

RESEARCH CENTER Sophia Antipolis - Méditerranée

FIELD

# Activity Report 2018

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### **AROMATH Project-Team**

## 6. New Results

### 6.1. Solving Polynomial Systems via Truncated Normal Forms

Participant: Bernard Mourrain.

In [12], we consider the problem of finding the isolated common roots of a set of polynomial functions defining a zero-dimensional ideal I in a ring R of polynomials over  $\mathbb{C}$ . We propose a general algebraic framework to find the solutions and to compute the structure of the quotient ring R/I from the null space of a Macaulay-type matrix. The affine dense, affine sparse, homogeneous, and multihomogeneous cases are treated. In the presented framework, the concept of a border basis is generalized by relaxing the conditions on the set of basis elements. This allows for algorithms to adapt the choice of basis in order to enhance the numerical stability. We present such an algorithm and show numerical results.

This is a joint work with Simon Telen and Marc Van Barel (Univ. Leuven, Belgium)

### 6.2. On supersolvable and nearly supersolvable line arrangements

Participant: Alexandru Dimca.

In the paper [3], we introduce a new class of line arrangements in the projective plane, called nearly supersolvable, and show that any arrangement in this class is either free or nearly free. More precisely, we show that the minimal degree of a Jacobian syzygy for the defining equation of the line arrangement, which is a subtle algebraic invariant, is determined in this case by the combinatorics. When such a line arrangement is nearly free, we discuss the splitting types and the jumping lines of the associated rank two vector bundle, as well as the corresponding jumping points, introduced recently by S. Marchesi and J. Vallès.

Joint work with Gabriel Sticlaru (Faculty of Mathematics and Informatics, Ovidius University, Romania).

# 6.3. Computing the monodromy and pole order filtration on Milnor fiber cohomology of plane curves

Participant: Alexandru Dimca.

In the paper [4], we describe an algorithm computing the monodromy and the pole order filtration on the Milnor fiber cohomology of any reduced projective plane curve C. The relation to the zero set of Bernstein-Sato polynomial of the defining homogeneous polynomial for C is also discussed. When C has some non weighted homogeneous singularities, then we have to assume that a conjecture holds in order to get some of our results. In all the examples computed so far this conjecture holds.

Joint work with Gabriel Sticlaru (Faculty of Mathematics and Informatics, Ovidius University, Romania).

### 6.4. Invariant Algebraic Sets and Symmetrization of Polynomial Systems

Participant: Evelyne Hubert.

Assuming the variety of a polynomial set is invariant under a group action, we construct, in [9], a set of invariants that cut the same variety. The construction can be seen as a generalization of the previously known construction for finite groups. The result though has to be understood outside an invariant variety which is independent of the polynomial set considered. We introduce the symmetrizations of a polynomial that are polynomials in a generating set of rational invariants. The generating set of rational invariants and the symmetrizations are constructed w.r.t. a section of the orbits of the group action.

### 6.5. Rational invariants of even ternary forms under the orthogonal group

Participant: Evelyne Hubert.

In [8], we determine a generating set of rational invariants of minimal cardinality for the action of the orthogonal group  $O_3$  on the space  $R[x, y, z]_{2d}$  of ternary forms of even degree 2d. The construction relies on two key ingredients: On the one hand, the Slice Lemma allows us to reduce the problem to determining the invariants for the action on a subspace of the finite subgroup  $B_3$  of signed permutations. On the other hand, our construction relies in a fundamental way on specific bases of harmonic polynomials. These bases provide maps with prescribed  $B_3$ -equivariance properties. Our explicit construction of these bases should be relevant well beyond the scope of this paper. The expression of the  $B_3$ -invariants can then be given in a compact form as the composition of two equivariant maps. Instead of providing (cumbersome) explicit expressions for the  $O_3$ -invariants to determine the  $O_3$ -orbit locus and provide an algorithm for the inverse problem of finding an element in  $R[x, y, z]_{2d}$  with prescribed values for its invariants. These are the computational issues relevant in brain imaging.

This is a joint work with P. Görlach (Max Planck institute, Leipzig) and T. Papadopoulo (EPI Athena, Inria SAM)

### 6.6. Algorithms for Computing Cubatures Based on Moment Theory

Participant: Evelyne Hubert.

Quadrature is an approximation of the definite integral of a function by a weighted sum of function values at specified points, or nodes, within the domain of integration. Gaussian quadratures are constructed to yield exact results for any polynomials of degree 2r - 1 or less by a suitable choice of r nodes and weights. Cubature is a generalization of quadrature in higher dimension. In [2] we elaborate algorithms to compute all minimal cubatures for a given domain and a given degree. We propose first an algorithm in symbolic computation to characterize all cubatures of a given degree with a fixed number of nodes. The determination of the nodes and weights is then left to the computation of the eigenvectors of the matrix identified at the characterization stage and can be performed numerically. The characterisation of cubatures on which our algorithms are based stems from moment theory. We formulate the results there in a basis independent way : rather than considering the moment matrix, the central object in moment problems, we introduce the underlying linear map from the polynomial ring to its dual, the Hankel operator. This makes natural the use of bases of polynomials other than the monomial basis, and proves to be computationally relevant, either for numerical properties or to exploit symmetry.

Joint work with M. Collowald, (previously Université Nice Sophia Antipolis).

### 6.7. Products of Euclidean Metrics and Applications to Proximity Questions among Curves

Participants: Ioannis Emiris, Ioannis Psarros.

In [18], we study Approximate Nearest Neighbor (ANN) search on 1-dimensional shapes. We start with distance functions between discretized curves in Euclidean space: they appear in a wide range of applications, from road segments and molecular backbones to time-series in general dimension. For p-products of Euclidean metrics, for any positive integer p, we design simple and efficient data structures for ANN, based on randomized projections, which are of independent interest. They serve to solve proximity problems under a notion of distance between discretized curves, which generalizes both discrete Fréchet and Dynamic Time Warping distances. These are the most popular and practical approaches to comparing such curves. We offer the first data structures and query algorithms for ANN with arbitrarily good approximation factor, at the expense of increasing space usage and preprocessing time over existing methods. Query time complexity is comparable or significantly improved by our algorithms.

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### 6.8. Efficient Random-Walk Methods for Approximating Polytope Volume

Participant: Ioannis Emiris.

In [5] we experimentally study the fundamental problem of computing the volume of a convex polytope given as an intersection of linear inequalities. We implement and evaluate practical randomized algorithms for accurately approximating the polytope's volume in high dimensions (e.g. one hundred). To carry out this efficiently we experimentally correlate the effect of parameters, such as random walk length and number of sample points, on accuracy and runtime. Moreover, we exploit the problem's geometry by implementing an iterative rounding procedure, computing partial generations of random points and designing fast polytope boundary oracles. Our publicly available code is significantly faster than exact computation and more accurate than existing approximation methods. We provide volume approximations for the Birkhoff polytopes of order 11 to 15, whereas exact methods have only computed that for order 10.

This is a joint work with Vissarion Fisikopoulos (Oracle Corp., Athens, Greece).

# 6.9. Randomized Embeddings with Slack and High-Dimensional Approximate Nearest Neighbor

Participants: Evangelos Anagnostopoulos, Ioannis Emiris, Ioannis Psarros.

In [1], we study the approximate nearest neighbor problem (e-ANN) in high dimensional Euclidean space with methods beyond Locality Sensitive Hashing (LSH), which has polynomial dependence in the dimension, sublinear query time, but subquadratic space requirement. In particular, we introduce a new definition of "lowquality" embeddings for metric spaces. It requires that, for some query point q, there exists an approximate nearest neighbor among the pre-images of the k approximate nearest neighbors in the target space. Focusing on Euclidean spaces, we employ random projections in order to reduce the original problem to one in a space of dimension inversely proportional to k. The k approximate nearest neighbors can be efficiently retrieved by a data structure such as BBD-trees. The same approach is applied to the problem of computing an approximate near neighbor, where we obtain a data structure requiring linear space, and query time in  $O(dn^{\rho})$ , for  $\rho \approx 1-e^2/\log(1/e)$ . This directly implies a solution for e-ANN, while achieving a better exponent in the query time than the method based on BBD-trees. Better bounds are obtained in the case of doubling subsets of  $\ell^2$ , by combining our method with r-nets. We implement our method in C++, and present experimental results in dimension up to 500 and  $10^6$  points, which show that performance is better than predicted by the analysis. In addition, we compare our ANN approach to E2LSH, which implements LSH, and we show that the theoretical advantages of each method are reflected on their actual performance.

### 6.10. Practical Volume Computation of Structured Convex Bodies, and an Application to Modeling Portfolio Dependencies and Financial Crises

Participants: Ioannis Emiris, Apostolos Chalkis.

In [16], we examine volume computation of general-dimensional polytopes and more general convex bodies, defined as the intersection of a simplex by a family of parallel hyperplanes, and another family of parallel hyperplanes or a family of concentric ellipsoids. Such convex bodies appear in modeling and predicting financial crises. The impact of crises on the economy (labor, income, etc.) makes its detection of prime interest for the public in general and for policy makers in particular. Certain features of dependencies in the markets clearly identify times of turmoil. We describe the relationship between asset characteristics by means of a copula; each characteristic is either a linear or quadratic form of the portfolio components, hence the copula can be constructed by computing volumes of convex bodies. We design and implement practical algorithms in the exact and approximate setting, we experimentally juxtapose them and study the tradeoff of exactness and accuracy for speed. We analyze the following methods in order of increasing generality: rejection sampling relying on uniformly sampling the simplex, which is the fastest approach, but inaccurate for small volumes; exact formulae based on the computation of integrals of probability distribution functions, which are the method of choice for intersections with a single hyperplane; an optimized Lawrence sign decomposition

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method, since the polytopes at hand are shown to be simple with additional structure; Markov chain Monte Carlo algorithms using random walks based on the hit-and-run paradigm generalized to nonlinear convex bodies and relying on new methods for computing a ball enclosed in the given body, such as a second-order cone program; the latter is experimentally extended to non-convex bodies with very encouraging results. Our C++ software, based on CGAL and Eigen and available on github, is shown to be very effective in up to 100 dimensions. Our results offer novel, effective means of computing portfolio dependencies and an indicator of financial crises, which is shown to correctly identify past crises. (The views expressed are those of the authors and do not necessarily reflect official positions of the European Commission.)

This is a joint work with Ludovic Calées (EU JRC, Ispra, Italy), and Vissarion Fisikopoulos (Oracle Corp., Athens, Greece).

# 6.11. On the maximal number of real embeddings of spatial minimally rigid graphs

Participants: Ioannis Emiris, Evangelos Bartzos.

In [15], we study the number of embeddings of minimally rigid graphs in Euclidean space  $R^D$ , which is (by definition) finite, modulo rigid transformations, for every generic choice of edge lengths. Even though various approaches have been proposed to compute it, the gap between upper and lower bounds is still enormous. Specific values and its asymptotic behavior are major and fascinating open problems in rigidity theory. Our work considers the maximal number of real embeddings of minimally rigid graphs in  $R^3$ . We modify a commonly used parametric semi-algebraic formulation that exploits the Cayley-Menger determinant to minimize the *a priori* number of complex embeddings, where the parameters correspond to edge lengths. To cope with the huge dimension of the parameter space and find specializations of the parameters that maximize the number of real embeddings, we introduce a method based on coupler curves that makes the sampling feasible for spatial minimally rigid graphs. Our methodology results in the first full classification of the number of real embeddings of graphs with 7 vertices in  $R^3$ , which was the smallest open case. Building on this and certain 8-vertex graphs, we improve the previously known general lower bound on the maximum number of real embeddings in  $R^3$ .

This is a joint work with J. Legersky (JK University, Linz, Austria) and E. Tsigaridas (PolSys, Inria).

### 6.12. Curved Optimal Delaunay Triangulation

Participant: Laurent Busé.

Meshes with curvilinear elements hold the appealing promise of enhanced geometric flexibility and higherorder numerical accuracy compared to their commonly-used straight-edge counterparts. However, the generation of curved meshes remains a computationally expensive endeavor with current meshing approaches: high-order parametric elements are notoriously difficult to conform to a given boundary geometry, and enforcing a smooth and non-degenerate Jacobian everywhere brings additional numerical difficulties to the meshing of complex domains. In the paper [6], we propose an extension of Optimal Delaunay Triangulations (ODT) to curved and graded isotropic meshes. By exploiting a continuum mechanics interpretation of ODT instead of the usual approximation theoretical foundations, we formulate a very robust geometry and topology optimization of Bézier meshes based on a new simple functional promoting isotropic and uniform Jacobians throughout the domain. We demonstrate that our resulting curved meshes can adapt to complex domains with high precision even for a small count of elements thanks to the added flexibility afforded by more control points and higher order basis functions.

Joint work Leman Feng (ENPC), Pierre Alliez (EPI Titane), Hervé Delingette (EPI Asclepios) and Mathieu Desbrun (CalTech, USA),

# 6.13. Convolution surfaces with varying radius: Formulae for skeletons made of arcs of circles and line segments

Participants: Evelyne Hubert, Alvaro Javier Fuentes Suárez.

In [19], we develop closed form formulae for the computation of the defining fields of convolutions surfaces. The formulae are obtained for power inverse kernels with skeletons made of line segments or arcs of circle. To obtain the formulae we use Creative Telescoping and describe how this technique can be used for other families of kernels and skeleton primitives. We apply the new formulae to obtain convolution surfaces around  $G^1$  skeletons, some of them closed curves. We showcase how the use of arcs of circles greatly improves the visualization of the surface around a general curve compared with a segment based approach.

### 6.14. Scaffolding a Skeleton with Quadrangular Tubes

Participant: Evelyne Hubert.

The goal of [22] is to construct a quadrilateral mesh around a one-dimensional skeleton that is as coarse as possible, the "scaffold". A skeleton allows one to quickly describe a shape, in particular a complex shape of high genus. The constructed scaffold is then a potential support for the surface representation: it provides a topology for the mesh, a domain for parametric representation (a quad mesh is ideal for tensor product splines) or, together with the skeleton, a grid support on which to project an implicit surface that is naturally defined by the skeleton through convolution. We provide a constructive algorithm to derive a quad-mesh scaffold with topologically regular cross-sections (which are also quads), and no T-junctions. We show that this construction is optimal in the sense that no coarser quad mesh with topologically regular cross-sections may be constructed. Finally, we apply an existing rotation minimization algorithm along the skeleton branches, which produces a mesh with a natural edge flow along the shape.

This is joint work with A. Panotopoulou (Dartmouth College), E. Ross (MESH consultants), K. Welker (University of Trier), G. Morin (Intitut de Recherche en Informatique de Toulouse).

# 6.15. Scaffolding skeletons using spherical Voronoi diagrams: feasibility, regularity and symmetry

Participants: Evelyne Hubert, Alvaro Javier Fuentes Suárez.

Given a skeleton made of line segments, in [7] we describe how to obtain a coarse quad mesh of a surface that encloses tightly the skeleton and follows its structure - the scaffold. We formalize as an Integer Linear Program the problem of constructing an optimal scaffold that minimizes the total number of quads on the mesh. We prove the feasibility of the Integer Linear Program for any skeleton. In particular we can generate these scaffolds for skeletons with cycles. We additionally show how to obtain regular scaffolds, i.e. with the same number of quad patches around each line segment, and symmetric scaffolds that respect the symmetries of the skeleton. An application to polygonization of skeleton-based implicit surfaces is also presented.

### 6.16. Exact conversion from Bézier tetrahedra to Bézier hexahedra

Participant: Bernard Mourrain.

