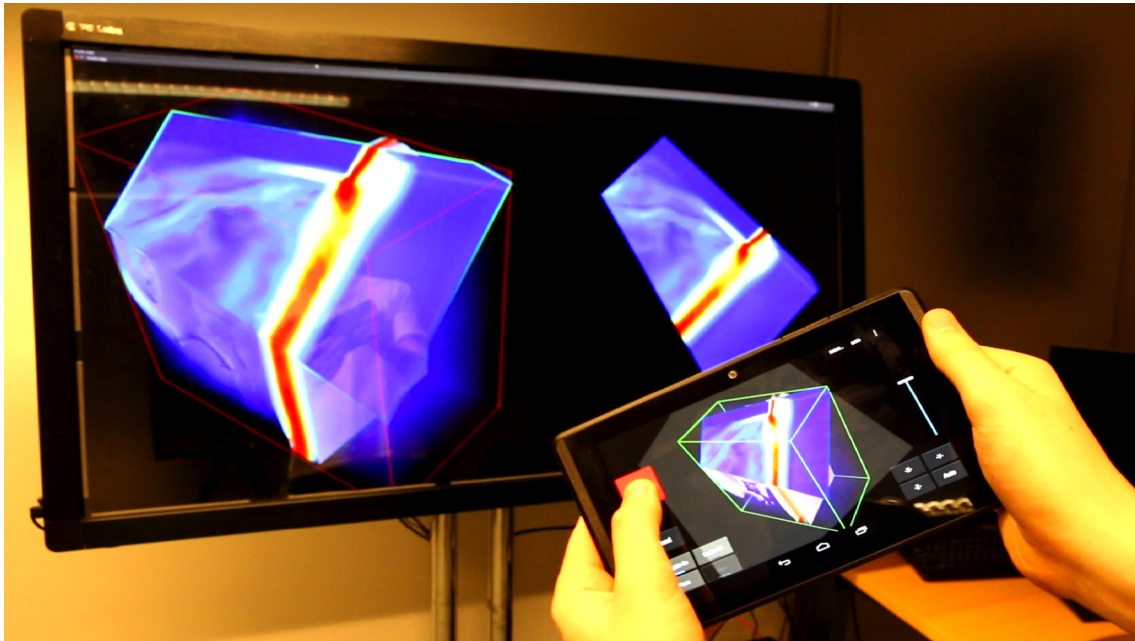


Figure 8. Picture of the hybrid interaction system.

We present the design and evaluation of an interface that combines tactile and tangible paradigms for 3D visualization. While studies have demonstrated that both tactile and tangible input can be efficient for a subset of 3D manipulation tasks, we reflect here on the possibility to combine the two complementary input types. Based on a field study and follow-up interviews, we present a conceptual framework of the use of these different interaction modalities for visualization both separately and combined—focusing on free exploration as well as precise control. We present a prototypical application of a subset of these combined mappings for fluid dynamics data visualization using a portable, position-aware device which offers both tactile input and tangible sensing. We evaluate our approach with domain experts and report on their qualitative feedback.

More on the project Web page: <http://lonni.besancon.pagesperso-orange.fr/Projects/HybridInteraction/HybridInteraction.html>.

## 6.7. Pressure-Based Gain Factor Control for Mobile 3D Interaction using Locally-Coupled Devices

**Participants:** Lonni Besançon [correspondant], Mehdi Ammi, Tobias Isenberg.

We present the design and evaluation of pressure-based interactive control of 3D navigation precision. Specifically, we examine the control of gain factors in tangible 3D interactions using locally-coupled mobile devices. By focusing on pressure as a separate input channel we can adjust gain factors independently from other input modalities used in 3D navigation, in particular for the exploration of 3D visualizations. We present two experiments. First, we determined that people strongly preferred higher pressures to be mapped to higher gain factors. Using this mapping, we compared pressure with rate control, velocity control, and slider-based control in a second study. Our results show that pressure-based gain control allows people to be more precise in the same amount of time compared to established input modalities. Pressure-based control was also clearly preferred by our participants. In summary, we demonstrate that pressure facilitates effective and efficient precision control for mobile 3D navigation.

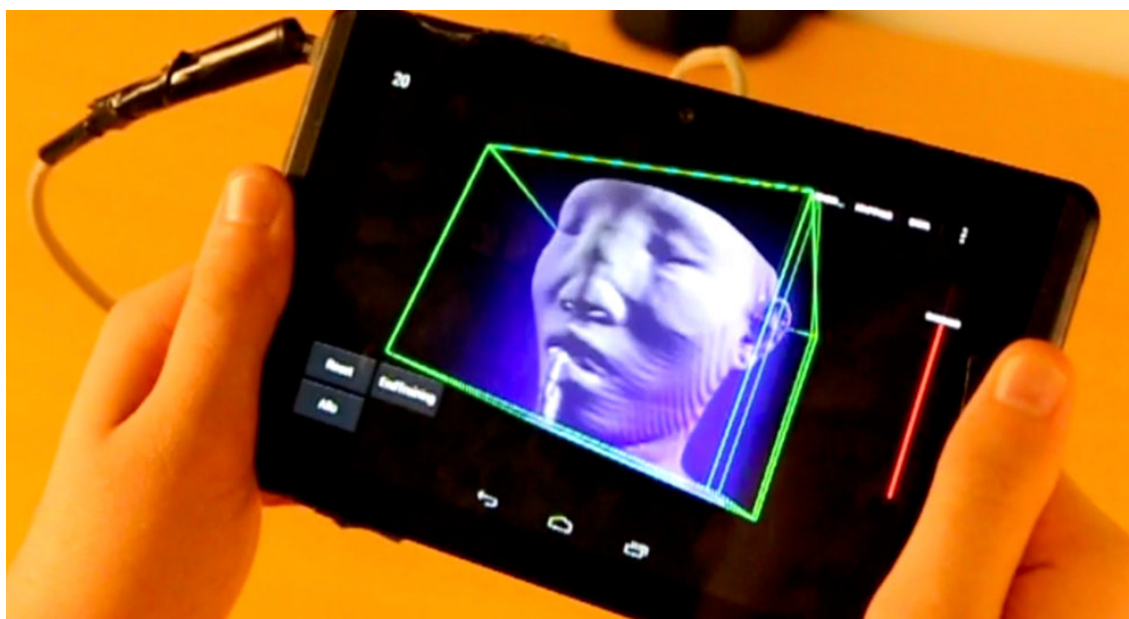


Figure 9. Picture of the pressure-based gain factor control prototype.

More on the project Web page: <http://lonni.besancon.pagesperso-orange.fr/Projects/Pressure/Pressure.html>.

## 6.8. Pressure-Based Gain Factor Control for Mobile 3D Interaction using Locally-Coupled Devices

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## 6.9. The Attraction Effect in Information Visualization

**Participants:** Evanthia Dimara [correspondant], Pierre Dragicevic, Anastasia Bezerianos.

The attraction effect is a well-studied cognitive bias in decision making research, where one's choice between two alternatives is influenced by the presence of an irrelevant (dominated) third alternative. We examine whether this cognitive bias, so far only tested with three alternatives and simple presentation formats such as numerical tables, text and pictures, also appears in visualizations. Since visualizations can be used to support decision making — e.g., when choosing a house to buy or an employee to hire — a systematic bias could have important implications. In a first crowdsourcing experiment, we indeed partially replicated the attraction effect