Modeling and computing of trivariate parametric volumes is an important research topic in the field of threedimensional isogeometric analysis. In [13], we propose two kinds of exact conversion approaches from Bézier tetrahedra to Bézier hexahedra with the same degree by reparametrization technique. In the first method, a Bézier tetrahedron is converted into a degenerate Bézier hexahedron, and in the second approach, a nondegenerate Bézier tetrahedron is converted into four non-degenerate Bézier hexahedra. For the proposed methods, explicit formulae are given to compute the control points of the resulting tensor-product Bézier hexahedra. Furthermore, in the second method, we prove that tetrahedral spline solids with  $C^k$ -continuity can be converted into a set of tensor-product Bézier volumes with  $G^k$ -continuity. The proposed methods can be used for the volumetric data exchange problems between different trivariate spline representations in CAD/CAE. Several experimental results are presented to show the effectiveness of the proposed methods.

This is a joint work with Gang Xu (Hanghzou, China), Yaoli Jin (Hanghzou, China), Zhoufang Xiao (Hanghzou, China), Qing Wu (Hanghzou, China), Timon Rabczuk (Weimar, Germany).

# 6.17. Constructing IGA-suitable planar parameterization from complex CAD boundary by domain partition and global/local optimization

### Participant: Bernard Mourrain.

In the paper [14], we propose a general framework for constructing IGA-suitable planar B-spline parameterizations from given complex CAD boundaries. Instead of the computational domain bounded by four B-spline curves, planar domains with high genus and more complex boundary curves are considered. Firstly, some pre-processing operations including Bézier extraction and subdivision are performed on each boundary curve in order to generate a high-quality planar parameterization; then a robust planar domain partition framework is proposed to construct high-quality patch-meshing results with few singularities from the discrete boundary formed by connecting the end points of the resulting boundary segments. After the topology information generation of quadrilateral decomposition, the optimal placement of interior Bézier curves corresponding to the interior edges of the quadrangulation is constructed by a global optimization method to achieve a patch-partition with high quality. Finally, after the imposition of  $C^1/G^1$ -continuity constraints on the interface of neighboring Bézier patches with respect to each quad in the quadrangulation, the highquality Bézier patch parameterization is obtained by a local optimization method to achieve uniform and orthogonal iso-parametric structures while keeping the continuity conditions between patches. The efficiency and robustness of the proposed method are demonstrated by several examples which are compared to results obtained by the skeleton-based parameterization approach.

This is a joint work with Gang Xu (Hanghzou, China), Ming Li (Zhejiang, China), Timon Rabczuk (Weimar, Germany), Jinlan Xu (Hangzhou, China), Stéphane P.A. Bordas (Luxembourg).

### 6.18. A Classification Approach to Efficient Global Optimization in Presence of Non-Computable Domains

### Participant: Elisa Berrini.

Gaussian-Process based optimization methods have become very popular in recent years for the global optimization of complex systems with high computational costs. These methods rely on the sequential construction of a statistical surrogate model, using a training set of computed objective function values, which is refined according to a prescribed infilling strategy. However, this sequential optimization procedure can stop prematurely if the objective function cannot be computed at a proposed point. Such a situation can occur when the search space encompasses design points corresponding to an unphysical configuration, an ill-posed problem, or a non-computable problem due to the limitation of numerical solvers. To avoid such a premature stop in the optimization procedure, we propose in [11] to use a classification model to learn non-computable areas and to adapt the infilling strategy accordingly. Specifically, the proposed method splits the training set into two subsets composed of computable and non-computable points. A surrogate model for the objective function is built using the training set of computable points, only, whereas a probabilistic classification model is built using the union of the computable and non-computable training sets. The classifier is then incorporated in the surrogate-based optimization procedure to avoid proposing new points in the non-computable domain while improving the classification uncertainty if needed. The method has the advantage to automatically adapt both the surrogate of the objective function and the classifier during the iterative optimization process. Therefore, non-computable areas do not need to be a priori known. The proposed method is applied to several analytical problems presenting different types of difficulty, and to the optimization of a fully nonlinear fluidstructure interaction system. The latter problem concerns the drag minimization of a flexible hydrofoil with cavitation constraints. The efficiency of the proposed method compared favorably to a reference evolutionary algorithm, except for situations where the feasible domain is a small portion of the design space.

This is joint work with Matthieu Sacher (IRENAV), Régis Duvigneau (ACUMES), Olivier Le Maitre (LIMSI), Mathieu Durand (K-Epsilon), Frédéric Hauville (IRENAV), Jacques-André Astolfi (IRENAV).

### 6.19. Compressions of a polycarbonate honeycomb

Participant: André Galligo.

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In [21], the in-plane compressive response of a polycarbonate honeycomb with circular close-packed cells is considered first experimentally then analytically. Under quasi-static uniaxial compression, we observed behaviors strongly depending on the orientation: for one of the two main orientations the compression is homogeneous, while for the other the deformation localizes in a very narrow band of cells. More surprisingly, for not crushing but extreme compression, when the load is released, the deformation is reversed, the localization disappears and the polycarbonate returns to its original shape. In order to explain this strange phenomena, we develop a geometric model of this honeycomb together with an expression of the bending energy. We focus on a basic mechanical element made of an elastica triangle. We also compare our description with previous experimental studies and simulations made with similar material. Finally, to illustrate mathematically this type of behavior, we present a simple model for buckling deformations with two degrees of freedom.

This is a joint work with Jean Rajchenbach (LPMC, UCA) and Bernard Rousselet (JAD, UCA).

### 6.20. Modeling and Computation of a liquid-vapor bubble formation

Participant: André Galligo.

The Capillary Equation correctly predicts the curvature evolution and the length of a quasi-static vapour formation. It describes a two-phase interface as a smooth curve resulting from a balance of curvatures that are influenced by surface tension and hydrostatic pressures. The present work provides insight into the application of the Capillary Equation to the prediction of single nu-cleate site phase change phenomena. In an effort to progress towards an application of the Capillary Equation to boiling events, a procedure to generating a numerical solution, in which the computational expense is reduced, is reported in [20].

This is a joint work with Frédéric Lesage (LCPI, UCA), Sebastian Minjeaud (JAD, UCA).

### 6.21. Axl, a geometric modeler for semi-algebraic shapes

Participants: Emmanouil Christoforou, Bernard Mourrain.

In [17], we describe the algebraic-geometric modeling platform Axl, which provides tools for the manipulation, computation and visualisation of semi-algebraic models. This includes meshes, basic geometric objects such as spheres, cylinders, cones, ellipsoids, torus, piecewise polynomial parameterisations of curves, surfaces or volumes such as B-spline parameterisations, as well as algebraic curves and surfaces defined by polynomial equations. Moreover, Axl provides algorithms for processing these geometric representations, such as computing intersection loci (points, curves) of parametric models, singularities of algebraic curves or surfaces, certified topology of curves and surfaces, etc. We present its main features and describe its generic extension mechanism, which allows one to define new data types and new processes on the data, which benefit from automatic visualisation and interaction facilities. The application capacities of the software are illustrated by short descriptions of plugins on algebraic curves and surfaces and on splines for Isogeometric Analysis.

This is a joint work with Angelos Mantzaflaris (JKU, Austria), Julien Wintz (SED, Inria).

### **DATASHAPE Project-Team**

## 7. New Results

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

### 7.1.1. DTM-based filtrations

Participants: Frédéric Chazal, Marc Glisse, Raphaël Tinarrage.

In collaboration with H. Anai, Y. Ike, H. Inakoshi and Y. Umeda of Fujitsu.

Despite strong stability properties, the persistent homology of filtrations classically used in Topological Data Analysis, such as, e.g. the Čech or Vietoris-Rips filtrations, are very sensitive to the presence of outliers in the data from which they are computed. In this paper [33], we introduce and study a new family of filtrations, the DTM-filtrations, built on top of point clouds in the Euclidean space which are more robust to noise and outliers. The approach adopted in this work relies on the notion of distance-to-measure functions, and extends some previous work on the approximation of such functions.

### 7.1.2. Persistent Homology with Dimensionality Reduction: k-Distance vs Gaussian Kernels Participants: Shreya Arya, Jean-Daniel Boissonnat, Kunal Dutta.

We investigate the effectiveness of dimensionality reduction for computing the persistent homology for both kdistance and kernel distance [34]. For k-distance, we show that the standard Johnson-Lindenstrauss reduction preserves the k-distance, which preserves the persistent homology upto a  $(1 - \varepsilon)^{-1}$  factor with target dimension  $O(k \log n/\varepsilon^2)$ . We also prove a concentration inequality for sums of dependent chi-squared random variables, which, under some conditions, allows the persistent homology to be preserved in  $O(\log n/\varepsilon^2)$ dimensions. This answers an open question of Sheehy. For Gaussian kernels, we show that the standard Johnson-Lindenstrauss reduction preserves the persistent homology up to an  $4(1 - \varepsilon)^{-1}$  factor.

### 7.1.3. Computing Persistent Homology of Flag Complexes via Strong Collapses Participants: Jean-Daniel Boissonnat, Siddharth Pritam.

### In collaboration with Divyansh Pareek (Indian Institute of Technology Bombay, India)

We introduce a fast and memory efficient approach to compute the persistent homology (PH) of a sequence of simplicial complexes. The basic idea is to simplify the complexes of the input sequence by using strong collapses, as introduced by J. Barmak and E. Miniam [DCG (2012)], and to compute the PH of an induced sequence of reduced simplicial complexes that has the same PH as the initial one. Our approach has several salient features that distinguishes it from previous work. It is not limited to filtrations (i.e. sequences of nested simplicial complexes) but works for other types of sequences like towers and zigzags. To strong collapse a simplicial complex, we only need to store the maximal simplices of the complex, not the full set of all its simplices, which saves a lot of space and time. Moreover, the complexes in the sequence can be strong collapsed independently and in parallel. Finally, we can compromize between precision and time by choosing the number of simplicial complexes of the sequence we strong collapse. As a result and as demonstrated by numerous experiments on publicly available data sets, our approach is extremely fast and memory efficient in practice [27].

### 7.1.4. Strong Collapse for Persistence

Participants: Jean-Daniel Boissonnat, Siddharth Pritam.

In this paper, we build on the initial success of and show that further decisive progress can be obtained if one restricts the family of simplicial complexes to flag complexes. Flag complexes are fully characterized by their graph (or 1-skeleton), the other faces being obtained by computing the cliques of the graph. Hence, a flag complex can be represented by its graph, which is a very compact representation. Flag complexes are very popular and, in particular, Vietoris-Rips complexes are by far the most widely simplicial complexes used in Topological Data Analysis. It has been shown in that the persistent homology of Vietoris-Rips filtrations can be computed very efficiently using strong collapses. However, most of the time was devoted to computing the maximal cliques of the complex prior to their strong collapse. In this paper [37], we observe that the reduced complex obtained by strong collapsing a flag complex is itself a flag complex, not the set of its maximal cliques. Finally, we show how to compute the equivalent filtration of the sequence of reduced flag simplicial complexes using again only 1-skeletons. x On the theory side, we show that strong collapses of flag complexes can be computed in time  $O(v^2k^2)$  where v is the number of vertices of the complex and k the maximal degree of its graph. The algorithm described in this paper has been implemented and the code will be soon released in the Gudhi library. Numerous experiments show that our method outperforms previous methods, e.g. Ripser.

### 7.1.5. Triangulating submanifolds: An elementary and quantified version of Whitney's method Participants: Jean-Daniel Boissonnat, Siargey Kachanovich, Mathijs Wintraecken.

We quantize Whitney's construction to prove the existence of a triangulation for any  $C^2$  manifold, so that we get an algorithm with explicit bounds. We also give a new elementary proof, which is completely geometric [36].

### 7.1.6. Randomized incremental construction of Delaunay triangulations of nice point sets Participants: Jean-Daniel Boissonnat, Kunal Dutta, Marc Glisse.

In collaboration with Olivier Devillers (Inria, CNRS, Loria, Université de Lorraine).

*Randomized incremental construction* (RIC) is one of the most important paradigms for building geometric data structures. Clarkson and Shor developed a general theory that led to numerous algorithms that are both simple and efficient in theory and in practice.

Randomized incremental constructions are most of the time space and time optimal in the worst-case, as exemplified by the construction of convex hulls, Delaunay triangulations and arrangements of line segments.

However, the worst-case scenario occurs rarely in practice and we would like to understand how RIC behaves when the input is nice in the sense that the associated output is significantly smaller than in the worst-case. For example, it is known that the Delaunay triangulations of nicely distributed points in  $\mathbb{R}^d$  or on polyhedral surfaces in  $\mathbb{R}^3$  has linear complexity, as opposed to a worst-case complexity of  $\Theta(n^{\lfloor d/2 \rfloor})$  in the first case and quadratic in the second. The standard analysis does not provide accurate bounds on the complexity of such cases and we aim at establishing such bounds in this paper [35]. More precisely, we will show that, in the two cases above and variants of them, the complexity of the usual RIC is  $O(n \log n)$ , which is optimal. In other words, without any modification, RIC nicely adapts to good cases of practical value.

Along the way, we prove a probabilistic lemma for sampling without replacement, which may be of independent interest.

### 7.1.7. Approximate Polytope Membership Queries

Participant: Guilherme Da Fonseca.

In collaboration with Sunil Arya (Hong Kong University of Science and Technology) and David Mount (University of Maryland).

In the polytope membership problem, a convex polytope K in  $\mathbb{R}^d$  is given, and the objective is to preprocess K into a data structure so that, given any query point  $q \in \mathbb{R}^d$ , it is possible to determine efficiently whether  $q \in K$ . We consider this problem in an approximate setting. Given an approximation parameter  $\epsilon$ , the query can be answered either way if the distance from q to K's boundary is at most  $\epsilon$  times K's diameter. We assume that the dimension d is fixed, and K is presented as the intersection of n halfspaces. Previous solutions to approximate polytope membership were based on straightforward applications of classic polytope approximation techniques by Dudley (1974) and Bentley et al. (1982). The former is optimal in the worstcase with respect to space, and the latter is optimal with respect to query time. We present four main results. First, we show how to combine the two above techniques to obtain a simple space-time trade-off. Second, we present an algorithm that dramatically improves this trade-off. In particular, for any constant  $\alpha \ge 4$ , this data structure achieves query time roughly  $O(1/\epsilon^{(d-1)/\alpha})$  and space roughly  $O(1/\epsilon^{(d-1)(1-\Omega(\log \alpha))/\alpha})$ . We do not know whether this space bound is tight, but our third result shows that there is a convex body such that our algorithm achieves a space of at least  $\Omega(1/\epsilon^{(d-1)(1-O(\sqrt{\alpha}))/\alpha})$ . Our fourth result shows that it is possible to reduce approximate Euclidean nearest neighbor searching to approximate polytope membership queries. Combined with the above results, this provides significant improvements to the best known space-time tradeoffs for approximate nearest neighbor searching in  $\mathbb{R}^d$ . For example, we show that it is possible to achieve a query time of roughly  $O(\log n + 1/\epsilon^{d/4})$  with space roughly  $O(n/\epsilon^{d/4})$ , thus reducing by half the exponent in the space bound [11].

### 7.1.8. Approximate Convex Intersection Detection with Applications to Width and Minkowski Sums

Participant: Guilherme Da Fonseca.

In collaboration with Sunil Arya (Hong Kong University of Science and Technology) and David Mount (University of Maryland).