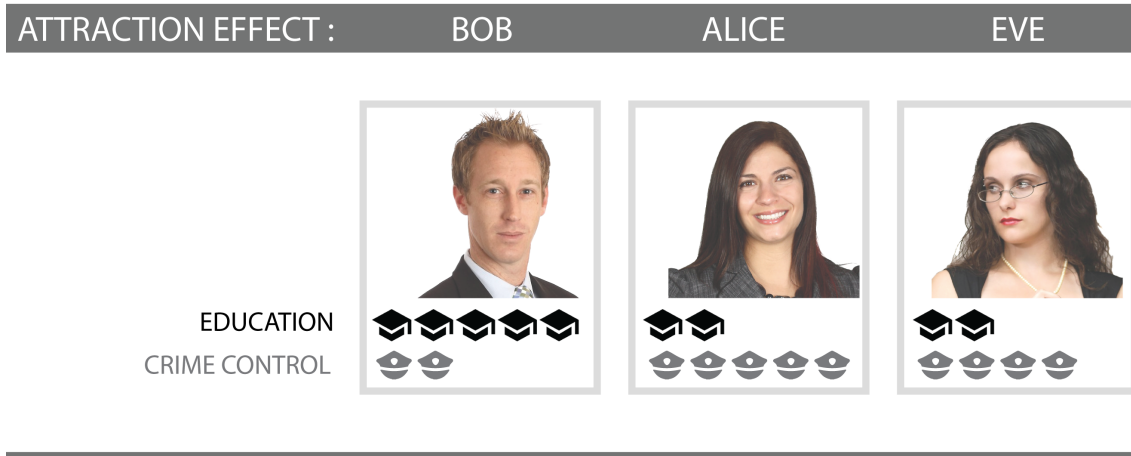


Figure 10. Example of an attraction effect in elections: Bob has an excellent education plan, while Alice is very strong in crime control. The addition of Eve, a candidate similar but slightly inferior to Alice, raises Alice's attractiveness as a candidate. This irrelevant option is called a decoy.

with three alternatives presented as a numerical table, and observed similar effects when they were presented as a scatterplot. In a second experiment, we investigated if the effect extends to larger sets of alternatives, where the number of alternatives is too large for numerical tables to be practical. Our findings indicate that the bias persists for larger sets of alternatives presented as scatterplots. We discuss implications for future research on how to further study and possibly alleviate the attraction effect.

More on the project Web page: <http://www.aviz.fr/decoy>.

## 6.10. Narratives in Crowdsourced Evaluation of Visualizations: A Double-Edged Sword?

**Participants:** Evanthia Dimara [correspondant], Pierre Dragicevic, Anastasia Bezerianos.

We explore the effects of providing task context when evaluating visualization tools using crowdsourcing. We gave crowdworkers i) abstract information visualization tasks without any context, ii) tasks where we added semantics to the dataset, and iii) tasks with two types of backstory narratives: an analytic narrative and a decision-making narrative. Contrary to our expectations, we did not find evidence that adding data semantics increases accuracy, and further found that our backstory narratives can even decrease accuracy. Adding dataset semantics can however increase attention and provide subjective benefits in terms of confidence, perceived easiness, task enjoyability and perceived usefulness of the visualization. Nevertheless, our backstory narratives did not appear to provide additional subjective benefits. These preliminary findings suggest that narratives may have complex and unanticipated effects, calling for more studies in this area.

More on the project Web page: <http://www.aviz.fr/narratives>.

## 6.11. Conceptual and Methodological Issues in Evaluating Multidimensional Visualizations for Decision Support.

**Participants:** Evanthia Dimara [correspondant], Pierre Dragicevic, Anastasia Bezerianos.

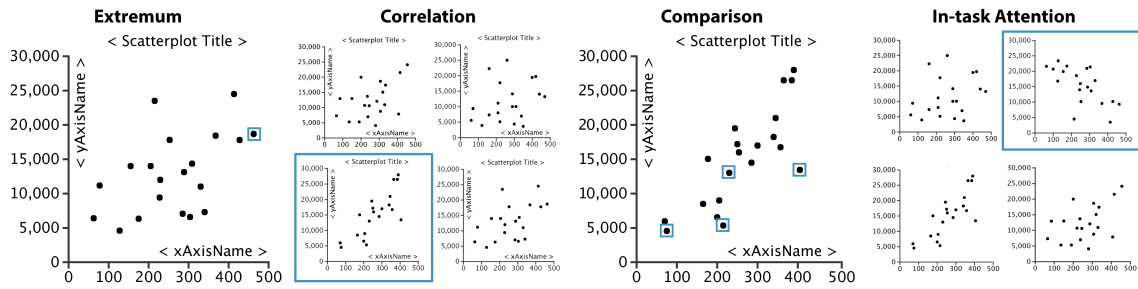


Figure 11. Stimuli used in each task (Ext, Cor and Com), and in the in-task attention test. Correct answers are annotated in blue. Axes were labeled (X,Y) for ABS, and (size m2, price (\$)) in all other context conditions. The title was Diagram Z : Datapoints in ABS, and was Diagram Z : Houses in SEM (all tasks) and DM-NAR (Ext, Cor tasks). In all other conditions the title was Agency Z : Houses. Z was an integer (1, 2, 3, or 4) identifying the scatterplot.

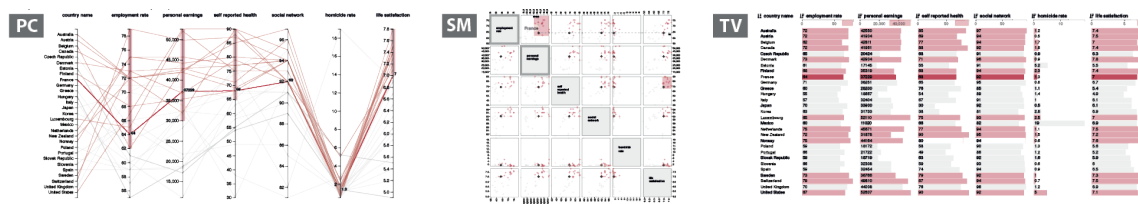


Figure 12. The visualizations we evaluated: Parallel Coordinates (PC), Scatterplot Matrix (SM) and Tabular Visualization (TV).

We explore how to rigorously evaluate multidimensional visualizations for their ability to support decision making. We first define multi-attribute choice tasks, a type of decision task commonly performed with such visualizations. We then identify which of the existing multidimensional visualizations are compatible with such tasks, and set out to evaluate three elementary visualizations: parallel coordinates, scatterplot matrices and tabular visualizations. Our method consists in first giving participants low-level analytic tasks, in order to ensure that they properly understood the visualizations and their interactions. Participants are then given multi-attribute choice tasks consisting of choosing holiday packages. We assess decision support through multiple objective and subjective metrics, including a decision accuracy metric based on the consistency between the choice made and self-reported preferences for attributes. We found the three visualizations to be comparable on most metrics, with a slight advantage for tabular visualizations. In particular, tabular visualizations allow participants to reach decisions faster. Thus, although decision time is typically not central in assessing decision support, it can be used as a tie-breaker when visualizations achieve similar decision accuracy. Our results also suggest that indirect methods for assessing choice confidence may allow to better distinguish between visualizations than direct ones. We finally discuss the limitations of our methods and directions for future work, such as the need for more sensitive metrics of decision support.

More on the project Web page: <http://www.aviz.fr/dm>.

## CEDAR Team

## 7. New Results

### 7.1. Semantic Query Answering

Building upon last year's work on regular path queries, we studied the complexity of answering conjunctive regular path queries under linear existential rules and under guarded existential rules. These queries generalized conjunctive queries by their ability to check for a path between two individuals which is labeled by a word belonging to a given regular language. Linear and guarded rules are widely recognized as two important classes of existential rules, that among other generalizes most popular Horn description logics. The results are quite positive, in the sense that the complexity is as good as we could hope for: we provided matching upper-bound that correspond to much less expressive query or ontology languages (i.e., they come from RPQs over linear rules or CQs over guarded rules). These results have been published at IJCAI'17 [13].

### 7.2. Representative Semantic Query Answers

The availability of large knowledge bases such as Yago or DBPedia allows theoretically anybody to tap in their resources through structured and semantics queries. This is still not as widespread as it could be, and we postulate this is mainly for two reasons. First, it is complex to write queries in such a setting. Second, the value added of such querying is improvable. We focused on the second point, with the rationale that increasing the value added may motivate more easily users to spend the time and energy necessary to learn to write SPARQL queries. More specifically, the internship of M. Buron [22] explored the possibility of exploiting the reasoning performed to find a tuple as an answer to cluster answers in a semantic (and explainable) way.