Approximation problems involving a single convex body in d-dimensional space have received a great deal of attention in the computational geometry community. In contrast, works involving multiple convex bodies are generally limited to dimensions  $d \leq 3$  and/or do not consider approximation. In this paper, we consider approximations to two natural problems involving multiple convex bodies: detecting whether two polytopes intersect and computing their Minkowski sum. Given an approximation parameter  $\epsilon > 0$ , we show how to independently preprocess two polytopes A, B into data structures of size  $O(1/\epsilon^{(d-1)/2})$  such that we can answer in polylogarithmic time whether A and B intersect approximately. More generally, we can answer this for the images of A and B under affine transformations. Next, we show how to  $\epsilon$ -approximate the Minkowski sum of two given polytopes defined as the intersection of n halfspaces in  $O(n \log (1/\epsilon) + 1/\epsilon^{(d-1)/2+\alpha})$  time, for any constant  $\alpha > 0$ . Finally, we present a surprising impact of these results to a well studied problem that considers a single convex body. We show how to  $\epsilon$ -approximate the width of a set of n points in  $O(n \log (1/\epsilon) + 1/\epsilon^{(d-1)/2+\alpha})$  time, for any constant  $\alpha > 0$ , a major improvement over the previous bound of roughly  $O(n + 1/\epsilon^{d-1})$  time, for any constant  $\alpha > 0$ .

### 7.1.9. Approximating the Spectrum of a Graph

Participant: David Cohen-Steiner.

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

The spectrum of a network or graph G = (V, E) with adjacency matrix A, consists of the eigenvalues of the normalized Laplacian  $L = I - D^{-1/2}AD^{-1/2}$ . This set of eigenvalues encapsulates many aspects of the structure of the graph, including the extent to which the graph posses community structures at multiple scales. We study the problem of approximating the spectrum,  $\lambda = (\lambda_1, \dots, \lambda_{|V|})$ , 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  $\tilde{\lambda} = (\tilde{\lambda}_1, \dots, \tilde{\lambda}_{|V|})$ , such that  $\|\tilde{\lambda} - \lambda\|_1 \le \varepsilon |V|$ . Our algorithm has query complexity and running time  $\exp(O(1/\varepsilon))$ , which is independent of the size of the graph, |V|. We demonstrate the practical viability of our algorithm on synthetically generated graphs, and 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. The spectra of these real-world networks reveal insights into the structural similarities and differences between them, illustrating the potential value of our algorithm for efficiently approximating the spectrum of large networks [29].

### 7.1.10. Spectral Properties of Radial Kernels and Clustering in High Dimensions

Participants: David Cohen-Steiner, Alba Chiara de Vitis.

In this paper [40], we study the spectrum and the eigenvectors of radial kernels for mixtures of distributions in  $\mathbb{R}^n$ . Our approach focuses on high dimensions and relies solely on the concentration properties of the components in the mixture. We give several results describing of the structure of kernel matrices for a sample drawn from such a mixture. Based on these results, we analyze the ability of kernel PCA to cluster high dimensional mixtures. In particular, we exhibit a specific kernel leading to a simple spectral algorithm for clustering mixtures with possibly common means but different covariance matrices. This algorithm will succeed if the angle between any two covariance matrices in the mixture (seen as vectors in  $\mathbb{R}^{n^2}$ ) is larger than  $\Omega(n^{-1/6} \log^{5/3} n)$ . In particular, the required angular separation tends to 0 as the dimension tends to infinity. To the best of our knowledge, this is the first polynomial time algorithm for clustering such mixtures beyond the Gaussian case.

### 7.1.11. Exact computation of the matching distance on 2-parameter persistence modules Participant: Steve Oudot.

### In collaboration with Michael Kerber (T.U. Graz) and Michael Lesnick (SUNY).

The matching distance is a pseudometric on multi-parameter persistence modules, defined in terms of the weighted bottleneck distance on the restriction of the modules to affine lines. It is known that this distance is stable in a reasonable sense, and can be efficiently approximated, which makes it a promising tool for practical applications. In [44] we show that in the 2-parameter setting, the matching distance can be computed exactly in polynomial time. Our approach subdivides the space of affine lines into regions, via a line arrangement. In each region, the matching distance restricts to a simple analytic function, whose maximum is easily computed. As a byproduct, our analysis establishes that the matching distance is a rational number, if the bigrades of the input modules are rational.

### 7.1.12. A Comparison Framework for Interleaved Persistence Modules

### Participant: Miroslav Kramár.

### In collaboration with Rachel Levanger (UPenn), Shaun Harker and Konstantin Mischaikow (Rutgers).

In [43], we present a generalization of the induced matching theorem of [1] and use it to prove a generalization of the algebraic stability theorem for R-indexed pointwise finite-dimensional persistence modules. Via numerous examples, we show how the generalized algebraic stability theorem enables the computation of rigorous error bounds in the space of persistence diagrams that go beyond the typical formulation in terms of bottleneck (or log bottleneck) distance.

### 7.1.13. Discrete Morse Theory for Computing Zigzag Persistence

Participant: Clément Maria.

In collaboration with Hannah Schreiber (Graz University of Technology, Austria)

We introduce a framework to simplify zigzag filtrations of general complexes using discrete Morse theory, in order to accelerate the computation of zigzag persistence. Zigzag persistence is a powerful algebraic generalization of persistent homology. However, its computation is much slower in practice, and the usual optimization techniques cannot be used to compute it. Our approach is different in that it preprocesses the filtration before computation. Using discrete Morse theory, we get a much smaller zigzag filtration with same persistence. The new filtration contains general complexes. We introduce new update procedures to modify on the fly the algebraic data (the zigzag persistence matrix) under the new combinatorial changes induced by the Morse reduction. Our approach is significantly faster in practice [45].

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

### 7.2.1. Robust Bregman Clustering

Participants: Claire Brécheteau, Clément Levrard.

### In collaboration with Aurélie Fischer (Université Paris-Diderot).

Using a trimming approach, in [38], we investigate a k-means type method based on Bregman divergences for clustering data possibly corrupted with clutter noise. The main interest of Bregman divergences is that the standard Lloyd algorithm adapts to these distortion measures, and they are well-suited for clustering data sampled according to mixture models from exponential families. We prove that there exists an optimal codebook, and that an empirically optimal codebook converges a.s. to an optimal codebook in the distortion sense. Moreover, we obtain the sub-Gaussian rate of convergence for k-means 1  $\sqrt{n}$  under mild tail assumptions. Also, we derive a Lloyd-type algorithm with a trimming parameter that can be selected from data according to some heuristic, and present some experimental results.

### 7.2.2. Statistical analysis and parameter selection for Mapper

Participants: Mathieu Carrière, Bertrand Michel, Steve Oudot.

In [15] 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.

### 7.2.3. A Fuzzy Clustering Algorithm for the Mode-Seeking Framework

### Participants: Thomas Bonis, Steve Oudot.

In [13] we propose a new soft clustering algorithm based on the mode-seeking framework. Given a point cloud in  $\mathbb{R}^d$ , we define regions of high density that we call cluster cores, then we implement a random walk on a neighborhood graph built on top of the data points. This random walk is designed in such a way that it is attracted by high-density regions, the intensity of the attraction being controlled by a temperature parameter  $\beta > 0$ . The membership of a point to a given cluster is then the probability for the random walk starting at this point to hit the corresponding cluster core before any other. While many properties of random walks (such as hitting times, commute distances, etc) are known to eventually encode purely local information when the number of data points grows to infinity, the regularization introduced by the use of cluster cores allows the output of our algorithm to converge to quantities involving the global structure of the underlying density function. Empirically, we show how the choice of  $\beta$  influences the behavior of our algorithm: for small values of  $\beta$  the result is really close to hard mode-seeking, while for values of  $\beta$  close to 1 the result is similar to the output of the (soft) spectral clustering. We also demonstrate the scalability of our approach experimentally.

### 7.2.4. Large Scale computation of Means and Clusters for Persistence Diagrams using Optimal Transport

Participants: Théo Lacombe, Steve Oudot.

#### In collaboration with Marco Cuturi (ENSAE).

Persistence diagrams (PDs) are at the core of topological data analysis. They provide succinct descriptors encoding the underlying topology of sophisticated data. PDs are backed-up by strong theoretical results regarding their stability and have been used in various learning contexts. However, they do not live in a space naturally endowed with a Hilbert structure where natural metrics are not even differentiable, thus not suited to optimization process. Therefore, basic statistical notions such as the barycenter of a finite sample of PDs are not properly defined. In [30] we provide a theoretically good and computationally tractable framework to estimate the barycenter of a set of persistence diagrams. This construction is based on the theory of Optimal Transport (OT) and endows the space of PDs with a metric inspired from regularized Wasserstein distances.

### 7.2.5. The k-PDTM : a coreset for robust geometric inference

Participants: Claire Brécheteau, Clément Levrard.

Analyzing the sub-level sets of the distance to a compact sub-manifold of  $\mathbb{R}^d$  is a common method in TDA to understand its topology. The distance to measure (DTM) was introduced by Chazal, Cohen-Steiner and Mérigot to face the non-robustness of the distance to a compact set to noise and outliers. This function makes possible the inference of the topology of a compact subset of  $\mathbb{R}^d$  from a noisy cloud of n points lying nearby in the Wasserstein sense. In practice, these sub-level sets may be computed using approximations of the DTM such as the q-witnessed distance or other power distance. These approaches lead eventually to compute the homology of unions of n growing balls, that might become intractable whenever n is large. To simultaneously face the two problems of large number of points and noise, we introduce in [39] the k-power distance to measure (k-PDTM). This new approximation of the distance to measure may be thought of as a k-coreset based approximation of the DTM. Its sublevel sets consist in union of k-balls, k << n, and this distance is also proved robust to noise. We assess the quality of this approximation for k possibly dramatically smaller than n, for instance k = n13 is proved to be optimal for 2-dimensional shapes. We also provide an algorithm to compute this k-PDTM.

### 7.2.6. The density of expected persistence diagrams and its kernel based estimation

Participants: Frédéric Chazal, Vincent Divol.

Persistence diagrams play a fundamental role in Topological Data Analysis where they are used as topological descriptors of filtrations built on top of data. They consist in discrete multisets of points in the plane  $\mathbb{R}^2$  that can equivalently be seen as discrete measures in  $\mathbb{R}^2$ . When the data come as a random point cloud, these discrete measures become random measures whose expectation is studied in this paper. In [28] we first show that for a wide class of filtrations, including the Čech and Rips-Vietoris filtrations, the expected persistence diagram, that is a deterministic measure on  $\mathbb{R}^2$ , has a density with respect to the Lebesgue measure. Second, building on the previous result we show that the persistence surface recently introduced by Adams et al can be seen as a kernel estimator of this density. We propose a cross-validation scheme for selecting an optimal bandwidth, which is proven to be a consistent procedure to estimate the density.

### 7.2.7. On the choice of weight functions for linear representations of persistence diagrams Participant: Vincent Divol.

### In collaboration with Wolfgang Polonik (UC Davis)

Persistence diagrams are efficient descriptors of the topology of a point cloud. As they do not naturally belong to a Hilbert space, standard statistical methods cannot be directly applied to them. Instead, feature maps (or representations) are commonly used for the analysis. A large class of feature maps, which we call linear, depends on some weight functions, the choice of which is a critical issue. An important criterion to choose a weight function is to ensure stability of the feature maps with respect to Wasserstein distances on diagrams. In [42], we improve known results on the stability of such maps, and extend it to general weight functions. We also address the choice of the weight function by considering an asymptotic setting; assume that  $X_n$  is an i.i.d. sample from a density on  $[0, 1]^d$ . For the Cech and Rips filtrations, we characterize the weight functions for which the corresponding feature maps converge as n approaches infinity, and by doing so, we prove laws

of large numbers for the total persistence of such diagrams. Both approaches lead to the same simple heuristic for tuning weight functions: if the data lies near a d-dimensional manifold, then a sensible choice of weight function is the persistence to the power  $\alpha$  with  $\alpha \ge d$ .

### 7.2.8. Estimating the Reach of a Manifold

Participants: Frédéric Chazal, Bertrand Michel.

In collaboration with E. Aamari (CNRS Paris 7), J.Kim, A. Rinaldo and L. Wasserman (Carnegie Mellon University).

Various problems in manifold estimation make use of a quantity called the reach, denoted by  $\tau_M$ , which is a measure of the regularity of the manifold. [32] is the first investigation into the problem of how to estimate the reach. First, 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  $\mathbb{X}_n$ ,  $\tau(\mathbb{X}_n)$  is showed to achieve uniform expected loss bounds over a  $\mathcal{C}^3$ -like model. Finally, we obtain upper and lower bounds on the minimax rate for estimating the reach.

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

Participants: Frédéric Chazal, Bertrand Michel.

In collaboration with B. Fasy (Univ. Montana) and F. Lecci, A. Rinaldo and L. Wasserman (Carnegie Mellon University).

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), introduced by Chazal et al. (2011), and the kernel distance, introduced by Phillips et al. (2014), are smooth functions that provide useful topological information but are robust to noise and outliers. Chazal et al. (2015) derived concentration bounds for DTM. Building on these results, in [16], we derive limiting distributions and confidence sets, and we propose a method for choosing tuning parameters.

### 7.3. Topological approach for multimodal data processing

### 7.3.1. Barcode Embeddings for Metric Graphs

Participants: Steve Oudot, Yitchzak Solomon.

Stable topological invariants are a cornerstone of persistence theory and applied topology, but their discriminative properties are often poorly-understood. In [46] we study a rich homology-based invariant first defined by Dey, Shi, and Wang, which we think of as embedding a metric graph in the barcode space. We prove that this invariant is locally injective on the space of metric graphs and globally injective on a GH-dense subset. Moreover, we define a new topology on MGraphs, which we call the fibered topology, for which the barcode transform is injective on a generic (open and dense) subset.

### 7.3.2. Inverse Problems in Topological Persistence: a Survey

Participants: Steve Oudot, Yitchzak Solomon.

In [47] we review the literature on inverse problems in topological persistence theory. The first half of the survey is concerned with the question of surjectivity, i.e. the existence of right inverses, and the second half focuses on injectivity, i.e. left inverses. Throughout, we highlight the tools and theorems that underlie these advances, and direct the reader's attention to open problems, both theoretical and applied.

### 7.4. Experimental research and software development

## 7.4.1. Activity recognition from stride detection: a machine learning approach based on geometric patterns and trajectory reconstruction.

Participants: Bertrand Beaufils, Frédéric Chazal, Bertrand Michel.

#### In collaboration with M. Grelet (Sysnav).

In [23] algorithm for activity recognition is proposed using inertial sensors worn on the ankle. This innovative approach based on geometric patterns uses a stride detector that 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. A technique inspired by Zero Velocity Update is used on the stride detection to compute the trajectory of the device. It allows to compute relevant features for the activity recognition learning task. Compared to most algorithms in the literature, this method does not use fixed-size sliding window that could be too short to provide enough information or too long and leads to overlapping issue when the window covers two different activities.

### 7.4.2. Dynamics of silo deformation under granular discharge

Participant: Miroslav Kramár.

### In collaboration with Claudia Colonnello.

In [17], we use Topological Data Analysis to study the post buckling behavior of laboratory scale cylindrical silos under gravity driven granular discharges. Thin walled silos buckle during the discharge if the initial height of the granular column is large enough. The deformation of the silo is reversible as long as the filling height does not exceed a critical value, Lc. Beyond this threshold the deformation becomes permanent and the silo often collapses. We study the dynamics of reversible and irreversible deformation processes, varying the initial filling height around Lc. We find that all reversible processes exhibit striking similarities and they alternate between regimes of slow and fast dynamics. The patterns that occur at the beginning of irreversible deformation processes are topologically very similar to those that arise during reversible processes. However, the dynamics of reversible processes is significantly different. In particular, the evolution of irreversible processes is much faster. This allows us to make an early prediction of the collapse of the silo based solely on observations of the deformation patterns.

### 7.4.3. Characterizing Granular Networks Using Topological Metrics

### Participant: Miroslav Kramár.

## In collaboration with Joshua Dijksman (Duke Physics), Lenka Kovalcinova and Lou Kondic (NJIT), Jie Ren (Merck Research Lab), Robert Behringer (Duke), and Konstantin Mischaikow (Rutgers).

In [18], we carry out a direct comparison of experimental and numerical realizations of the exact same granular system as it undergoes shear jamming. We adjust the numerical methods used to optimally represent the experimental settings and outcomes up to microscopic contact force dynamics. Measures presented here range form microscopic, through mesoscopic to system-wide characteristics of the system. Topological properties of the mesoscopic force networks provide a key link between mi-cro and macro scales. We report two main findings: the number of particles in the packing that have at least two contacts is a good predictor for the mechanical state of the system, regardless of strain history and packing density. All measures explored in both experiments and numerics, including stress tensor derived measures and contact numbers depend in a universal manner on the fraction of non-rattler particles, fNR. The force network topology also tends to show this universality, yet the shape of the master curve depends much more on the details of the numerical simulations. In particular we show that adding force noise to the numerical data set can significantly alter the topological features in the data. We conclude that both fNR and topological metrics are useful measures to consider when quantifying the state of a granular system.

### 7.5. Miscellaneous

### 7.5.1. On Order Types of Random Point Sets

Participant: Marc Glisse.

## In collaboration with Olivier Devillers and Xavier Goaoc (Inria team Gamble) and Philippe Duchon (LaBRI, Université de Bordeaux).

Let P be a set of n random points chosen uniformly in the unit square. In this paper [41], we examine the typical resolution of the order type of P. First, we show that with high probability, P can be rounded to the grid of step  $\frac{1}{n^{3+\epsilon}}$  without changing its order type. Second, we study algorithms for determining the order type of a point set in terms of the number of coordinate bits they require to know. We give an algorithm that requires on average  $4n \log_2 n + O(n)$  bits to determine the order type of P, and show that any algorithm requires at least  $4n \log_2 n - O(n \log \log n)$  bits. Both results extend to more general models of random point sets.

### **KAIROS Team**

### 7. New Results

### 7.1. Schedulability of CCSL specifications via SMT

Participants: Frédéric Mallet, Robert de Simone.

The full expressive power of the CCSL language makes it very complex, if not impossible, to also find good, or even optimal, schedules as results of solving the CCSL constraints. Nevertheless, important subclasses can be devised, or efficient heuristics can be attempted. The study of CCSL scheduling decidability and efficient is a long-term source of theoretical developments in the team, here is a record of this year advances, split in two parts.

We have made progress on the inherent complexity of finding a schedule with a general CCSL specification. We have proved that the schedulability problem of CCSL is NP-hard. Then it makes sense to find whether there are still some practical ways to find solutions in specific cases. It turns out that in many cases, we can still find solutions in a reasonable duration. To do so, we have proposed [8] an encoding of CCSL specifications as an SMT (Satisfiability Modulo Theory) specification and we use Z3 and CVC4 as solvers for our experiments. Using a pure SAT solver is not possible for CCSL, as CCSL combines Boolean operations with arithmetics on unbounded integers. Using SMT allows to combine both. This encoding uses a sublogic called UFLIA that relies on quantified variables (boolean or integer), undefined functions on boolean and integers, and linear integer arithmetics. This logics is undecidable in the general case and the use of quantified variables makes it difficult to deal with, but we have found some interesting examples where we still get some results in a reasonable amount of time. We have also tried to identify subdomains where we get interesting results and we have focused on pure real-time schedulability problems. In that context, we showed that the schedulability problem for a set of real-time tasks reduces to the schedulability problem of CCSL specifications with a specific form (to be published).

The Clock Constraint Specification Language (CCSL) is a clock-based specification language for capturing causal and chronometric constraints between events in Real-Time Embedded Systems (RTESs). Due to the limitations of the existing verification approaches, CCSL lacks a full verification support for 'unsafe CCSL specifications' and a unified proof framework. In this paper [18], we propose a novel verification approach based on theorem proving and SMT-checking. We firstly build a logic called CCSL Dynamic Logic (CDL), which extends the traditional dynamic logic with 'signals' and 'clock relations' as primitives, and with synchronous execution mechanism for modelling RTESs. Then we propose a sound and relatively complete proof system for CDL to provide the verification support. We show how CDL can be used to capture RTES and verify CCSL specifications by analyzing a simple case study.

### 7.2. Logical Time for the semantics of Reactive Languages

Participants: Frédéric Mallet, Robert de Simone.

This work was initiated during the sabbatical period of Reihard von Hanxleden, on leave from the University of Kiel (Germany), funded by the the UMR I3S laboratory.

The results won Best Paper Award at the Federated Design Languages (FDL) conference edition of 2018 [16]. The paper abstract follows:

Synchronous languages, such as the recently proposed SCCharts language, have been designed for the rigorous specification of real-time systems. Their sound semantics, which builds on an abstraction from physical execution time, make these languages appealing, in particular for safety-critical systems. However, they traditionally lack built-in support for physical time. This makes it rather cumbersome to express things like time-outs or periodic executions within the language. We here propose several mechanisms to reconcile the synchronous paradigm with physical time. Specifically, we propose extensions to the SCCharts language to express clocks and execution periods within the model. We draw on several sources, in particular timed automata, the Clock Constraint Specification Language, and the recently proposed concept of dynamic ticks. We illustrate how these extensions can be mapped to the SCChart language core, with minimal requirements on the run-time system, and we argue that the same concepts could be applied to other synchronous languages such as Esterel, Lustre or SCADE.

### 7.3. Dealing with uncertainty in logical time

Participants: Frédéric Mallet, Robert de Simone.

When uplifting the target of models to heterogeneous Cyber-Physical Systems, the relations from physical time (which governs Physical components) to logical time becomes an issue for proper abstraction in the design. Often, the other engineering discipline may know of "proto-logical" timing abstraction, but involving probabilistic/stochastic ingredients to link the declared logical clocks/events. As a results, several attempts have been made at extending the language to allow perceptive probabilistic structuring operators, that may link (unreachable) physical rhythms with their discretized, manageable counter-parts. Of course the feasibility of constraint solving remains the key issue for allowing extensions scarcely. Nevertheless, it should be noted that the focus on relevancy of relations between physical and logical times may in some case be an important concerns for non-IT scientists.

The reports on how early attempts can be found in [6], [10], [12]. The topic is far from closed, but as such these are valuable starts.

In the future, we plan to exploit these model extensions on practical application fields, including car trajectory computation with Renault Software Lab, security properties "with Time"in the ILP SPAI with other Inria teams, and micro-satellites in the ATIPPIC IRT Saint-Exupery project with Thales Alenia Space.

### 7.4. Behavioral semantics and equivalence notions for Open Systems

Participants: Eric Madelaine, Tengfei Li, Zechen Hou.

Model-Based Design naturally implies model transformations. To be proven correct, they require equivalence of "Open" terms, in which some individual component models may be omitted. Such models take into account various kind of data parameters, including, but not limited to, time. The middle term goal is to build a formal framework, but also an effective tool set, for the compositional analysis of such programs. Following last year results we have published an experience paper [23] showing the applicability of this approach to show properties of a piece of the control software of a nano-satellite, specified using BIP architectures. Our work now turns on designing specific symbolic algorithms for model checking and equivalence checking (bisimulation) of such open systems, and also, as a specific application domain, to formalize the encoding of BIP architecture, extended with data constraints, into open pNets, aiming at a full approach for compositional verification of such systems. This work is done in collaboration with researchers from ENS Lyon and Inria Lille, and from ECNU Shanghai [23].

### 7.5. Logical Time for Safety Analysis and dependability

Participants: Paul Bouche, Amin Oueslati, Robert de Simone.

We have studied in the past the relevance of Logical Time for modeling of dynamic Non-Functional Properties (NFP) aspects of functional applications and/or execution platforms. In this setting, any recurring events may be seen as generating its own "rythm", as a logical clock. The most obvious NFP aspects to consider were performance and power consumption, as important concerns of Real-Time Embedded systems. Recently we have turned towards fault tolerance and availability/dependability aspects. This was motivated by demands from industrial partners inside IRT Saint-Exupery, who tried to design in real terms the digital computing structure of micro-satellites using ordinary processor components from the Shelf (COTS), extremely sensible to solar radiations (creatings faults). We have put up a full model-based design of the proposed use case, which includes modeling of the fault-tolerant features, but also the independent modeling of waterfall propagation schemes from incidental faults to fully recognized dysfunctions, where the system is no longer operational. Current results are encouraging, as they build up natural specification styles using logical time on top of existing formalisms such as AltaRica, widely used in industry. Methodological advances are proposed to industrial partners in IRT Saint-Exupery, and primarily Thales Alenia Space. We plan to comfort our approach next year with dedicated tools for modeling and analysis, as well as translation towards existing formalisms such as AltaRica, seen as lower level in our context.

### 7.6. Co-Simulation of Cyber-Physical Systems

Participants: Julien Deantoni, Giovanni Liboni, Robert de Simone.

While we continued to study and envision the past, present and future of co-simulation in [11], we already obtained promising results. In [14], we highlighted the current problems of the FMI co-simulation standards and more generally of existing coordination between actors of the co-simulation. We also shown that providing appropriate mean to communicate with the actors according to their internal semantics allows for dedicated coordinator providing better results than existing ones (speed up can reach 25 with a perfect accuracy). As shown in [14], the functional correctness of co-simulation can be violated by a non appropriate coordination of co-simulation actors. To avoid such phenomenon, we explored in [17] the possibility to formally prove the correctness of a coordinator according to properties defined by the actors. This last work is greatly exploratory but Julien Deantoni did a Short Term Scientific Mission (in the context of the MPM4CPS cost action <sup>0</sup>) in the MSDL Lab in Antwerp to understand more deeply the problem and potential solutions. Preliminary interesting results have been obtained <sup>0</sup> and may be published in 2019.

### 7.7. Early Interconnect Contention Analysis

Participants: Amin Oueslati, Julien Deantoni.

In the context of the Atippic project, industrial partners are using the Capella system engineering language (http://polarsys.org/capella) to migrate a satellite control software on a totally new architecture platform based on "COTS" dual core processors. In order to better deal with the potential contention on the interconnect between the different cores, it was required to help for contention analysis. In this context and based on one of our software (GEMOC Studio: http://eclipse.org/gemoc) we developed an executable extension to Capella, from which simulation of Capella model can be used to obtain bus latency and bandwidth.

We are currently extending this simulation approach to ease Design Space Exploration based on variation of some parameters (typically parameters of the tasks that create traffic like for instance, periods or consumed/produced data size). First results have already been demonstrated to the IRT Saint-Exupery and should be published early 2019.

### 7.8. Process network models with explicit data size handling

Participants: Amin Oueslati, Robert de Simone.

<sup>&</sup>lt;sup>0</sup>http://mpm4cps.eu/

<sup>&</sup>lt;sup>0</sup>http://mpm4cps.eu/STSM/reports/material/STSM\_DeantoniJulien\_Report\_527.pdf

We concluded our activities in the definition of a process network, inspired from established formalisms such as Ptolemy's SDF, StreaMIT, and Thales Array-OL task graph languages. Our next formalisms described accurately how regular data structures (2-dimensional arrays or matrices mostly) get assembled or deassembled in actual data-flow computations for streaming intensive data/signal processing. This allows to allocate these computations to similar dedicated architectures (GPUs, TPUs) while making all kinds of parallelism (data-, task-, streaming) explicit. The resulting forms of specification are intently very close to representations that may be expressed in OpenMP or MPI, and cover the important class of Deep Networks filter stream models, which have raised tremendous interest lately in Artificial Intelligence.

### **7.9.** Union and Intersection constraints

Participants: Luigi Liquori, Claude Stolze.

In [21], we introduced an explicitly typed  $\lambda$ -calculus with strong pairs, projections and explicit type coercions. The calculus can be parameterized with different intersection type theories, producing a family of calculi with related intersection typed systems. We proved the main properties like Church-Rosser, unicity of type, subject reduction, strong normalization, decidability of type checking and type reconstruction. We stated the relationship between the intersection type assignment systems and the corresponding intersection typed systems by means of an essence function translating an explicitly typed Delta-term into a pure  $\lambda$ -term one. We finally translated a term with type coercions into an equivalent one without them; the translation is proved to be coherent because its essence is the identity. The resulting generic calculus can be parametrized to take into account other intersection type theories as the ones in the Barendregt *et al.* book.

### 7.10. Logical frameworks with Union and Intersection constraints and Oracles

Participants: Luigi Liquori, Claude Stolze.

In [13], we introduced the  $\Delta$ -framework, DLF, a dependent type theory based on the Edinburgh Logical Framework LF, extended with the *strong proof-functional connectives*, i.e. strong intersection, minimal relevant implication and strong union. Strong proof-functional connectives take into account the shape of logical proofs, thus reflecting polymorphic features of proofs in formulæ. This is in contrast to classical or intuitionistic connectives where the meaning of a compound formula depends only on the truth value or the provability of its subformulæ. Our framework encompasses a wide range of type disciplines. Moreover, since relevant implication permits to express subtyping, DLF subsumes also Pfenning's refinement types. We discuss the design decisions which have led us to the formulation of DLF, study its metatheory, and provide various examples of applications. Our strong proof-functional type theory can be plugged in existing common interactive proof assistants.

Moreover, in [7], we introduced two further extensions of LF, featuring monadic *locks*. A lock is a monadic type construct that captures the effect of an *external call to an oracle*. The oracle can be invoked either to check that a constraint holds or to provide a suitable witness. Such calls are the basic tool for *plugging-in*, i.e. gluing together, different type theories and proof development environments.

### 7.11. Object reclassification

### Participant: Luigi Liquori.

In [19], we investigated, in the context of *functional prototype-based languages*, a calculus of objects which might extend themselves upon receiving a message, a capability referred to by Cardelli as a *self-inflicted* operation. We introduced a sound type system for this calculus which guarantees that evaluating a well-typed expression will never yield a *message-not-found* run-time error. The resulting calculus is an attempt towards the definition of a language combining the safety advantage of static type checking with the flexibility normally found in dynamically typed languages.

### 7.12. Object discovery

Participant: Luigi Liquori.

In [20], we proposed a Content Name System (CNS) discovery service, extending the current TCP/IP hourglass Internet architecture, that provides a new network aware content discovery service. Contents are addressed using "hypernames", whose rich syntax allow to specify hosts, PKI, fingerprint and optional logical attributes (tags) attached to the content name, such as e.g. mutable vs. immutable contents, digital signatures, owner, availability, price, etc. The CNS behavior and architecture is, partly, inspired by the Domain Name Service (DNS), and whose discovery process logic uses the Border Gateway Protocol (BGP) information allowing Internet to route between different Autonomous Systems (AS). The service registers and discovers object names in each Autonomous System (AS), and the content discovery process is inspired to the so called "valley-free" property. In the routing among different ASes (i.e., the BGP protocol) this is a property that avoids unjustified AS transit costs.

### 7.13. Code optimization for HPC and CPS programs

Participants: Sid Touati, Carsten Bruns, Robert de Simone.

Optimising HPC applications is a classical research area in computer science, complementary to intensive computation (which is an adjacent research community to HPC). Since decades, the most used languages are imperative ones (FORTRAN, C, etc). These languages are the closest to formal algorithms and low-level assembly codes. In intensive computing area, other kinds of languages and programming paradigms are used (interpreted languages for instance), but are far from HPC challenges, which tackle low level optimization (close to back-end compilation and processor micro-architectures).

We started a while ago to work on optimisation of HPC applications at C++ program level, where code and data are mixed in the same objects, allowing sophisticated programming methods that were not traditionally tackled in classical HPC programming (such as virtual classes, exception handling, etc). Currently, we are working on performance analysis and optimisation of linear algebra codes (BLAS) programmed with classes: this allows to extend BLAS computation to any kind of data (such as complex numbers) not only floating points. Our final aim is to apply and adjust this type of general C++ code optimization, to cover the spectrum of typical Kairos applications expressed from in C++ from high level formal specifications.