### 7.3. Interactive Data Exploration at Scale

To respond to increasing user information needs in the era of Big Data, we aim to build interactive data exploration as a new database service, using an approach called "explore-by-example". In particular, we cast the "explore-by-example" problem in a principled "active learning" framework, and bring the properties of important classes of database queries to bear on the design of new algorithms and optimizations for active learning based database exploration. We introduce a dual-space (data and version space) model for convex pattern queries, leverage the factorized dual-space model and online feature selection to handle high dimensional exploration, and design a new active learning algorithm based on version space reduction. These new techniques allow the database system to not only gain improved accuracy but also overcome fundamental limitations of traditional active learning, in particular, the slow convergence problem. Evaluation results using real-world datasets and user interest patterns show that our new system significantly outperforms state-of-the-art active learning techniques and data exploration systems in accuracy while achieving desired efficiency for interactive performance. In addition, we will extend current data exploration system to handle more complex inputs, such as pictures, by adding a active representation learning phase via neural networks to the existing system. Part of this work was explored during the M2 internship of Alexandre Sevin [25].

### 7.4. A Quotient Framework for Summarizing RDF Graphs

RDF is the data model of choice for Semantic Web applications. RDF graphs are often large and heterogeneous, thus users may have a hard time determining whether a graph is useful for a certain application. We consider answering such questions by inspecting a *graph summary*, a compact structure conveying as much information as possible about the input graph. A summary is *representative* of a graph if it represents both its explicit and implicit triples, the latter resulting from RDF Schema constraints. To ensure representativeness, we defined a novel RDF-specific summarization framework based on *RDF node equivalence* and *graph quotients*; our framework can be instantiated with many different RDF node equivalence relations. We have shown



that our summaries are representative, and establish a *sufficient condition* on the RDF equivalence relation to ensure that a graph can be *efficiently summarized*, without materializing its implicit triples. We illustrate our framework on *bisimulation* equivalence relations between graph nodes, and demonstrate the performance benefits of our efficient summarization method through a set of experiments. These results appeared in [17] and are extended in [20], [19].

## 7.5. Exploring RDF Graphs through Aggregation

RDF graphs may be large and their structure is heterogeneous and complex, making them very hard to explore and understand. To help users discover valuable insights from RDF graph, we have developed Dagger, a tool which automatically recommends *interesting aggregation queries* over the RDF graphs; Dagger evaluates the queries and graphically shows their results to the user, in the ranked order of their interestingness. To specify aggregate RDF queries, we rely on a dialect of SPARQL 1.1, the standard Semantic Web query language, which has been recently enhanced with the capability to specify aggregation; for the interestingness measure, we relied on variance (or second statistic moment). Dagger was developed as part of the M2 internship of Shu Shang [26] and was demonstrated at the International Semantic Web Conference [15]. A short video of our demo appears online at: <https://team.inria.fr/cedar/projects/dagger>.

## 7.6. Models and Algorithms for Fact-Checking and Data Journalism

We have advanced toward a generic definition of a computational fact-checking platform, and identified the set of core functionalities it should support: (i) extraction of a claim from a larger document (typically a text published online in some media, social network etc.); this may require identifying the time and space context in which the claim is supposed to hold; (ii) checking the accuracy of the claim against a set of reference data sources; (iii) putting the claim into perspective by checking its significance in a broader context, for instance by checking if the claim still holds after some minor modification of its temporal, spatial or numeric parameters. Checking a claim is not possible in the absence of a set of reference sources, containing data we consider to be true; thus reference source construction, refinement and selection are also central tasks in such an architecture. We have carried this work as part of the ANR ContentCheck project (Section 8.1.1) and also within our associated team with AIST Japan (Section 8.2.1.1). The architecture of the generic platform we envision has been presented in the Paris DB Day event in May 2017, in an ERCIM News [21] and in a keynote [24].

Within this architecture, an important task is to construct reference data sources and to make them more accessible. Toward this goal, we have devised an approach to extract Linked Open Data (RDF graphs) from Excel tables published by INSEE, the French national statistics institute [14]; the resulting data has been published online. Another ongoing line of work explored within the PhD of Ludivine Duroyon concerns establishing new models for temporal beliefs and statements, allowing journalists to increase the value of reference sources on which to check who said what when.

## 7.7. Design and optimization for population genomics

As mentioned above, the area of genomics experiences a massive increase in the amount of data to be processed. Furthermore the data generated can sometimes hard to interpret (in particular NGS data for CNV detection).

We investigate new means to discover Copy Number Variation in the human population using methods from the deep learning community. Indeed, great success has been achieved in that area within projects such as DeepVariant; such projects managed to considerably lower the latency for getting results (about 10 fold) but at a higher computational cost. Such methods are currently attracting significant attention in the biology / bioinformatics community, as witnessed by an editorial in Cell Systems (December 2017)<sup>0</sup>.

<sup>0</sup>[http://www.cell.com/cell-systems/fulltext/S2405-4712\(17\)30554-9](http://www.cell.com/cell-systems/fulltext/S2405-4712(17)30554-9)



As the area of population genomics is fairly new, we hope to help design a complete framework allowing for better optimisations and integration with database tools. This work is carried by Yanlei Diao and Felix Raimundo, together with Dr. Avinash Abhyankar at the New York Genome Center (NYGC) who co-advises the PhD of F. Raimundo and Dr. Toby Bloom (head of informatics at NYGC).

## **7.8. Performance Modeling and Multi-Objective Optimization For the Cloud**

We study cloud service models based on attaining user's performance objectives; these immediately lead to problems of multi-objective optimization.

Given different cost models, we consider the optimizer will search a multi-dimensional space, compute execution plans that are not dominated by others (known as Pareto plans) and explore meaningful tradeoffs between different objectives to find the optimal plan for each analytical task. We focused on analytical tasks encoded as dataflow programs as in Hadoop and Spark systems. When such dataflow programs are submitted to the cloud, we aim to provide a multi-objective optimizer that can automatically find an optimal execution plan of the dataflow program, which meets specific user performance objectives. Developing an optimizer for dataflow programs in the cloud raises two major challenges: The optimizer needs cost models for running complex dataflow programs in the cloud, and, it further needs a new algorithmic foundation for multi-objective optimization across user-specific objectives.

We have worked to develop a performance model for the optimizer in order to build the skylines for the user-objectives. We found that deep learning offers an incremental prediction framework (using embedding architecture) or online prediction framework (using auto-encoder along with a gradient boosting regressor) that are not available in a baseline regressor approach. However, there is a tradeoff between using the online prediction framework and having good performance, since of course retraining improves results. That said, the online prediction framework gave us acceptable generalization power over unseen jobs. This work has been carried in the M2 internship of Khaled Zaouk [27], and it continues through his PhD.

## EX-SITU Project-Team

# 7. New Results

## 7.1. Fundamentals of Interaction

**Participants:** Michel Beaudouin-Lafon [correspondant], Marianela Ciolfi Felice, Sarah Fdili Alaoui, Cédric Fleury, Carla Griggio, Wanyu Liu, Wendy Mackay, Nolwenn Maudet, Philip Tchernavskij, Theophanis Tsandilas.

In order to better understand fundamental aspects of interaction, ExSitu studies interaction under extreme situations. We conduct in-depth observational studies and controlled experiments which contribute to theories and frameworks that unify our findings and help us generate new, advanced interaction techniques.

On the theoretical side, in collaboration with Telecom ParisTech, we are bringing the tools and concepts from Information Theory to HCI. We conducted an information-theoretic analysis of human performance for command selection [21]. While a number of studies have focused on improving rapid command selection through novel interaction techniques, new interface design and innovative devices, user performance in this context has received little attention. We ran a controlled experiment to test the theory that the transmitted information from the user to the computer levels off as difficulty increases. Our reasoning is based on basic information-theoretic concepts such as entropy, mutual information and Fano's inequality. The important result is the bell-shaped behavior of the throughput as a function of command entropy, which shows that there is an optimal level of difficulty for a given input technique.

We also used the information-theoretic concept of mutual information, also known as information gain, in our BIG (Bayesian Information Gain) framework. We created *BIGnav* [20], a new multiscale navigation technique based on Bayesian Experimental Design where the criterion is to maximize the expected information gain from the next user input. In a controlled experiment, *BIGnav* was up to 40% faster than the standard pan-and-zoom technique. *BIGnav* creates a form of human-computer partnership (see below) where the computer challenges the user in order to maximize the amount of information extracted from the user's input. This work received a Best Paper Award at ACM CHI 2017, and the first prize for doctoral research from the Paris-Saclay doctoral school in computer science.

Finally, we continued our long-standing line of work on Fitts' law, with a novel analysis of minimal, as opposed to average, movement time in human aimed movement [18]. We showed that both metrics have a lot of support from theoretical and empirical perspectives and gave two examples, one in a controlled experiment and the other in a field study of pointing, where making the minimum versus average distinction is fruitful.

On the empirical side, we conducted two observational studies to better understand how people interact with technology. The first study [23] targeted expert graphic designers and their use of advanced computer tools. Traditional graphic design tools emphasize the grid for structuring layout. Interviews with professional graphic designers revealed that they use surprisingly sophisticated structures that go beyond the grid, which we call *graphical substrates*. These structures are not well supported by existing tools, so we developed two technology probes to explore how to embed graphical substrates into tools. *Contextify* lets designers tailor layouts according to each reader's intention and context, while *Linkify* lets designers create dynamic layouts based on relationships among content properties. We tested the probes with professional graphic designers, who all identified novel uses in their current projects. We incorporated their suggestions into *StyleBlocks*, a prototype that reifies CSS declarations into interactive graphical substrates. This work demonstrates that graphical substrates offer an untapped design space for tools that can help graphic designers generate personal layout structures.

The second study [30] targeted the operating system upgrade process that most users regularly have to go through to keep their system up to date. While current research has focused primarily on the security aspect of upgrades, we investigated the user's perspective of upgrading software. We found that users delay major upgrades by an average of 80 days, and an extensive field study revealed that very few participants prepare for upgrades (e.g., by backing up files), and over half had negative reactions to the upgrade process and other changes (e.g., bugs, lost settings, unwanted features). During the upgrade process, waiting times were too long, feedback was confusing or misleading, and few had clear mental models of what was happening. Moreover, users almost never mentioned security as a concern or reason for upgrading, while interviews with technical staff responsible for one organization's upgrades focused only on security and licensing, not user interface changes. This work shows that upgrades should be handled differently, offering users more control and decoupling security updates from the introduction of new features or the update of existing features.

These two sets of studies support our strong commitment to re-inventing interactive systems by identifying fundamental principles of interaction that unify, rather than separate, interaction styles in order to support the diversity of uses and users [33]. For example, most of our interactions with the digital world are mediated by apps: desktop, web, or mobile applications. Apps impose artificial limitations on collaboration among users, distribution across devices, and the changing procedures that constantly occur in real work. These limitations are partially due to the engineering principles of encapsulation and program-data separation, calling for new architectural principles [29]. Shareable dynamic media, which we have explored in our earlier work on Webstrates[5], provides an interesting approach as it blurs the limits between apps and documents and supports collaboration, distribution and flexibility as fundamental features [28]. In connection with these issues, we ran a workshop at the ACM CHI 2017 conference on HCI toolkits [37] where we discussed challenges and opportunities to develop new methods and approaches to design, evaluate, disseminate and share toolkits, as well as the technical, methodological and enabling role of toolkits for HCI research.

## 7.2. Human-Computer Partnerships

**Participants:** Wendy Mackay [correspondant], Jessalyn Alvina, Marianela Ciolfi Felice, Carla Griggio, Shu Yuan Hsueh, Wanyu Liu, John Maccallum, Nolwenn Maudet, Joanna McGrenere, Midas Nouwens, Andrew Webb.

ExSitu is interested in designing effective human-computer partnerships, in which expert users control their interaction with technology. Rather than treating the human users as the 'input' to a computer algorithm, we explore human-centered machine learning, where the goal is to use machine learning and other techniques to increase human capabilities. Much of human-computer interaction research focuses on measuring and improving productivity: our specific goal is to create what we call 'co-adaptive systems' that are discoverable, appropriable and expressive for the user. Jessalyn Alvina, under the supervision of Wendy Mackay, successfully defended her thesis, *Increasing The Expressive Power of Gesture-based Interaction on Mobile Devices* [38], on this topic.

We are interested in helping users create their own custom gesture-based commands for mobile devices. This raises two competing requirements: gestures must be both personally memorable for the user, while reliably recognizable by the system. We created two dynamic guides [22], *Fieldward* and *Pathward*, which use progressive feedforward to interactively visualize the "negative space" of unused gestures. The Pathward technique suggests four possible completions to the current gesture, whereas the Fieldward technique uses color gradients to reveal optimal directions for creating recognizable gestures (Figure 2 ). We ran a two-part experiment in which 27 participants each created 42 personal gesture shortcuts on a smartphone, using *Pathward*, *Fieldward* or *No Feedforward*. The Fieldward technique best supported the most common user strategy, i.e. to create a memorable gesture first and then adapt it to be recognized by the system. Users preferred the Fieldward technique to Pathward or No Feedforward, and remembered gestures more easily when using the technique. Dynamic guides can help developers design novel gesture vocabularies and support users as they design custom gestures for mobile applications.

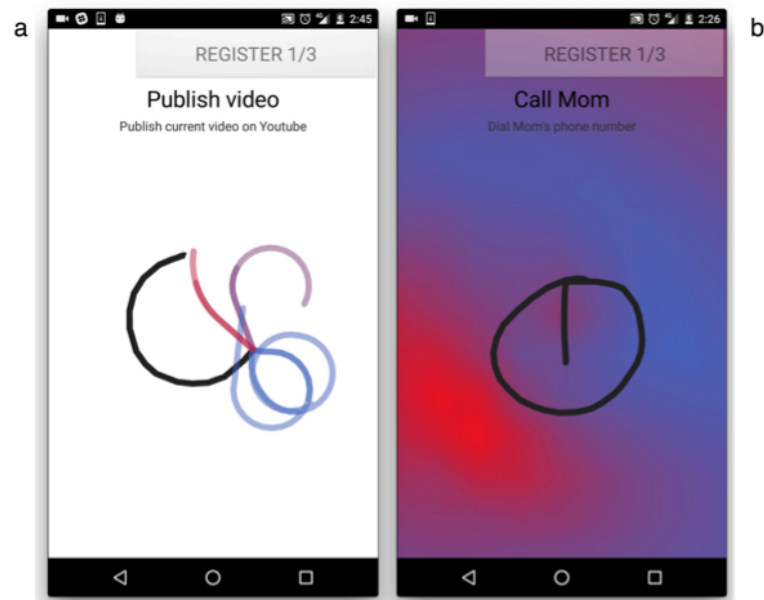


Figure 2. The Pathward (a) & Fieldward (b) dynamic guides help users create their own easy-to-remember gesture commands that are also recognizable by the system.

We are also interested in letting users use simple gestures to generate commands on a mobile device. *CommandBoard* [14] offers a simple, efficient and incrementally learnable technique for issuing gesture commands from a soft keyboard. We transform the area above the keyboard into a command-gesture input space that lets users draw unique command gestures or type command names followed by execute (Fig 3 ). Novices who pause see an in-context dynamic guide, whereas experts simply draw. Our studies show that *CommandBoard*'s inline gesture shortcuts are significantly faster (almost double) than markdown symbols and significantly preferred by users. We demonstrate additional techniques for more complex commands, and discuss trade-offs with respect to the user's knowledge and motor skills, as well as the size and structure of the command space. We filed a patent for the *CommandBoard* technique.



Figure 3. *CommandBoard* creates a new command gesture input space above a soft keyboard. Users can: a) type 'happy' and use a dynamic guide to style it as bold; b) type 'brightn', draw an execute gesture and adjust the brightness slider; c) type 'sans', choose 'sans mono' and draw an execute gesture to change the font; d) type 'color', select yellow in the marking menu to change the brush color.

In the context of an art-science project with the *n+1* theater group and the Théâtre de l'Agora d'Evry, we created an interactive installation that was exhibited at Fête de la Science, at the Agora d'Evry for an entire month, and at the Festival Curiositas. We were interested in understanding what makes public art installations interactive, so that they are engaging both for the individual user and the surrounding public. More specifically, we experimented with the principle of 'shaping' from behavioral psychology to create a human-computer partnership: an animated Santa character mirrors the exact movements of the user, but also offers different types of reinforcing or punishing feedback that in turn shapes the user's behavior (Figure 4 ). From the user's perspective, the user is always in control. Yet, from the system's perspective, the user moves through successive approximations to a specific desired behavior. Thus, we explore the dynamic nature of shared control between users and technology.