### **MARELLE Project-Team**

## 6. New Results

### 6.1. Extension language for Coq

**Participants:** Enrico Tassi, Feruccio Guidi [University of Bologna], Claudio Sacerdoti Coen [University of Bologna].

We continued our work on the design of a language mixing  $\lambda$ -prolog and constraint programming. This year, we redesigned and provided a new implementation of the constraint handling rules, leading to a first public release of the software. We are starting to have users beyond our own team:

- (Inria/Parsifal) MLTS https://github.com/voodoos/mlts
- (Inria/Parsifal) proofcert https://github.com/proofcert/checkers
- (UML.eu) Lang-n-play https://github.com/mcimini/lang-n-play

In an article submitted for publication [24], we showed that Elpi could be used to give a short implementation of Type Theory.

We are also starting a collaboration to construct an elaborator for HOL-Light using Elpi.

### 6.2. Deriving equality tests

Participant: Enrico Tassi.

In type theory, for most inductive types, it is possible to construct a two-argument boolean function that tests when two terms of the type are equal. When inductive types have constructors containing sub-components from another inductive, this needs to be done in a modular way. This year, we studied how this problem could be solved in a modular way using Elpi. It turns out that the unary parametricity translation can serve as a tool to make the derivation compositional. This is described in a pre-print [25].

### **6.3.** Parametricity proofs

**Participants:** Cyril Cohen, Abishek Anand [Cornell University], Simon Boulier [Inria Gallinette], Matthieu Sozeau [Inria Pi.r2], Nicolas Tabareau [Inria Gallinette], Robert Y. Lewis [Vrije Universiteit Amsterdam], Johannes Hölzl [CMU, Pittsburgh, USA and Vrije Universiteit, Amsterdam, the Netherlands].

After our previous experiment using Elpi to develop a tool that produces parametricity proofs, we investigated the use of the *Template-Coq* framework to implement this kind of algorithm. This work is described in [11]. A similar experiment has been performed using the Lean theorem prover.

### 6.4. Proving Expected Sensitivity of Probabilistic Programs

**Participants:** Benjamin Grégoire, Gilles Barthe [IMDEA], Thomas Espitau [UPMC Paris 6], Justin Hsu [University of Pennsylvania], Pierre-Yves Strub [Ecole Polytechnique].

Program sensitivity, also known as Lipschitz continuity, describes how small changes in a program's input lead to bounded changes in the output. We propose an average notion of program sensitivity for probabilistic programs—expected sensitivity—that averages a distance function over a probabilistic coupling of two output distributions from two similar inputs. This work is described in [8].

### 6.5. An Assertion-Based Program Logic for Probabilistic Programs

**Participants:** Benjamin Grégoire, Gilles Barthe [IMDEA], Thomas Espitau [UPMC Paris 6], Marco Gaboardi [University at Buffalo, SUNY], Justin Hsu [University of Pennsylvania], Pierre-Yves Strub [Ecole Polytechnique].

We have developed Ellora, a sound and relatively complete assertion-based program logic, and demonstrate its expressivity by verifying several classical examples of randomized algorithms using an implementation in the EasyCrypt proof assistant. Ellora features new proof rules for loops and adversarial code, and supports richer assertions than existing program logics. We also show that Ellora allows convenient reasoning about complex probabilistic concepts by developing a new program logic for probabilistic independence and distribution law, and then smoothly embedding it into Ellora. This is described in article [14].

### 6.6. Vectorizing Higher-Order Masking

**Participants:** Benjamin Grégoire, Kostas Papagiannopoulos [Radboud University], Peter Schwabe [Radboud University], Ko Stoffelen [Radboud University].

The cost of higher-order masking as a countermeasure against side-channel attacks is often considered too high for practical scenarios, as protected implementations become very slow. At Eurocrypt 2017, we have proposed the bounded moment leakage model to study the (theoretical) security of parallel implementations of masking schemes. In this work we show how the NEON vector instructions of larger ARM Cortex-A processors can be exploited to build much faster masked implementations of AES based on the bounded moment model. This work is described in publication [18].

### 6.7. Masking the GLP Lattice-Based Signature Scheme at Any Order

**Participants:** Benjamin Grégoire, Gilles Barthe [IMDEA], Sonia Belaïd [CryptoExpert], Thomas Espitau [UPMC Paris 6], Pierre-Alain Fouque [Université Rennes 1], Mélissa Rossi [ENS Paris], Mehdi Tibouchi [NTT].

Recently, numerous physical attacks have been demonstrated against lattice based schemes, often exploiting their unique properties such as the reliance on Gaussian distributions, rejection sampling and FFT-based polynomial multiplication. In this work, we describe the first masked implementation of a lattice-based signature scheme. Since masking Gaussian sampling and other procedures involving contrived probability distribution would be prohibitively inefficient, we focus on the GLP scheme. This work is described in [13].

### 6.8. Symbolic Proofs for Lattice-Based Cryptography

**Participants:** Benjamin Grégoire, Gilles Barthe [IMDEA], Xiong Fan [Cornell], Joshua Gancher [Cornell], Charlie Jacomme [LSV], Elaine Shi [Cornell].

Symbolic methods have been used extensively for proving security of cryptographic protocols in the Dolev-Yao model, and more recently for proving security of cryptographic primitives and constructions in the computational model. However, existing methods for proving security of cryptographic constructions in the computational model often require significant expertise and interaction, or are fairly limited in scope and expressivity. In this work we introduce a symbolic approach for proving security of cryptographic constructions based on the Learning With Errors assumption. This work is described in [15].

### 6.9. Formal Security Proof of CMAC and Its Variants

**Participants:** Benjamin Grégoire, Cécile Baritel-Ruet, François Dupressoir [University of Surrey], Pierre-Alain Fouque [Université Rennes 1].

The CMAC standard, when initially proposed by Iwata and Kurosawa as OMAC1, was equipped with a complex game-based security proof. Following recent advances in formal verification for game-based security proofs, we have formalized a proof of unforgeability for CMAC in EasyCrypt. This work is described in [12].

# 6.10. Secure Compilation of Side-Channel Countermeasures: The Case of Cryptographic "Constant-Time"

Participants: Benjamin Grégoire, Gilles Barthe [IMDEA], Vincent Laporte [IMDEA].

Software-based countermeasures provide effective mitigation against side-channel attacks, often with minimal efficiency and deployment overheads. Their effectiveness is often amenable to rigorous analysis: specifically, several popular countermeasures can be formalized as information flow policies, and correct implementation of the countermeasures can be verified with state-of-the-art analysis and verification techniques. However, in absence of further justification, the guarantees only hold for the language (source, target, or intermediate representation) on which the analysis is performed. We consider the problem of preserving side-channel counter-measures by compilation for cryptographic "constant-time", a popular countermeasure against cachebased timing attacks. We have presented a general method, based on the notion of constant-time-simulation, for proving that a compilation pass preserves the constant-time countermeasure. This work was described in [16]. At the conference, this work received the "distinguished paper" award.

### 6.11. Hypotheses of Decisional Diffie-Hellmann

Participants: Benjamin Grégoire, Mohamad El Laz, Tamara Rezk [Inria, Indes project team].

In the thesis work of Mohamad El Laz, co-supervised by Benjamin Grégoire and Tamara Rezk (Indes projectteam), we studied the cryptographic hypothesis of DDH (Decisional Diffie-Hellman) and implementations that would break this hypothesis. We focused on ElGamal encryption cryptosystem implementations to assess they use the DDH hypothesis correctly. We analyzed a number of implementations including Botan, Belenios and Libgcrypt. The lessons learned from this analysis are that the hypotheses are not always well understood.

In a second stage we considered message encoding methods. We investigated several approaches such as DCDH (Decisional Class Diffie-Hellman) in Encoding-Free ElGamal Encryption.

### 6.12. Proving the domain management protocol

**Participants:** José Bacelar Almeida [INESC TEC], Manuel Barbosa [INESC TEC], Gilles Barthe [IMDEA], Benjamin Grégoire, Vitor Pereira [INESC TEC], Bernardo Portela [INESC TEC], Benedikt Schmidt [Google Inc.], François-Xavier Standaert [Université Catholique de Louvain], Pierre-Yves Strub [Ecole Polytechnique].

We have performed a machine-checked proof of security for the domain management protocol of Amazon Web Services KMS (Key Management Service), a critical security service used throughout AWS and by AWS customers. Domain management is at the core of KMS; it governs the long-term keys that anchor the security of encryption services at AWS. Informally, we show that the protocol securely implements a distributed encryption mechanism. Formally, the proof shows that the domain management protocol is indistinguishable from an ideal encryption functionality under standard cryptographic assumptions.

### 6.13. Formalized graph theory algorithms

**Participants:** Cyril Cohen, Laurent Théry, Ran Chen [Chinese Academy of Science], Jean-Jacques Lévy [Inria Pi.r2], Stephan Merz [Inria Veridis].

We formalise the correctness proof of Tarjan's algorithm for computing strongly connected components using the Mathematical Component Library. This leads to a comparison of formalisation between various systems described in [22].

### 6.14. Formal study of a triangulation algorithm

Participant: Yves Bertot.

In work from 2010, a formal description of Delaunay triangulations was presented where the input was a triangulation not satisfying the Delaunay criterion and where the output was a triangulation satisfying this criterion.

In this work, we wish to complete the previous work by describing an algorithm that produces the initial triangulation. We plan this work in several phases, where the first phase only uses simple data-structures, more advanced structures being introduced only later. This work was presented partially in an invited talk at the ICTAC conference [10].

### 6.15. Formalizing Bourbaki-style mathematics

Participant: José Grimm.

Most of the work described here is inspired by the experiment of giving formal proofs in Coq of the exercises found in Bourbaki's exposition of set theory. However, some of the results go beyond what can be found in Bourbaki.

We implemented a paper of Sierpinski about properties of continuous ordinal functions and limits of such functions.

We implemented a paper on sums of sequences of ordinals, showing that the value obtained (which depends on the order) lies in a finite set. We also showed that this result does not hold when replacing ordinals by order types.

We implemented a paper by Tarski that says if every infinite cartinal is equal to its square, then every set can be well-ordered (this is the axiom of choice). We had to modify our library to make the use of the axiom of choice more explicit.

We continued implementing in Coq the Exercises of Set Theory of Bourbaki. We solved two of them, and proved by a counter example that three of them are false.

### 6.16. Formal study of double-word arithmetic algorithms

**Participants:** Laurence Rideau, Jean-Michel Muller [CNRS and ENS Lyon], Valentina Popescu [CNRS and ENS Lyon], Mioara Joldes [CNRS LAAS].

As part of the ANR Fastrelax project, we are formalizing double-word arithmetic algorithms, in particular the sum of a double-word and a floating point number and the sum of two double-word numbers described in the article " Tight and rigourous error bounds for basic building blocks of double-word arithmetic" [27]. The formalization is progressing, moving from addition to multiplication. The progress is slowed down because minor errors in the informal proofs are regularly uncovered, which requires a dialog with the initial authors.

### 6.17. Proofs of transcendence

Participants: Sophie Bernard, Yves Bertot, Laurence Rideau.

The work on proofs of transcendence that was started the previous year was completed this year by an effort to integrate generic part of the proofs in the Mathematical Components library. A public package for easy re-use by other researchers was also developed.

### 6.18. Abel's theorem

**Participants:** Sophie Bernard, Yves Bertot, Cyril Cohen, Laurence Rideau, Assia Mahboubi [Inria Gallinette], Russell O'Connor [McMaster University].

A natural extension of the work on group theory is a proof that polynomials of degree higher than 5 cannot be solved by radicals. This is known as Abel's theorem. We have started an experiment to give a formal proof of this result on top of the Mathematical Components library.

### 6.19. Formalizing Hermitian Forms

Participants: Cyril Cohen, Laurence Rideau.

We updated the representation and relevant theorems for bilinear, sesquilinear, and hermitian forms in the Mathematical Components library and updated the archived proof of the odd-order theorem (Feit-Thompson) to use the new presentation. This work also includes a proof of the Spectral Theorem.

### 6.20. Mathematical Components Analysis

**Participants:** Cyril Cohen, Damien Rouhling, Reynald Affeldt [AIST Japan], Assia Mahboubi [Inria Gallinette], Pierre-Yves Strub [Ecole Polytechnique].

As a synthesis of the lessons learned in the usage of Mathematical Components and Coquelicot, we develop an extension of the Mathematical Components library to cover questions of analysis. This work includes a new tactic called near to handle reasoning steps around limits and filters and little-o notation (following Landau's style of asymptotic reasoning). This work is described in [6]. There also contains a new formalization of topoligical structures, Rolle's theorem, the intermediate value theorem, and Heine Borel's theorem. Ongoing work concentrates on a better design of the topological hierarchy and a simplification of the properties expected from real numbers (following a design by A. Mahboubi and P.-Y. Strub).

Some of this work also includes experiments performed with the LEAN theorem prover (developed at Microsoft Research).

### 6.21. Rigorous Polynomial Approximation

Participants: Florian Steinberg, Laurent Théry.

We have developed a certified library for computing Chebyshev models for formulas composed of polynomials, exponential, logarithm, and trigonometric function. This work is part of the ANR project FastRelax. The code is available at https://github.com/FlorianSteinberg/Cheby

### 6.22. Formalization of proofs in control theory

Participants: Damien Rouhling, Cyril Cohen.

Damien Rouhling presented his work on formalizing control theory for an inverted pendulum at an international conference in January [19].

The original development was based on Coquelicot. An analysis of the difficulties in formalizing led to the design of Mathematical Components Analysis. The development on control was then ported to this new library. This work was presented at the Coq Workshop in July.

### 6.23. Formalizing Cylindrical Algebraic Decomposition

Participants: Boris Djalal, Yves Bertot, Cyril Cohen.

Our study of cylindrical algebraic decomposition requires that we find a good representation of semi-algebraic sets. An article on this topic was published [17]. This is also the one of the main topics of Boris Djalal's thesis, which was defended in December.

### 6.24. A type theory for Algebraic Structures

Participants: Cyril Cohen, Assia Mahboubi, Xavier Montillet.

In collaboration with members of the Inria Gallinette team, we are investigating the properties that a type theory should enjoy to support algebraic structures better than what is currently available.

### **ACUMES Project-Team**

## 7. New Results

### 7.1. Macroscopic traffic flow models on networks

**Participants:** Guillaume Costeseque, Nikodem Dymski, Paola Goatin, Nicolas Laurent-Brouty, Shuxia Tang, Yunzhi Wu, Alexandre Bayen [UC Berkeley, CA, USA], Alexander Keimer [UC Berkeley, CA, USA], Antonella Ferrara [U Pavia, Italy], Giulia Piacentini [U Pavia, Italy].

**The relaxation limit for ARZ model.** The Aw-Rascle-Zhang model [55], [157] can now be considered as a classical traffic flow model. In [27], we detail the mathematical behavior of the Aw-Rascle-Zhang model with relaxation [54]. In a Lagrangian setting, we use the Wave-Front-Tracking method with splitting technique to construct a sequence of approximate solutions. We prove that this sequence admits a limit. We then show that the limit is a weak entropy solution of the relaxed system associated to a given initial datum with bounded variation. Finally, we prove that this limit converges to a weak solution of the scalar conservation law when the relaxation parameter goes to zero.

**Bounded acceleration.** In [29], we propose a new mathematical model accounting for the boundedness of traffic acceleration at a macroscopic scale. Our model is built on a first order macroscopic PDE model coupled with an ODE describing the trajectory of the leader of a platoon accelerating at a given constant rate. We use Wave Front Tracking techniques to construct approximate solutions to the Initial Value Problem. We present some numerical examples including the case of successive traffic signals on an arterial road and we compare the solution to our model with the solution given by the classical LWR equation in order to evaluate the impact of bounded acceleration.