Finally, with *BIGnav* [20], we experimented with a different kind of partnership. *BIGnav* is a new multi-scale navigation technique based on Bayesian Experimental Design where the criterion is to maximize the information-theoretic concept of mutual information, also known as information gain. Rather than simply executing user navigation commands, *BIGnav* interprets user input to update its knowledge about the user's intended target. It then navigates to a new view that maximizes the information gain provided by the user's expected subsequent input. *BIGnav* creates a novel form of human-computer partnership, where the computer challenges the user in order to extract more information from the user's input, making interaction more efficient. We showed that *BIGnav* is significantly faster than conventional pan and zoom and requires fewer



Figure 4. The interactive Christmas window: the Santa character mimics the movements of the user in front of the window, but also uses reinforcement feedback to shape the movements of the user.

commands for distant targets, especially in non-uniform information spaces. We also applied *BIGnav* to a realistic application and showed that users can navigate to highly probable points of interest on a map with only a few steps.

### 7.3. Creativity

**Participants:** Sarah Fdili Alaoui [correspondant], Marianela Ciolfi Felice, Carla Griggio, Shu Yuan Hsueh, Ghita Jalal, Germán Leiva, John Maccallum, Wendy Mackay, Nolwenn Maudet, Joanna McGrenere, Midas Nouwens, Jean-Philippe Riviere, Nicolas Taffin, Philip Tchernavskij, Theophanis Tsandilas, Andrew Webb, Michael Wessely.

ExSitu is interested in understanding the work practices of creative professionals, particularly artists, designers, and scientists, who push the limits of interactive technology. Nolwenn Maudet, under the supervision of Wendy Mackay and Michel Beaudouin-Lafon, successfully defended her thesis, *Designing Design Tools* [40], on this topic. Her research includes observational studies of graphic designers and developers ([24] described in the *Collaboration* section below), as well as the creation of variety of creativity support tools to support professional designers [23] (described in the *Fundamentals of Interaction* section above).

We designed and evaluated computational models of movement's expressive qualities as defined in the framework of Laban Efforts [13] for dancer and movement practitioners. We included experts in Laban Movement Analysis (LMA) in our design process, in order to select a set of suitable multimodal sensors as well as to compute features that closely correlate to the definitions of Efforts in LMA. Evaluation of our model showed that multimodal data combining positional, dynamic and physiological information allows for a better characterization of Laban Efforts. Inspired by movement practices and dance, we designed an interactive sound installation that supports kinesthetic awareness of a participant's micro-movements [17] and discussed perspectives of such an installation from somatic practices and embodied cognition [16]. We discussed [25] the ethical and aesthetic implications of the appropriation of biomedical sensors in artistic practices, in particular dance. We also traced the history and new perspective of HCI in Dance and body based practices [11].

In collaboration with Inria Lille, we developed a versioning and annotation system for supporting collaborative, iterative design of mapping layers for digital musical instruments (DMIs) [31]. We also collaborated with Saarland University, TU Berlin and MIT to digitally fabricate Directional screens, devices and surfaces that maximize perceived image quality (e.g., resolution, brightness, and color reproduction) for large audiences [27]. Finally, Michael Wessely participated in the *MIT Summer School for Computational Fabrication and Smart Matter* and was then invited by its organizers to co-author an article [35] that presents and discusses the results of the summer school.

### 7.4. Collaboration

**Participants:** Cédric Fleury [correspondant], Ignacio Avellino Martinez, Michel Beaudouin-Lafon, Marianela Ciolfi Felice, Carla Griggio, Germán Leiva, Can Liu, Wendy Mackay, Nolwenn Maudet, Joanna McGrenere, Midas Nouwens, Yujiro Okuya.

ExSitu is interested in exploring new ways of supporting collaborative interaction, especially within and across large interactive spaces such as those of the Digiscope network (<http://digiscope.fr/>). Multi-touch wall-sized displays afford collaborative exploration of large datasets and re-organization of digital content. However, standard touch interactions, such as dragging to move content, do not scale well to large surfaces and were not designed to support collaboration, such as passing objects around. We created *CoReach* [19], a set of collaborative gestures that combine input from multiple users in order to manipulate content, facilitate data exchange and support communication. *Throw-and-catch* (Figure 5) lets users send digital objects to each other, *Preview* lets one user show content to another, and *SharedClipboard* lets users gather content. We conducted an observational study to inform the design of *CoReach*, and a controlled study showing that it reduced physical fatigue and facilitated collaboration when compared with traditional multi-touch gestures. A final study assessed the value of also allowing input through a handheld tablet to manipulate content from a distance.



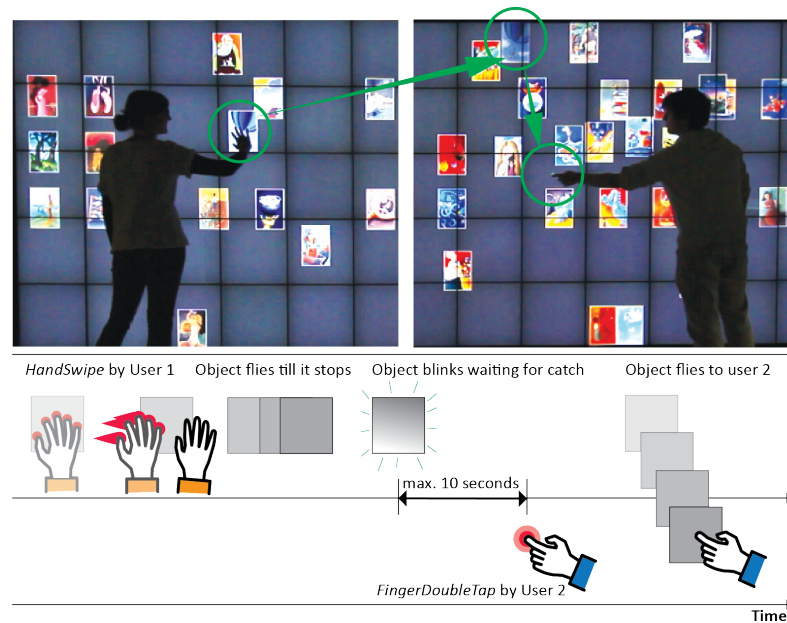


Figure 5. One of the three CoReach gestures: sending an object to the partner.

We also studied remote collaboration across wall-sized displays, where the challenge is to support audio-video communication among users as they move in front of the display. We created *CamRay* [15], a platform that uses camera arrays embedded in wall-sized displays (Figure 6) to capture video of users and present it on remote displays according to the users' positions. We investigated two settings: in *Follow-Remote*, the position of the video window follows the position of the remote user; in *Follow-Local*, the video window always appears in front of the local user. A controlled experiment showed that with *Follow-Remote*, participants were faster, used more deictic instructions, interpreted them more accurately, and used fewer words. However, some participants preferred the virtual face-to-face created by *Follow-Local* when checking for their partners' understanding. An ideal system should therefore combine both modes, in a way that does not hinder the collaborative process. Ignacio Avellino, under the supervision of Michel Beaudouin-Lafon and Cédric Fleury, successfully defended his thesis *Supporting Collaborative Practices Across Wall-Sized Displays with Video-Mediated Communication* [39] on this topic.

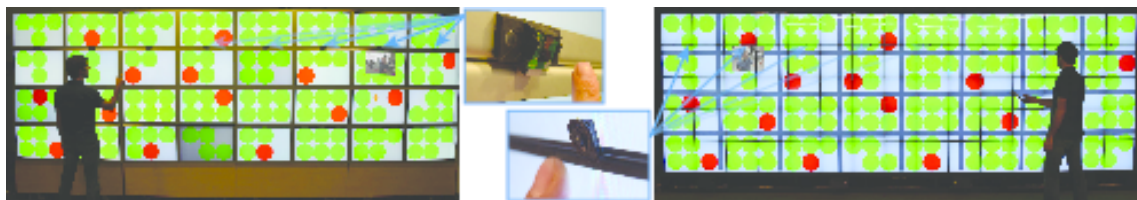


Figure 6. CamRay: the video cameras embedded in the wall-sized display (middle), and the two wall-sized displays (left, right) showing the video feed from the partner.

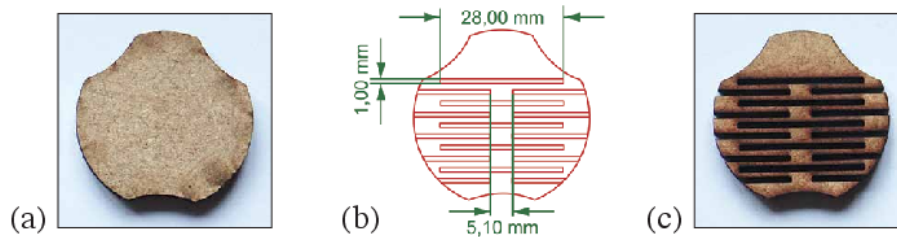
We are also interested in the collaboration between professional interaction designers and software developers when they create novel interactive systems [24]. Although designers and developers have different skills and training, they need to collaborate closely to create interactive systems. Our studies highlighted the mismatches among their processes, tools and representations: We found that current practices create unnecessary rework and cause discrepancies between the original design and the implementation. We identified three types of design breakdowns: omitting critical details, ignoring edge cases, and disregarding technical limitations. In a follow-up study, we found that early involvement of the developer helped mitigate potential design breakdowns but new ones emerged as the project unfolded. Finally, we ran a participatory design session and found that the designer/developer pairs had difficulty representing and communicating pre-existing interactions. This work will inform our future work on tools for designers and developers of interactive systems, in the context of our overall theoretical framework.

We also studied the use of social networks, with an indepth study of how users communicate via multiple apps that offer almost identical functionality [26]. We studied how and why users distribute their contacts within their app ecosystem. We found that the contacts in an app affect a user's conversations with other contacts, their communication patterns in the app, and the quality of their social relationships. Users appropriate the features and technical constraints of their apps to create idiosyncratic communication places, each with its own recursively defined membership rules, perceived purposes, and emotional connotations. Users also shift the boundaries of their communication places to accommodate changes in their contacts' behaviour, the dynamics of their relationships, and the restrictions of the technology. We argue that communication apps should support creating multiple communication places within the same app, relocating conversations across apps, and accessing functionality from other apps.

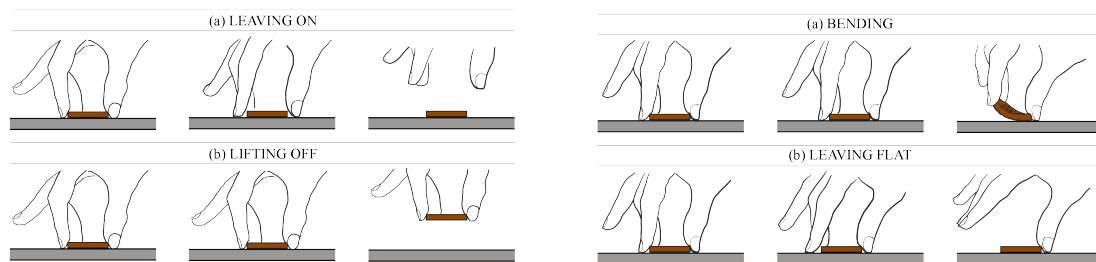
## ILDA Project-Team

# 7. New Results

## 7.1. Gestures and Tangibles



Making a TouchToken flexible: (a) original, rigid TouchToken (circle, 4cm in diameter), (b) schematics of lattice-hinges, (c) flexible TouchToken.



Micro-movements when leaving a token *on* the surface (a), and when lifting it *off* (b)      Micro-movements when (a) bending a token, and when leaving it flat (b)

Figure 3. Flexible TouchTokens

- As a follow-up to our work on TouchTokens [6], we investigated a way to augment the expressiveness of passive tokens for tangible interaction. This work was published at CHI 2017 [23]. TouchTokens are passive tokens that can be recognized on any capacitive surface based on the spatial configuration of the fingers that hold them. However, interaction with these tokens is confined to the basic two-state model of touch interaction as the system only knows the tokens' position and cannot detect tokens that are not touched. We increased the expressive power of TouchTokens by introducing laser-cut lattice hinges in their design, so as to make them flexible (Figure 3). A new recognizer, that analyzes the micro-movements of the fingers that hold the tokens, enables the system to detect when a token is left on the surface rather than taken off it. It can also detect bend events that can be mapped to command triggers, and a squeezed state that can be used for quasi-modal interaction.
- With MarkPad, presented at CHI 2017 [20] and demoed at IHM 2017, we propose a novel interaction technique taking advantage of the touchpad. MarkPad allows creating a large number of size-dependent gestural shortcuts that can be spatially organized as desired by the user. It relies on

the idea of using visual or tactile marks on the touchpad or a combination of them. Gestures start from a mark on the border and end on another mark anywhere (see Figure 4 ). MarkPad does not conflict with standard interactions and provides a novice mode that acts as a rehearsal of the expert mode. A study showed that an accuracy of 95% could be achieved for a dense configuration of tactile and/or visual marks allowing 680 possible gestures, more than all existing techniques with a comparable input channel. Performance was 5% lower in a second study where the marks were only on the borders, and subjective results suggest that a mixed interface (borders with tactile marks and center with visual marks) is a promising solution. A working prototype is freely available at <http://brunofruchard.com/markpad.html>.

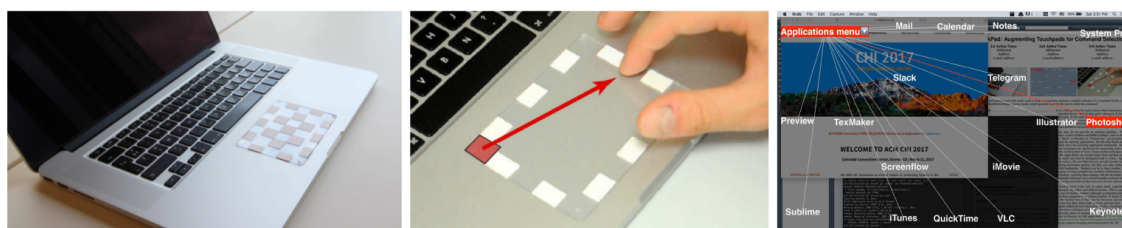


Figure 4. Tactile or visual marks on the touchpad help performing gestures: (Left) Dense configuration of tactile marks, (Middle) Light configuration with marks only on the borders, (Right) Example of a menu in novice mode. This menu and the selected shortcut on its right side correspond to the red area and the red gesture line in the middle picture.

## 7.2. Interacting with Linked Data and the Semantic Web

- As part of the team's novel research theme on Semantics-Driven Data Manipulation 3.2, Emmanuel Pietriga worked jointly with colleagues from Linköping University on a visualization technique for the comparative evaluation of ontology alignments produced by different algorithms, that was published at the International Semantic Web Conference [21]. Ontology alignment is an area of active research where many algorithms and approaches are being developed. Their performance is usually evaluated by comparing the produced alignments to a reference alignment in terms of precision, recall and F-measure. These measures, however, only provide an overall assessment of the quality of the alignments, but do not reveal differences and commonalities between alignments at a finer-grained level such as, e.g., regions or individual mappings. Furthermore, reference alignments are often unavailable, which makes the comparative exploration of alignments at different levels of granularity even more important. Making such comparisons efficient calls for a human-in-the-loop approach, best supported through interactive visual representations of alignments. Our approach extended previous work by Inria on Matrix Cubes [32], used for visualizing dense dynamic networks. We identified use cases for ontology alignment evaluation that could benefit from interactive visualization, and then detailed how *Alignment Cubes* could support interactive exploration of multiple ontology alignments. We then showed how alignment cubes could support common tasks identified in these use cases.