**Second order models with moving bottlenecks.** In [25], we study the Aw-Rascle-Zhang (ARZ) model with non-conservative local point constraint on the density flux introduced in [Garavello, M., and Goatin, P. The Aw-Rascle traffic model with locally constrained flow. Journal of Mathematical Analysis and Applications 378, 2 (2011), 634-648], its motivation being, for instance, the modeling of traffic across a toll gate. We prove the existence of weak solutions under assumptions that result to be more general than those required in [Garavello, M., and Villa, S. The Cauchy problem for the Aw-Rascle-Zhang traffic model with locally constrained flow. Journal of Hyperbolic Differential Equations 14, 03 (2017), 393-414]. More precisely, we do not require that the waves of the first characteristic family have strictly negative speeds of propagation. The result is achieved by showing the convergence of a sequence of approximate solutions constructed via the wave-front tracking algorithm. The case of solutions attaining values at the vacuum is considered. We also present an explicit numerical example to describe some qualitative features of the solutions.

**Traffic control by autonomous vehicles.** We consider the possibility of properly controlling a moving bottleneck to improve the traffic flow. The traffic is represented by means of a macroscopic model able to take into account the interactions with the bottleneck. This latter interacts with the surrounding flow modifying the traffic density and the flow speed profiles. An optimal control problem is stated by using the speed of the moving bottleneck as control variable. Specifically, in [30] the MPC (Model Predictive Control) approach is used to get a fuel consumption reduction when the traffic is congested due to the presence of a fixed bottleneck on the highway. In addition we have demonstrated that no increase of the travel time is caused by the control application. The concept illustrated in this paper suggests a future innovative traffic control approach. Indeed the prospective of exploiting special vehicles with manipulable speed to control the traffic flow is particularly attractive given the expected increasing penetration rate of autonomous vehicles in traffic networks in future years.

Well-posedness of conservation laws on networks with finite buffers. In collaboration with A. Bayen and A. Keimer (UC Berkeley), we introduce a model capable of dealing with conservation laws on networks and the coupled boundary conditions at the junctions. To that end we introduce a buffer of fixed arbitrary size and time dependent split ratios at the junctions which represent how traffic should be routed. One of the most important and interesting property of the presented model is its capability of showing spill-back phenomena over junctions. Having defined the dynamics on the level of conservation laws we lift them up to Hamilton Jacobi equations. The corresponding formulation in terms of H-J allows us to attack the problem that boundary datum of in and out-going junctions is a function of the queue size and vice versa. We do this by defining a fixed-point problem in a proper Banach space setting and prove the existence of a solution. Thus, the problem is solved on the level of Conservation laws with boundary datum in the sense of Bardos-Leroux-Nédélec.

Altogether, the system of conservation laws – locally coupled via the boundary conditions is studied for analytical questions of well-posedness, uniqueness and existence.

Finally we detail how to use this framework on a non-trivial road network, with several intersections and finite-length links.

**Minimum time boundary controls.** In collaboration with A. Bayen and A. Keimer (UC Berkeley), we are investigating the minimum time control problem for traffic flow. More precisely, we seek for the inflow upstream boundary condition that drives congested traffic to free flow condition on a stretch of road in minimum time.

**Big Data analysis and modeling of road Traffic.** Yunzhi Wu's internship, funded by Inria under the program "Transverse Actions", was co-supervised by Acumes (P. Goatin and G. Costeseque) and Zenith (F. Masseglia and R. Akbarinia). In this project, we processed the traffic data collected by loop detectors in the Mediterranean region during 3 months in 2015 (provided by DIRMED). We aimed at finding out the characteristics of traffic data and provide a new way of traffic prediction and estimation. The method of Motif Discovery was used for abnormality detection and pattern discovery. A modified method was also used for congestion prediction. Then we use the Co-Clustering method to group the data by day and loop. The clustering results were used to do a grouped calibration of fundamental diagram.

### 7.2. Non-local conservation laws

Participants: Felisia Angela Chiarello, Paola Goatin, Elena Rossi, Florent Berthelin [COFFEE, Inria].

F.A. Chiarello's PhD thesis focuses on non-local conservation laws. In [22], we proved the stability of entropy weak solutions, considering smooth kernels. We obtained an estimate on the dependence of the solution with respect to the kernel function, the speed and the initial datum, applying the doubling of variables technique. We also provided some numerical simulations illustrating the dependencies above for some cost functionals derived from traffic flow applications.

In the paper [21], we proved the existence for small times of weak solutions for a class of non-local systems in one space dimension, arising in traffic modeling. We approximated the problem by a Godunov type numerical scheme and we provided uniform  $L^{\infty}$  and BV estimates for the sequence of approximate solutions. We showed some numerical simulations illustrating the behavior of different classes of vehicles and we analyzed two cost functionals measuring the dependence of congestion on traffic composition.

We also conducted a study on Lagrangian-Antidiffusive Remap schemes (previously proposed for classical hyperbolic systems) for the above mentioned non-local multi-class traffic flow model. The error and convergence analysis show the effectiveness of the method, which is first order, in sharply capturing shock discontinuities, and better precision with respect to other methods as Lax-Friedrichs or Godunov (even 2nd order). A journal article about these results is submitted [40].

In the setting of Florent Berthelin's secondement, we studied the regularity properties of solutions of a nonlocal traffic model involving a convolution product. Unlike other studies, the considered kernel is discontinuous on  $\mathbb{R}$ . We proved Sobolev estimates and the convergence of approximate solutions solving a viscous and regularized non-local equation. It leads to weak,  $C([0,T], L^2(\mathbb{R}))$ , and smooth,  $W^{2,2N}([0,T] \times \mathbb{R})$ , solutions for the non-local traffic model [16].

### 7.3. Well-posedness results for Initial Boundary Value Problems

Participants: Paola Goatin, Elena Rossi.

We focused on the IBVP for a general scalar balance law in one space dimension and proved its well-posedness and the stability of its solutions with respect to variations in the flux and in the source terms. For both results, the initial and boundary data are required to be bounded functions with bounded total variations. The existence of solutions is obtained from the convergence of a Lax-Friedrichs type algorithm, while the stability follows from an application of Kruzkov's doubling of variables method [33].

Exploiting the same techniques, we focused also on a non local version of the scalar IBVP for a conservation law. The flux is indeed assumed to depend non locally on the unknown, and the non local operator is "aware of boundaries". For this non local problem, existence and uniqueness of solutions are provided. In particular, the uniqueness follows from the Lipschitz continuous dependence on initial and boundary data, which is proved exploiting the results on the local IBVP [43].

### 7.4. Isogeometric analysis

**Participants:** Régis Duvigneau, Stefano Pezzano, Maxime Stauffert, Asma Azaouzi [ENIT], Maher Moakher [ENIT].

High-order isogeometric solvers are developed, based on CAD representations for both the geometry and the solution space, for applications targeted by the team, in particular hyperbolic or convection-dominated problems. Specifically, we investigate a Discontinuous Galerkin method for hyperbolic systems such as compressible Euler, or Navier-Stokes equations, based on an isogeometric formulation[24]: the partial differential equations governing the flow are solved on rational parametric elements, that preserve exactly the geometry of boundaries defined by Non-Uniform Rational B-Splines (NURBS) thanks to Bézier extraction techniques, while the same rational approximation space is adopted for the solution.

This topic has been studied in the context of A. Azaouzi's PhD work defended in December 2018, in co-supervision with M. Moakher at ENIT. Current works concern local refinement strategies by splitting algorithms, the arbitrary Lagrangian-Eulerian formulation in the isogeometric context (PhD work of S. Pezzano) and high-order shape sensitivity analysis (Post-doc of M. Stauffert, PRE "GeoSim").

### 7.5. Sensitivity equation method for hyperbolic systems

Participants: Régis Duvigneau, Camilla Fiorini [UVST], Christophe Chalons [UVST].

While the sensitivity equation method is a common approach for parabolic systems, its use for hyperbolic ones is still tedious, because of the generation of discontinuities in the state solution, yielding Dirac distributions in the sensitivity solution. To overcome this difficulty, we investigate a modified sensitivity equation, that includes an additional source term when the state solution exhibits discontinuities, to avoid the generation of delta-peaks in the sensitivity solution. We consider as typical example the one-dimensional compressible Euler equations. Different approaches are tested to integrate the additional source term: a Roe solver, a Godunov method and a moving cells approach[18].

This study is achieved in collaboration with C. Chalons from University of Versailles, in the context of C. Fiorini's PhD work, defended in July 2018.

### 7.6. Classification algorithms in Bayesian optimization

**Participants:** Régis Duvigneau, Matthieu Sacher [Ecole Navale], Frédéric Hauville [Ecole Navale], Olivier Le Maître [CNRS-LIMSI].

A Gaussian-Process based optimization algorithm is proposed to efficiently determine the global optimum for expensive simulations, when some evaluations may fail, due to unrealistic configurations, solver crash, degenerated mesh, etc. The approach is based on coupling the classical Bayesian optimization method with a classification algorithm, to iteratively identify the regions where the probability of failure is high[35].

The method is applied to the optimization of foils and sails in the context of racing yachts[34], in particular for the America's Cup in collaboration with Groupama team. This work was part of M. Sacher's PhD work at Ecole Navale, defended in September 2018.

## 7.7. Solving with games the coupled problems of conductivity or obstacle identification and data recovery

**Participants:** Abderrahmane Habbal, Rabeb Chamekh [PhD, LAMSIN, Univ. Tunis Al Manar], Marwa Ouni [PhD, LAMSIN, Univ. Tunis Al Manar], Moez Kallel [LAMSIN, Univ. Tunis Al Manar], Nejib Zemzemi [Inria Bordeaux, EPI CARMEN].

We extend in two directions our previous successful attempts [112], [121] to tackle ill posed inverse problems as Nash games.

In a first direction, a Nash game algorithm is used for the solution of coupled conductivity identification and data completion in cardiac electrophysiology. In [19], we consider the identification problem of the conductivity coefficient for an elliptic operator using an incomplete over-specified measurements on the surface. We define three players with three corresponding criteria. The two first players use Dirichlet and Neumann strategies to solve the completion problem, while the third one uses the conductivity coefficient as strategy, and uses a cost which basically relies on an established identifiability theorem. The implemented algorithm is used for the electrocardiography ECG imaging inverse problem, dealing with inhomogeneities in the torso domain. The inverse problem of ECG consists in finding the electric potential distribution on the heart's surface given the one on the torso, so that it is a data completion problem. Furthermore, in our approach, the conductivity coefficients are known only by an approximate values. we conduct numerical experiments on a 2D torso case including noisy measurements. Results illustrate the ability of our computational approach to tackle the difficult problem of joint identification and data completion.

The second direction deals with Nash strategies for the inverse inclusion Cauchy-Stokes problem. We introduce in [44] a new algorithm to solve the problem of detecting unknown cavities immersed in a stationary viscous fluid, using partial boundary measurements. The considered fluid obeys a steady Stokes regime, the cavities are inclusions and the boundary measurements are a single compatible pair of Dirichlet and Neumann data, available only on a partial accessible part of the whole boundary. This inverse inclusion Cauchy-Stokes problem is ill-posed for both the cavities and missing data reconstructions, and designing stable and efficient algorithms is not straightforward. We reformulate the problem as a three-player Nash game. Thanks to an identifiability result derived for the Cauchy-Stokes inclusion problem, it is enough to set up two Stokes BVP, then use them as state equations. The Nash game is then set between 3 players, the two first targeting the data completion while the third one targets the inclusion detection. We used a level-set approach to get rid of the tricky control dependence of functional spaces, and we provided the third player with the level-set function as strategy, with a cost functional of Kohn-Vogelius type. We propose an original algorithm, which we implemented using Freefem++. We present 2D numerical experiments for three different test-cases. The obtained results corroborate the efficiency of our 3-player Nash game approach to solve parameter or shape identification for Cauchy problems.

### 7.8. The Kalai-Smorodinski solution for many-objective Bayesian optimization

Participants: Mickael Binois [Univ. Chicago], Victor Picheny [INRA, Toulouse], Abderrahmane Habbal.

Game theory finds nowadays a broad range of applications in engineering and machine learning. However, in a derivative-free, expensive black-box context, very few algorithmic solutions are available to find game equilibria. In [31], we propose a novel Gaussian-process based approach for solving games in this context. We follow a classical Bayesian optimization framework, with sequential sampling decisions based on acquisition functions. Two strategies are proposed, based either on the probability of achieving equilibrium or on the Stepwise Uncertainty Reduction paradigm. Practical and numerical aspects are discussed in order to enhance the scalability and reduce computation time. Our approach is evaluated on several synthetic game problems with varying number of players and decision space dimensions. We show that equilibria can be found reliably for a fraction of the cost (in terms of black-box evaluations) compared to classical, derivative-based algorithms.

Another ongoing scope of research in multi-objective Bayesian optimization is to extend its applicability to a large number of objectives : the so-called many-objective optimization. Regarding the harsh many-objective optimization problems, the recovering of the set of optimal compromise solution generally requires lots of observations while being less interpretable, since this set tends to grow larger with the number of objectives. We thus propose to focus on a choice of a specific solution originating from game theory, the Kalai-Smorodinsky solution, that possesses attractive properties. In particular, it ensures equal marginal gains over all objectives in the copula space. A novel tailored algorithm is proposed to search for the solution, in the form of a Bayesian optimization algorithm: sequential sampling decisions are made based on acquisition functions that derive from an instrumental GP prior. Our approach is tested on three problems with respectively four, six and ten objectives.

The Nash and Kalai-Smorodinsky methods are available in the R package GPGame available on CRAN at https://cran.r-project.org/package=GPGame.

### 7.9. Stochastic multiple gradient descent algorithm

**Participants:** Jean-Antoine Désidéri, Fabrice Poirion [ONERA Châtillon, Aeroelasticity and Structural Dynamics Dept.], Quentin Mercier [ONERA Châtillon, Aeroelasticity and Structural Dynamics Dept.].

We have proposed a new method for multi-objective optimization problems in which the objective functions are expressed as expectations of random functions. The present method is based on an extension of the classical stochastic gradient algorithm and a deterministic multi-objective algorithm, the Multiple Gradient Descent Algorithm (MGDA). In MGDA a descent direction common to all specified objective functions is identified through a result of convex geometry. The use of this common descent vector and the Pareto stationarity definition into the stochastic gradient algorithm makes the algorithm able to solve multi-objective problems. The mean square and almost sure convergence of this new algorithm are proven considering the classical stochastic gradient algorithm hypothesis. The algorithm efficiency is illustrated on a set of benchmarks with diverse complexity and assessed in comparison with two classical algorithms (NSGA-II, DMS) coupled with a Monte Carlo expectation estimator [129]

### 7.10. Non-convex multiobjective optimization under uncertainty

**Participants:** Jean-Antoine Désidéri, Fabrice Poirion [ONERA Châtillon, Aeroelasticity and Structural Dynamics Dept.], Quentin Mercier [ONERA Châtillon, Aeroelasticity and Structural Dynamics Dept.].

A novel algorithm for solving multi-objective design optimization problems with non-smooth objective functions and uncertain parameters is presented. The algorithm is based on the existence of a common descent vector for each sample of the random objective functions and on an extension of the stochastic gradient algorithm. The proposed algorithm is applied to the optimal design of sandwich material. Comparisons with the genetic algorithm NSGA-II and the DMS solver are given and show that it is numerically more efficient due to the fact that it does not necessitate the objective function expectation evaluation. It can moreover be entirely parallelized. Another simple illustration highlights its potential for solving general reliability problems, replacing each probability constraint by a new objective written in terms of an expectation. Moreover, for this last application, the proposed algorithm does not necessitate the computation of the (small) probability of failure [129].