## 7.3. Wall Displays

Ultra-high-resolution wall displays feature a very high pixel density over a large physical surface, which makes them well-suited to the collaborative, exploratory visualization of large datasets (see Section 6.3.1 ). We have continued working on the design, implementation and evaluation of interactive visualization techniques

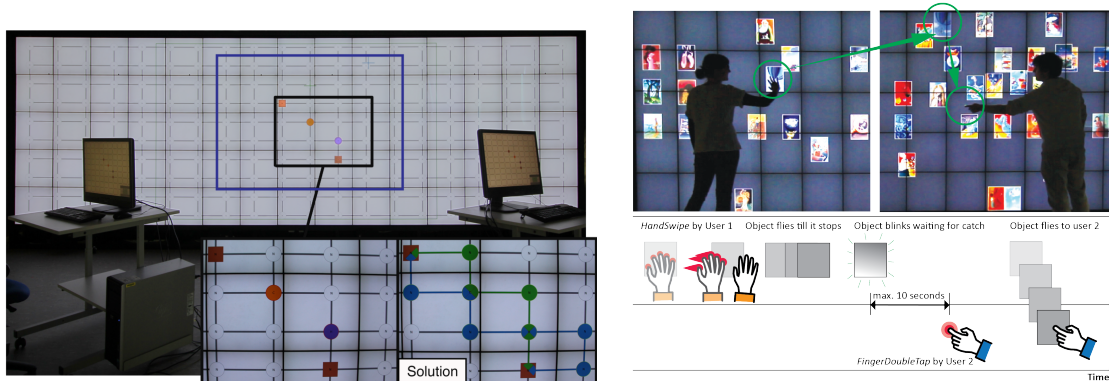


Figure 5. (Left) The setup for comparing a wall display with two desktops. Participants had to construct paths between the two brown nodes, that only crossed at the other colored nodes. The lower part of the image shows the closeup of a possible solution. (Right) An example of cooperative a gesture: throw-and-catch.

for such ultra-high-resolution wall-sized displays, focusing, in some of these projects, on the collaboration between users who perform different data manipulation and analysis tasks.

- We first studied if wall displays indeed provide advantages over more classic collaboration setups, such as multiple desktops [24]. Very few studies that empirically assess the differences of collaboration in front of a shared display compared to a non-shared setup, such as multiple desktops with a common view. We compared the use of the wall compared to two desktops, when pairs of users learn to perform a path-planning task (see Figure 5 -(Left)). Path planning tasks are common in critical situations (e.g., rerouting resources). We focused on learning, to approach exceptional and unexpected events in critical systems. Our results did not indicate a significant difference in learning time between the two setups, but found that participants adopted different task strategies and that quality was more consistent in the wall setup.
- We also continued our work on shared interaction techniques (see [56]). Multi-touch wall-sized displays afford collaborative exploration of large datasets and re-organization of digital content. However, standard touch interactions, such as dragging to move content, do not scale well to large surfaces and were not designed to support collaboration, such as passing an object around. With *CoReach* [22], published at CHI 2017, we introduce a set of collaborative gestures that combine input from multiple users in order to manipulate content, facilitate data exchange and support communication (see Figure 5 -(Right) for an example). We conducted an observational study to inform the design of *CoReach*, and a controlled study showing that it reduced physical fatigue and facilitated collaboration when compared with traditional multi-touch gestures. A final study assessed the value of also allowing input through a handheld tablet to manipulate content from a distance.
- We also studied more explicitly how interaction techniques affect collaboration. We investigated how pairs explore graphs on a touch enabled wall-display [18], using two selection techniques adapted for collaboration: a basic localized selection, and a propagation selection technique that uses the idea of diffusion/transmission from an origin node. Results from this work were accepted for publication in 2016 (and was part of the previews report), but the work appeared in print this year.

## 7.4. Visualization

- In the context of ANR-funded collaborative project MapMuxing (see Section 9.2.1 ), we investigated novel dynamic map compositing techniques for geovisualization. GIS software applications and





Figure 6. A proof-of-concept implementation of the MapMosaic dynamic compositing model and interaction techniques. (a) Toolbar to navigate the map, and to create & select areas. (b) Map viewer. (c) Access to individual layers. (d) Compositing area inspector. (e) Query builder for compositing region filters.

other mapping tools enable users to correlate data from multiple layers and gain insight from the resulting visualizations. However, most of these applications only feature basic, monolithic layer compositing techniques. These techniques do not always support users effectively in their tasks, as we observed during interviews with GIS experts at IGN (French national cartographic institute). We designed MapMosaic (Figure 6), a novel approach based on dynamic visual compositing that enables users to interactively create and manipulate local composites of multiple vector and raster map layers, taking into account the semantics and attribute values of objects and fields in the compositing process. We evaluated MapMosaic's interaction model against that of QGIS (a widely used desktop GIS) and MAPublisher (a professional cartography tool) using the Cognitive Dimensions framework, showing that MapMosaic's model is more flexible and can support users more effectively in their tasks. Feedback obtained from experts further confirmed the potential of this highly dynamic approach to map layer compositing.

- We also explored how different interactive visualizations of multidimensional datasets can affect how we make decisions [15]. We evaluated three elementary visualizations: parallel coordinates, scatterplot matrices and tabular visualizations. Our method consisted in first giving participants low-level analytic tasks, in order to ensure that they properly understood the visualizations and their interactions. Participants were then given multi-attribute choice tasks consisting of choosing holiday packages. We assessed decision support through multiple objective and subjective metrics, including a decision accuracy metric based on the consistency between the choice made and self-reported preferences for attributes. We found the three visualizations to be comparable on most metrics, with a slight advantage for tabular visualizations. In particular, tabular visualizations allow participants to reach decisions faster. Our results also suggest that indirect methods for assessing choice confidence may allow to better distinguish between visualizations than direct ones. Related to this topic, is our previous work on studying how biases can affect our decision making when using visualizations [14], work that was accepted in 2016 (and thus was part of last year's report) but appeared in print this year.
- Beyond the actual interactive visualizations themselves, we studied how framing the questions to participants may affect the results of evaluating visualizations [19]. More specifically we explored the effects of providing task context when evaluating visualization tools in crowdsourced studies. We gave participants abstract information visualization tasks without any context; tasks where we added semantics to the dataset; and tasks with two types of backstory narratives: an analytic narrative and a decision-making narrative. We did not find evidence that adding data semantics increases accuracy, but that it increases attention and provides subjective benefits in terms of confidence, perceived

easiness, task enjoyability and perceived usefulness of the visualization. Interestingly, we also found that backstory narratives, often used to motivate study participants, can even decrease accuracy.

- Finally, we are interested in understanding how people understand more general multidimensional visualisations. We mention here again work with colleagues both from University of Konstanz [16] on a review of multidimensional visualizations in the forms of glyphs; and with colleagues from INRA on a mixed initiative system that aids navigation of complex multi-dimensional datasets [41]. Both these results were accepted for publication in 2016 (and were part of the previous report), but the work appeared in print this year.



## PETRUS Project-Team

## 6. New Results

### 6.1. Personal Cloud Architecture Based on Trusted Execution Environments (Axis 1)

**Participants:** Nicolas Anciaux [correspondent], Luc Bouganim, Riad Ladjel, Julien Loudet, Benjamin Nguyen, Philippe Pucheral, Iulian Sandu Popa, Guillaume Scerri, Paul Tran Van.

**The Personal Cloud paradigm and its challenges:** The time of individualized management and control over one's personal data is upon us. Thanks to smart disclosure initiatives, we can access our personal data from the companies or government agencies that collected them. Concurrently, Personal Cloud solutions are flourishing. Their goal is to empower us to leverage our personal data for our own good. However, managing our own personal data constitutes a considerable burden. We must now: (1) ensure the security of the data we gather; and (2) manage the disclosed data and control its usage. We inherit the combined responsibility of an information security expert and a database administrator. Since very few users are actually IT experts, personal cloud providers propose solutions to manage personal data on behalf of their customers. Thus, paradoxically, instead of empowering users, smart disclosure and personal clouds create new privacy risks. In this work, we formulate this paradox and the problems it creates. Our central contribution is a reference architecture for the Personal Cloud, instantiated on several hardware configuration using trusted execution environments (paper in preparation).