### **ECUADOR Project-Team**

## 6. New Results

### 6.1. Towards Algorithmic Differentiation of C++

Participants: Laurent Hascoët, Valérie Pascual, Frederic Cazals [ABS team, Inria Sophia-Antipolis].

We made progress towards the extension of Tapenade for C++. Last year, an external parser for C++ was built on top of Clang-LLVM https://clang.llvm.org/ and connected to the input formalism "IL" of Tapenade, but the internals of Tapenade were not able to handle the new constructs present in this input. This year, integration of C++ was pushed further by taking into account many of the new constructs (namespaces, classes, constructors and destructors) in the Internal Representation(IR) of Tapenade. Not surprisingly, this implied deep changes in several areas of Tapenade code. The IR of Tapenade now contains classes, constructors and destructors, and also has a faithful representation for namespaces. The textual nested structure and the control-flow parts of the IR are correct. The symbol tables and the representation for memory locations are still under development.

As a result, Tapenade is now able to input its first C++ files and is able to output them, but without transformation. Although not advertised nor documented, the functionality is present in the latest release 3.14. Data-Flow analysis and code transformation (e.g. AD) will not be possible until we have a correct IR about variables and their memory locations. This work is going on.

This work benefited from the expertise in C++ of Frederic Cazals (Inria ABS team). The ABS team provided a large test application code (SBL, https://sbl.inria.fr/) for Molecular Dynamics, which will be our first C++ target.

### 6.2. AD of mixed-language codes

Participants: Valérie Pascual, Laurent Hascoët.

Last year Tapenade was extended to differentiate codes that mix different languages, beginning with the tangent mode of AD. Our motivating application here is Calculix, a 3-D Structural Finite Element code that mixes Fortran and C. This year, we continued development towards Adjoint Differentiation. Although more complete testing is needed, we now have a first correct adjoint of Calculix.

Tapenade can now routinely differentiate Fortran+C codes, and accepts and takes advantage of the interoperability directives provided by the Fortran 2003 standard. It can handle not only procedure parameters correspondence, but also interoperability between C struct and Fortran COMMON blocks. Laurent Hascoët presented the advancement of this work at the ISMP 2018 congress in Bordeaux https://ismp2018.sciencesconf.org/.

C files (aka "translation units") and Fortran modules are two instances of the more general notion of "package" for which we are looking for a unified representation in Tapenade. It appears that this common representation could also handle C++ namespaces.

### 6.3. Differentiation of non-smooth programs

Participants: Laurent Hascoët, Sri Hari Krishna Narayanan [Argonne National Lab. (Illinois, USA)].

Algorithmic Differentiation can be used to derive tangent models that cope with a certain class of nonsmoothness, through the use of the so-called Abs-Normal Form (ANF) [23]. These tangent models incorporate some knowledge of the nearby discontinuities of the derivatives. These models bring some additional power to processes that use tangent approximations, such as simulation, optimization, or solution of differential equations. The mechanics to derive these special tangent models can be built as an extension of standard tangent linear Algorithmic Differentiation. This has been first demonstrated by the AD tool AdolC which, being based on Operator Overloading, is more flexible and seems a natural choice for implementation. Together with Krishna Narayanan, we recently tried a similar adaption on Source-Transformation AD tools. It appears that very little development is needed in the AD-tool. Specifically for Tapenade, it appears that no development at all is needed in the tool itself. Any end-user can already produce ANF tangent without needing any access to the tool source. All it requires is a customized derivative of the absolute-value function (ABS), which is currently less than 40 lines of code.

Building the ANF of a given program introduces one new variable per run-time execution of the ABS function. As the number of rows and columns of the constructed extended Jacobian both grow like the number of variables, it may become unreasonably large for large codes. To overcome this issue, we explore the possibility of finding at run-time the "important" ABS calls that deserve this treatment, and those that don't. We base this decision on a notion of distance to the kink induced by this ABS call as illustrated by Figure 2. We presented these experiments at a Shonan meeting on this question (Shonan, Japan, June 25-29) and at a workshop of ISMP 2018 (Bordeaux, July 2-6)

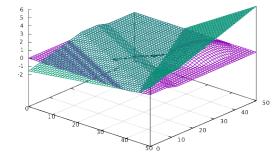


Figure 2. Abs-Normal Form of a non-smooth function: purple:original function, green ANF computed at (30,30). The ANF is linearized around the point of interest, and at the same time captures the non-smooth behavior. Notice the ANF divergence from the original function on the left, due to neglecting the leftmost kink which was decided "far" enough from the point of interest. The ANF divergence on the right is the natural effect of linearization

### 6.4. AD-adjoints and C dynamic memory management

Participants: Laurent Hascoët, Sri Hari Krishna Narayanan [Argonne National Lab. (Illinois, USA)].

One of the current frontiers of AD research is the definition of an adjoint AD model that can cope with dynamic memory management. This research is central to provide reliable adjoint differentiation of C, and for our distant goal of AD of C++. This research is conducted in collaboration with the MCS department of Argonne National Lab. Our partnership is formalized by joint participation in the Inria joint lab JLESC, and partly funded by the Partner University Fund (PUF) of the French embassy in the USA.

Adjoint AD must reproduce in reverse order the control decisions of the original code. In languages such as C, allocation of dynamic memory and pointer management form a significant part of these control decisions. Reproducing memory allocation in reverse means reallocating memory, possibly receiving a different memory

chunk. Reproducing pointer addresses in reverse thus requires to convert addresses in the former memory chunks into equivalent addresses in the new reallocated chunks. Together with Krishna Narayanan from Argonne, we experiment on real applications to find the most efficient solution to this address conversion problem. We jointly develop a library (called ADMM, ADjoint Memory Management) whose primitives are used in AD adjoint code to handle this address conversion. Both our AD tool Tapenade and Argonne's tool OpenAD use ADMM in the adjoint code they produce.

This year, trying to prove correctness of our current address conversion, we discovered some limitations that indeed made the proof impossible. To solve these issues, it seems necessary to assign at run-time a unique identifier to each chunk of memory used by the code, and to carry this identifier along with every pointer. This results in a code transformation which, although more complex than expected, can still be described by a small set of rewrite rules. Moreover, this alternative method should reduce the run-time overhead that we observed previously. Implementation and measurements are still under way. We presented this recent research in the form of a catalogue of alternatives for Data-Flow reversal of memory addresses, at the 21<sup>st</sup> EuroAD workshop (Jena, Germany, November 19-20).

### 6.5. Application to large industrial codes

**Participants:** Valérie Pascual, Laurent Hascoët, Bruno Maugars [ONERA], Sébastien Bourasseau [ONERA], Bérenger Berthoul [ONERA].

We support industrial users with their first experiments of Algorithmic Differentiation of large in-house codes.

This year's main application is with ONERA on their ElsA CFD platform (Fortran 90). Both tangent and adjoint models of the kernel of ElsA were built successfully by Tapenade. It is worth noticing that this application was performed inside ONERA by ONERA engineers (Bruno Maugars, Sébastien Bourasseau, Bérenger Berthoul) with no need for installation of ElsA inside Inria. We take this as a sign of maturity of Tapenade. Apart from a few minor corrections, our contributon was essentially during development meetings, to point out some strategies and tool options to obtain efficient differentiated code. One emphasis was on adjoint of vectorized code, which was produced as vectorized code too by means of a seldom-used Tapenade option that stores intermediate values statically, i.e. not on a global stack. Sébastien Bourasseau presented the first results at the 21<sup>st</sup> EuroAD workshop (Jena, Germany, November 19-20), with convincing performance on industrial-size test cases. A joint article is in preparation.

## 6.6. Multirate methods

Participants: Alain Dervieux, Bruno Koobus, Emmanuelle Itam, Stephen Wornom.

This study is performed in collaboration with IMAG-Montpellier. It addresses an important complexity issue in unsteady mesh adaptation and took place in the work done in the ANR Maidesc (ended 2017). Unsteady high-Reynolds computations are strongly penalized by the very small time step imposed by accuracy requirements on regions involving small space-time scales. Unfortunately, this is also true for sophisticated unsteady mesh adaptive calculations. This small time step is an important computational penalty for mesh adaptive methods of AMR type. This is also the case for the Unsteady Fixed-Point mesh adaptive methods developed by Ecuador in cooperation with the Gamma3 team of Inria-Saclay. In the latter method, the loss of efficiency is even more crucial when the anisotropic mesh is locally strongly stretched since only very few cells are in the regions of small time-step constraint. This loss is evaluated as limiting the numerical convergence order for discontinuities to 8/5 instead of second-order convergence. An obvious remedy is to design time-consistent methods using different time steps on different parts of the mesh, as far as they are efficient and not too complex. The family of time-advancing methods in which unsteady phenomena are computed with different time steps in different regions is referred to as the multirate methods. In our collaboration with university of Montpellier, a novel multirate method using cell agglomeration has been designed and developed in our AIRONUM CFD platform. A series of large-scale test cases show that the new method is much more efficient than an explicit method, while retaining a similar time accuracy over the whole computational domain. A novel analysis shows that the proposed multirate algorithm indeed solves the unsteady mesh adaptation barrier identified in previous works. This work is being published in a journal [13].

## 6.7. Control of approximation errors

**Participants:** Eléonore Gauci, Alain Dervieux, Adrien Loseille [Gamma3 team, Inria-Rocquencourt], Frédéric Alauzet [Gamma3 team, Inria-Rocquencourt], Anca Belme [university of Paris 6], Gautier Brèthes [university of Montreal], Alexandre Carabias [Lemma].

Reducing approximation errors as much as possible is a particular kind of optimal control problem. We formulate it exactly this way when we look for the optimal metric of the mesh, which minimizes a user-specified functional (goal-oriented mesh adaptation). In that case, the usual methods of optimal control apply, using adjoint states that can be produced by Algorithmic Differentiation.

This year, two conference papers were written on the methods of the team, including new analyses in [11],[10], a work on correctors in CFD in an AIAA paper. A detailed study of adjoint-based mesh adaptation for Navier-Stokes flows has been completed and published in a journal [9].

Following participation of Gamma3 and Ecuador to the European project UMRIDA (ended 2017), we wrote chapters 20, 21, 45, and 48 of the book "Uncertainty Management for Robust Industrial Design in Aeronautics", edited by C. Hirsch et al. in the Springer series Notes on Numerical Fluid Mechanics and Multidisciplinary Design (2019).

## **6.8.** Turbulence models

Participants: Alain Dervieux, Bruno Koobus, Stephen Wornom, Maria-Vittoria Salvetti [University of Pisa].

Modeling turbulence is an essential aspect of CFD. The purpose of our work in hybrid RANS/LES (Reynolds Averaged Navier-Stokes / Large Eddy Simulation) is to develop new approaches for industrial applications of LES-based analyses. In the applications targetted (aeronautics, hydraulics), the Reynolds number can be as high as several tens of millions, far too high for pure LES models. However, certain regions in the flow can be predicted better with LES than with usual statistical RANS (Reynolds averaged Navier-Stokes) models. These are mainly vortical separated regions as assumed in one of the most popular hybrid models, the hybrid Detached Eddy Simulation model. Here, "hybrid" means that a blending is applied between LES and RANS. An important difference between a real life flow and a wind tunnel or basin is that the turbulence of the flow upstream of each body is not well known.

The development of hybrid models, in particular DES in the litterature, has raised the question of the domain of validity of these models. According to theory, these models should not be applied to flow involving laminar boundary layers (BL). But industrial flows are complex flows and often present regions of laminar BL, regions of fully developed turbulent BL and regions of non-equilibrium vortical BL. It is then mandatory for industrial use that the new hybrid models give a reasonable prediction for all these types of flow. We concentrated on evaluating the behavior of hybrid models for laminar BL and for vortical wakes. While less predictive than pure LES on laminar BL, some hybrid models still give reasonable predictions for rather low Reynolds numbers.

This year, we have developed a new model relying on the hybridation of a DDES model based on a k- $\epsilon$  closure with our dynamic VMS model. This model shows improvement in most situations and in particular for laminar flows.

We have also addressed this year a challenging test case, the flow around tandem cylinders with a distance between the cylinders of 12 diameters. The accurate capture of the vortices traveling along this path of 12 diameters requires that the LES filter does not accumulate any dissipation along this trajactory. This is a noticeable property or our DVMS model. Further, the numerics need be as accurate as possible. We use a superconvergent approximation, up to fifth order accurate on Cartesian regions of the computational domain. This combination allowed for an accurate prediction of the drag of the second cylinder. This result has been presented at the workshop ETMM12 [12]

## **FACTAS Team**

# 6. New Results

## 6.1. Inverse problems for Poisson-Laplace equations

**Participants:** Laurent Baratchart, Sylvain Chevillard, Juliette Leblond, Jean-Paul Marmorat, Konstantinos Mavreas.

#### 6.1.1. Inverse magnetization issues from planar data

This work has been carried out in the framework of the Inria Associate Team IMPINGE, comprising Cauê Borlina, Eduardo Andrade Lima and Benjamin Weiss from the Earth Sciences department at MIT (Boston, USA) and Douglas Hardin, Edward Saff and Cristobal Villalobos from the Mathematics department at Vanderbilt University (Nashville, USA).

The overall goal of IMPINGE was to determine magnetic properties of rock samples (*e.g.* meteorites or stalactites), from weak field measurements close to the sample that can nowadays be obtained using SQUIDs (superconducting quantum interference devices). Depending on the geometry of the rock sample, the magnetization distribution can either be considered to lie in a plane or in a parallelepiped of thickness r. Some of our results apply to both frameworks (the former appears as a limiting case when r goes to 0), while others concern the 2-D case and have no 3-D counterpart as yet.

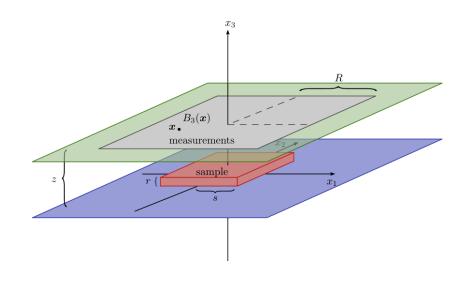


Figure 3. Schematic view of the experimental setup

Figure 3 presents a schematic view of the experimental setup: the sample lies on a horizontal plane at height 0 and its support is included in a parallelepiped. The vertical component  $B_3$  of the field produced by the sample is measured in points of a horizontal square at height z.

We pursued our research efforts towards designing algorithms for net moment recovery. The net moment is the integral of the magnetization over its support, and it is a valuable piece of information to physicists which has the advantage of being determined solely by the field: whereas two different magnetizations can generate the same field, the net moment depends only on the field and not on which magnetization produced it. Hence the goal may be described as to build a numerical magnetometer, capable of analyzing data close to the sample. This is in contrast to classical magnetometers which regard the latter as a single dipole, an approximation which is only valid away from the sample and is not suitable to handle weak fields which get quickly blurred by ambient magnetic sources if one measures the field at a distance from the sample.

The first approach consists in using the fact that the integral of  $B_3$  against polynomials of order less or equal to 1 on some domains symmetric with respect to the origin provides an estimate of the net moment, asymptotically when R grows large [20], [72]. This year, on the one hand, we conducted with our colleagues at MIT a campaign of fairly systematic tests (with various sensitivity parameters for the sensor, step size between measurement points, overall size of the measurement rectangle, etc.) to observe how our method behaves on true data. The results are overall very good when the signal-to-noise ratio is not poor; however, this revealed a few situations where the observed asymptotics does not fit the theoretical one, and we have currently no clue of the reason of this phenomenon (is it a manipulation error on some of the samples of our campaign? a bug in our implementation? a noise on the data with a surprisingly large effect on the asymptotic? the fact that the asymptotic regime was not yet reached?) Understanding this phenomenon is still an on-going work. On the other hand, we spotted in the literature approaches that are somehow similar to ours: they compute the same integral, but on the whole plane, and try to account for the finiteness of the measurement rectangle by more or less heuristic methods. As the finiteness of the rectangle is built-in in our approach (we exploit the fact the nature of the asymptotic behavior with respect to R is analytically known), we have good hope that our method should compare favorably against its competitors, but we did not conduct systematic tests yet.