### 6.2. Data Management in Secure Hardware (Axis 1)

**Participants:** Nicolas Anciaux, Philippe Pucheral, Iulian Sandu Popa [correspondent].

**Secure keyword search in the Personal Cloud:** The Personal Cloud paradigm has emerged as a solution that allows individuals to manage under their control the collection, usage and sharing of their data. However, by regaining the full control over their data, the users also inherit the burden of protecting it against all forms of attacks and abusive usages. The Secure Personal Cloud architecture relieves the individual from this security task by employing a secure token (i.e., a tamper-resistant hardware device) to control all the sensitive information (e.g., encryption keys, metadata, indexes) and operations (e.g., authentication, data encryption/decryption, access control, and query processing). However, secure tokens are usually equipped with extremely low RAM but have significant Flash storage capacity (Gigabytes), which raises important barriers for embedded data management. This work [11] proposes a new embedded search engine specifically designed for secure tokens, which applies to the important use-case of managing and securing documents in the Personal Cloud context. Conventional search engines privilege either insertion or query scalability but cannot meet both requirements at the same time. Moreover, very few solutions support data deletions and updates in this context. In this work, we introduce three design principles, namely Write-Once Partitioning, Linear Pipelining and Background Linear Merging, and show how they can be combined to produce an embedded search engine matching the hardware constraints of secure tokens and reconciling high insert/delete/update rate and query scalability. Our experimental results, obtained with a prototype running on a representative hardware platform, demonstrate the scalability of the approach on large datasets and its superiority compared to state of the art methods. Finally, the integration of our solution in another important real use-case related to performing information retrieval in smart objects has been previously discussed in [5] and demonstrated at [25].

### 6.3. Data Management in Flash Memory (Axis 1)

**Participant:** Luc Bouganim [correspondent].

**Understanding Flash I/O Patterns on Open-Channel Solid-State Drives:** Solid-State Drives (SSDs) have gained acceptance by providing the same block device abstraction as magnetic hard drives, at the cost of suboptimal resource utilization and unpredictable performance. Recently, Open-Channel SSDs have emerged as a means to obtain predictably high performance, based on a clean break from the block device abstraction. Open-channel SSDs embed a minimal flash translation layer (FTL) and expose their internals to the host. The Linux open-channel SSD subsystem, LightNVM, lets kernel modules as well as user-space applications control data placement and I/O scheduling. This way, it is the host that is responsible for SSD management. But what kind of performance model should the host rely on to guide the way it manages data placement and I/O scheduling? For addressing this question we have defined uFLIP-OC, a benchmark designed to identify the I/O patterns that are best suited for a given open-channel SSD. Our experiments on a Dragon- Fire Card (DFC) SSD, equipped with the OX controller, illustrate the performance impact of media characteristics and parallelism. In [17], we present uFLIP-OC and how it can be used to guide the design of host-based data systems on open-channel SSDs.

## 6.4. Data Sharing architecture for the Personal Cloud (Axis 2)

**Participants:** Nicolas Anciaux [correspondent], Philippe Pucheral, Paul Tran Van.

**SWYSWYK Architecture:** Pushed by recent legislation and smart disclosure initiatives, Personal Cloud platforms emerge and hold the promise of giving the control back to the individual on her data. However, this shift leaves the privacy and security issues in user's hands, a role that few people can properly endorse. Indeed, existing sharing models are difficult to administrate and securing their implementation in user's computing environment is an unresolved challenge. This study advocates the definition of a Privacy-by-Design sharing architecture, called SWYSWYK (Share What You See with Who You Know), dedicated to the Personal Cloud context. This architecture allows each user to physically visualize the net effects of sharing rules on her Personal Cloud and automatically provides tangible guarantees about the enforcement of the defined sharing policies. The architecture relies on a secure reference monitor, a set of user defined functions only interacting with the secure monitor and isolated from the unsecure environment, and an unsecure personal cloud platform managing encrypted personal data. The SWYSWYK architecture is presented in [20]. A validation of this architecture combining PlugDB to host the secure reference monitor, a RaspberryPI to launch the isolated user defined functions and a personal computer to host the untrusted personal cloud software was demonstrated in [19]. It shows the practicality of the approach and a performance evaluation on a real Personal Cloud platform.

## 6.5. Data sharing model for the Personal Cloud (Axis 2)

**Participants:** Nicolas Anciaux [correspondent], Paul Tran Van, Philippe Pucheral.

**SWYSWYK Semantics:** The personal cloud content intrinsically describes the individual's acquaintances under different forms (e.g., contact files, agendas, identity pictures, address book entries, etc.). Conversely, acquaintances are associated with pieces of information in the user's space (e.g., photos on which a friend appears). New sharing models should be thus able to map personal data to acquaintances (or subjects) and exploit their links with the stored documents (or objects) to produce authorizations satisfying users' sharing desires such as those expressed above. Interesting and common sharing rules could also be published and adopted by the members of a community of interest. In [18], we propose SWYSWYK, a new data sharing model which builds upon the transversal nature of the content of a personal cloud and makes easy and intuitive the definition and administration of sharing policies. Beyond the definition of the sharing policy, SWYSWYK provides means to the personal cloud owner to easily understand the net effects of a sharing policy, identify suspicious permissions and sanitize the sharing policy accordingly, and finally, to trust the way the policy is practically enforced. In [21] we demonstrate the semantics of the model with the goal to assess its practical interest for the personal cloud owner. To this end, we have integrated SWYSWYK in a real personal cloud platform (namely Cozy) and apply it to a smart surrounding scenario.

## 6.6. Privacy-preserving Computation Protocols on Asymmetric Architectures (Axis 3)

**Participant:** Iulian Sandu Popa [correspondent].

**Distributed Vehicular Traffic Re-routing System for Congestion Avoidance:** Centralized solutions for vehicular traffic re-routing to alleviate congestion suffer from two intrinsic problems: scalability, as the central server has to perform intensive computation and communication with the vehicles in real-time; and privacy, as the drivers have to share their location as well as the origins and destinations of their trips with the server. In this work [12], we proposed DIVERT, a distributed vehicular re-routing system for congestion avoidance. DIVERT offloads a large part of the re-routing computation at the vehicles, and thus, the re-routing process becomes practical in real-time. To take collaborative re-routing decisions, the vehicles exchange messages over vehicular ad hoc networks. DIVERT is a hybrid system because it still uses a server and Internet communication to determine an accurate global view of the traffic. In addition, DIVERT balances the user privacy with the re-routing effectiveness. The simulation results demonstrate that, compared with a centralized system, the proposed hybrid system increases the user privacy by 92 percent on average. In terms of average travel time, DIVERT's performance is slightly less than that of the centralized system, but it still achieves substantial gains compared to the no re-routing case. In addition, DIVERT reduces the CPU and network load on the server by 99.99 and 95 percent, respectively.

## 6.7. Privacy-preserving Anonymization Protocols on Asymmetric Architectures (Axis 3)

**Participants:** Axel Michel, Benjamin Nguyen [correspondent], Philippe Pucheral.

**Managing Distributed Queries under Personalized Anonymity Constraints** The benefit of performing Big data computations over individual's microdata is manifold, in the medical, energy or transportation fields to cite only a few, and this interest is growing with the emergence of smart disclosure initiatives around the world. However, these computations often expose microdata to privacy leakages, explaining the reluctance of individuals to participate in studies despite the privacy guarantees promised by statistical institutes. In this work [22], we propose a novel approach to push personalized privacy guarantees in the processing of database queries so that individuals can disclose different amounts of information (i.e. data at different levels of accuracy) depending on their own perception of the risk. Moreover, we propose a decentralized computing infrastructure based on secure hardware enforcing these personalized privacy guarantees all along the query execution process. A performance analysis conducted on a real platform shows the effectiveness of the approach.

## 6.8. Economic, legal and societal issues (Axis 4)

**Participants:** Nicolas Anciaux [correspondent], Philippe Pucheral.

**Data Portability and Users' Empowerment as a Privacy Incentive.** The principle of 'data portability' recently introduced in regulations (smart disclosure in the US, data portability in France and EU) is tightly coupled with the notion of Personal Cloud. We conduct a study of this principle in common with the DANTE Lab at UVSQ, in particular with Prof. Celia Zolynski (jurist, member of the CNN), within the DATAIA convergence institute at Inria and in the SIHS CNRS federation at UVSQ. Our recent contributions analyze the technical conditions under which individuals can get their data back from service providers according to this data portability principle, and examine its technical feasibility and legal opportunity. We also explain how data portability favors a form of users' empowerment, which can be viewed as a potential privacy incentive. Our recent results are presented in multi-disciplinary papers appeared in prestigious French journals like DALLOZ [14] and 'Revue Contrats, Concurrence, Consommation' [13] [15].