The second approach attempts to generalize the previous expansions in the case when R is moderately large (but only in the thin slab framework, modeling the sample as a rectangle). For this purpose, we setup a bounded extremal problem (BEP, see Section 3.3.1) and submitted an article last year on the subject. It has been accepted for publication this year, see [12].

A third approach developed during the previous years was to design an alternate procedure to compute a good linear estimator, dwelling on expansions on a family of piecewise affine functions, with a restricted number of pieces. A key point here is that it is possible to derive explicit formulas for the adjoint operator  $B_3^*$  (in appropriate  $L^2$  spaces) to the operator  $B_3$  mapping a magnetization to the vertical component of the field, when applied to polynomials. We derived this year explicit recurrence formulas that allow one to efficiently compute  $B_3^*$  of a polynomial of any degree in linear time with respect to the number of monomials. We currently only have draft notes of this research.

Concerning full inversion of thin samples, after preliminary experiments on regularization with  $L^1$  constraints (a heavy trend in linear inverse problems today to favor sparse solutions), we started studying magnetizations modeled by signed measures. A loop decomposition of silent sources was obtained, which sharpens in 2-D setting the structure theorem of [76]. Moreover, a characterization of equivalent sources having minimal total variation has been obtained when the support of the magnetization is very scattered (namely: purely 1-unrectifiable, which holds in particular for dipolar models) and also for certain magnetizations of physical interest like unidirectional ones. Thus, it seems that constraining the total variation to regularize the recovery process is appropriate in some important cases. The theoretical analysis has shown that the optimum is then always sparse, in that it has Hausdorff dimension at most 1. This stems from the real analyticity of the operators relating the magnetization to the field, which prevents them from assuming constant level on large sets. Moreover, we proved that the argument of the minimum of the regularized criterion  $||f-B_3\mu||_2^2 + \lambda ||\mu||_{TV}$ is unique; here,  $\mu$  is the measure representing the magnetization with respect to which the criterion gets optimized, f is the data and  $\lambda > 0$  a regularization parameter, while  $\|\mu\|_{TV}$  is the total variation of  $\mu$ . An implementation is currently being set up with promising results, discretization beforehand on a fixed grid. Yet, a deeper understanding on how to adjust the parameters of the method is required. This topic is studied in collaboration with D. Hardin and C. Villalobos from Vanderbilt University. [21].

Besides, we considered a simplified 2-D setup for magnetizations and magnetic potentials (of which the magnetic field is the gradient). When both the sample and the measurement set are parallel intervals, some best approximation issues related to inverse recovery and relevant BEP problems in Hardy classes of holomorphic functions (see Section 3.3.1). Note that, in the present case, the criterion no longer acts on the boundary of the holomorphy domain (namely, the upper half-plane), but on a strict subset thereof, while the constraint acts on the support of the approximating function. Both involve functions in the Hilbert Hardy space of the upper half-plane. This is the subject of ongoing work with E. Pozzi (Department of Mathematics and Statistics, St Louis Univ., St Louis, Missouri, USA).

For magnetizations supported in a volume  $\Omega$  with boundary  $\partial\Omega$ , there is a greater variety of silent sources, since they have much more space to live in. Now, to each magnetization m supported in  $\Omega$  there is a unique magnetization supported on  $\partial\Omega$  (the balayage of m) and producing the same field outside  $\Omega$ . Thus, describing silent sources supported on  $\partial\Omega$  is a way to factor out some of the complexity of the situation. When m is located in the plane, the Hardy-Hodge decomposition introduced in [35] (see Section 3.3.1) was used there to characterize all silent magnetizations from above (resp. below) as being those having no harmonic gradient from below (resp. above) in their decomposition. When m is supported on a closed compact surface, a similar decomposition exists for  $\mathbb{R}^3$ -valued vector fields on  $\partial\Omega$ , (see Section 6.4), that allows us to characterize all magnetizations on  $\partial\Omega$  which are silent from outside as being those harmonic components satisfy a certain spectral relation for the double layer potential on  $\partial\Omega$ . The significance and the algorithmic implications of that equation are under study.

Other types of inverse magnetization problems can be tackled using such techniques, in particular global Geomagnetic issues which arise in spherical geometry. In collaboration with C. Gerhards from the Technische Universität Bergakademie Freiberg (Germany), we developed a method to separate the crustal component of the Earth's magnetic field from its core component, if an estimate of the field is known on a subregion of the globe [33]. This assumption is not unrealistic: parts of Australia and of northern Europe are considered as fairly well understood from the magnetostatic view point. We are currently working to test the algorithm against real data, in collaboration with Geophysicists.

#### 6.1.2. Inverse magnetization issues from sparse cylindrical data

The team Factas is a partner of the ANR project MagLune on Lunar magnetism, headed by the Geophysics and Planetology Department of Cerege, CNRS, Aix-en-Provence (see Section 8.2.1). Recent studies let geoscientists think that the Moon used to have a magnetic dynamo for a while. However, the exact process that triggered and fed this dynamo is still not understood, much less why it stopped. The overall goal of the project is to devise models to explain how this dynamo phenomenon was possible on the Moon.

The geophysicists from Cerege went a couple of times to NASA to perform measurements on a few hundreds of samples brought back from the Moon by Apollo missions. The samples are kept inside bags with a protective atmosphere, and geophysicists are not allowed to open the bags, nor to take out samples from NASA facilities. Moreover, the process must be carried out efficiently as a fee is due to NASA by the time when handling these moon samples. Therefore, measurements were performed with some specific magnetometer designed by our colleagues from Cerege. This device measures the components of the magnetic field produced by the sample, at some discrete set of points located on circles belonging to three cylinders (see Figure 4). The objective of Factas is to enhance the numerical efficiency of post-processing data obtained with this magnetometer.

Under the hypothesis that the field can be well explained by a single magnetic pointwise dipole, and using ideas similar to those underlying the FindSources3D tool (see Sections 3.4.2 and 6.1.3), we try to recover the position and the moment of the dipole using the available measurements. This is still on-going work which constitutes the main topic of the PhD thesis of K. Mavreas.

In a given cylinder, using the associated cylindrical system of coordinates, recovering the position of the dipole boils down to determine its height z, its radial distance  $\rho$  and its azimuth  $\phi$ . We use a rational approximation technique which, for the circle of measurements at height h, gives us an estimate of the complex number  $u_h = \frac{1+\rho^2 + (h-z)^2}{\rho} e^{i\phi}$ , from which  $\phi$  is directly obtained. Besides, from the relation  $\rho |u_h| = 1 + \rho^2 + (h-z)^2$ , we see that the point  $(\rho, z)$  lies on a circle  $C_h$ . Therefore, with measurements

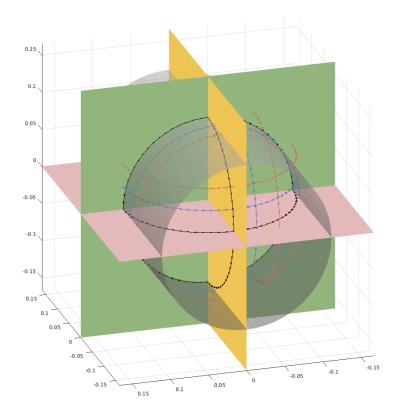


Figure 4. Typical measurements obtained with the instrument of Cerege. Measurements of the field are performed on nine circles, given as sections of three cylinders. On each circle, only one component of the field is measured: the component  $B_h$  along the axis of the corresponding cylinder (blue points), the component  $B_n$  radial with respect to the circle (black points), or the component  $B_{\tau}$  tangential to the circle (red points).

at three different heights  $h_i$  (i = 1, 2, 3), we can in principle recover  $(\rho, z)$  as the intersection of the three circles  $C_{h_1}, C_{h_2}$  and  $C_{h_3}$ .

In practice, due to the many sources of imprecision (the first of all being that the field is not truly generated by a single dipole), the circles do not all truly intersect. This year, we studied three different strategies to estimate the pseudo-intersection point of the circles. In the plane, for a point P and a circle C of center O and radius R, we define d(P,C) = ||PO|| - R| where  $|| \cdot ||$  denotes the Euclidean distance, and  $h(P,C) = ||PO||^2 - R^2$  and we formulate the problem of finding a pseudo-intersection point between  $C_{h_1}$ ,  $C_{h_2}$  and  $C_{h_3}$  as either:

- 1. finding a point P that minimizes  $d(P, C_{h_1}) + d(P, C_{h_2}) + d(P, C_{h_3})$ ;
- 2. finding a point *P* for which  $h(P, C_{h_1}) = h(P, C_{h_2}) = h(P, C_{h_3});$
- 3. finding a point *P* that minimizes  $h(P, C_{h_1})^2 + h(P, C_{h_2})^2 + h(P, C_{h_3})^2$ .

The first case turns out to actually be a generalization of two classical concepts: the Fermat point (or Torricelli point) of a triangle, and the Alhazen optical problem. The second case corresponds to a classical notion called the *radical center* of three circles (intersection of the three corresponding radical axes). Finally, the third case does not seem to have a documented solution. We solve it by writing the algebraic system of two equations corresponding to the critical points of the function, after an appropriate change of coordinates in order to reduce the degree. Finally, we get a superset of the solutions by estimating the roots of the resultant of both polynomials. First experiments showed that the third formulation led to the most satisfying estimate of the pseudo-intersection. We also implemented a heuristic numerical procedure (without theoretical formulas for its solution) to estimate the point P that minimizes  $d(P, C_{h_1})^2 + d(P, C_{h_2})^2 + d(P, C_{h_3})^2$ , and it also gives fairly acceptable estimates. This work has not yet been submitted for publication.

Another important part of our work this year has been to extensively test our implementation of the rational approximation procedure which is at the heart of our method (and which is also used for the problem described in Section 6.1.3). These tests allowed us to detect situations in which the algorithm was falling into an infinite loop or was converging towards a local minimum that was not really the best approximation. It also revealed that all initialization strategies for the iterative optimization algorithm were not equally sensitive to the noise. This led us to redesign our implementation.

Finally, the article that we submitted last year, with a rudimentary approach to recover  $\rho$  and z from the data obtained at several heights, has been accepted and will be published soon, see [14].

#### 6.1.3. Inverse problems in medical imaging

In 3-D, functional or clinically active regions in the cortex are often modeled by pointwise sources that have to be localized from measurements, taken by electrodes on the scalp, of an electrical potential satisfying a Laplace equation (EEG, electroencephalography). In the works [7], [40] on the behavior of poles in best rational approximants of fixed degree to functions with branch points, it was shown how to proceed via best rational approximation on a sequence of 2-D disks cut along the inner sphere, for the case where there are finitely many sources (see Section 4.3).

In this connection, a dedicated software FindSources3D (FS3D, see Section 3.4.2) is being developed, in collaboration with the Inria team Athena and the CMA - Mines ParisTech. In addition to the Matlab version of FS3D, a new (C++) version of the software that automatically performs the estimation of the quantity of sources is being built, specifically this year in the framework of the AMDT Bolis2 ("Action Mutualisée de Développement Technologique", "Boîte à Outils Logiciels pour l'Identification de Sources"), together with engineers from the SED (Service d'Expérimentation et de Développement) of the Research Center. This new version, still under development, is modular, portable and possesses a nice GUI (using Qt5, dtk, vtk), while non regression (continuous integration) is ensured.

It appears that, in the rational approximation step, *multiple* poles possess a nice behavior with respect to branched singularities. This is due to the very physical assumptions on the model from dipolar current sources: for EEG data that correspond to measurements of the electrical potential, one should consider *triple* poles; this will also be the case for MEG – magneto-encephalography – data. However, for (magnetic) field data produced by magnetic dipolar sources, like in Section 6.1.2, one should consider poles of order five.

Though numerically observed in [8], there is no mathematical justification so far why multiple poles generate such strong accumulation of the poles of the approximants. This intriguing property, however, is definitely helping source recovery and will be the topic of further study. It is used in order to automatically estimate the "most plausible" number of sources (numerically: up to 3, at the moment). Last but not least, the version of the software currently under development takes as inputs actual EEG measurements, like time signals, and performs a suitable singular value decomposition in order to separate independent sources.

Magnetic data from MEG recently became available along with EEG data, by our medical partners at INS in Marseille; indeed, it is now possible to use simultaneously both measurement devices, in order to measure both the electrical potential and a component of the magnetic field (its normal component on the MEG helmet, that can be assumed to be spherical). This should enhance the accuracy of our source recovery algorithms. We will add the treatment of MEG data as another functionality of the software FS3D.

Concerning dipolar source estimation from EEG, joint work with Marion Darbas (Univ. Picardie Jules Verne, Laboratoire Amiénois de Mathématique Fondamentale et Appliquée, LAMFA) is in progress for neonates data and models. Their specificity is that the skull does not have a constant conductivity (at the fontanels location, the bone is spongy). We pursue together a study of the influence of the skull conductivity on the inverse EEG problem, using in particular FS3D, see also [70].

We also consider non quasi-static models in order to more precisely analyze the time influence on the behavior of the solutions to the inverse source problems in EEG and MEG. This is current work with Iannis Stratis and Atanasios Yannacopoulos (National and Kapodistrian University of Athens, Greece, Department of Mathematics).

## 6.2. Matching problems and their applications

Participants: Laurent Baratchart, Martine Olivi, Gibin Bose, David Martinez Martinez, Fabien Seyfert.

Filter synthesis is usually performed under the hypothesis that both ports of the filter are loaded on a constant resistive load (usually 50 Ohm). In complex systems, filters are however cascaded with other devices, and end up being loaded, at least at one port, on a non purely resistive frequency varying load. For example, in an emitter-receiver, the antenna is followed by a filter. Whereas the antenna can usually be regarded as a resistive load at some frequencies, this is far from being true on the whole pass-band. A mismatch between the antenna and the filter, however, causes irremediable power losses, both in emission and transmission. Antennas are not the only systems where matching is of importance: in multiplexer design, one of the most complicated problems among microwave device synthesis, each filter is plugged at one of its accesses on a load made of the common manifold and all other channel filters. This load is far from being matched, and leads to a complex simultaneous matching problem, of all filters connected via the common manifold junction. Our goal is therefore to develop a method for filter synthesis that allows us to match varying loads on specific frequency bands, while enforcing some rejection properties away from the pass-band.

Figure 5 shows a filter with scattering matrix S, plugged at its right port on a frequency varying load with reflection parameter  $L_{1,1}$ . If the filter is lossless, simple algebraic manipulations show that on the frequency axis the reflex-ion parameter satisfies:

$$|G_{1,1}| = \left|\frac{S_{2,2} - \overline{L_{1,1}}}{1 - S_{2,2}L_{1,1}}\right| = \delta(\overline{L_{1,1}}, S_{2,2}).$$

The matching problem of minimizing  $|G_{1,1}|$  amounts therefore to minimize the pseudo-hyperbolic distance  $\delta$  between the filter's reflection parameter  $S_{2,2}$  and the conjugate of the load's reflection  $\overline{L_{1,1}}$ , on a given frequency band. On the contrary enforcing a rejection level on a stop band, amounts to maintaining the value of  $\delta(L_{1,1}, S_{2,2})$  above a certain threshold on this frequency band. For a broad class of filters, namely those that can be modeled by a circuit of n coupled resonators, the scattering matrix S is a rational function of McMillan degree n in the frequency variable. The matching problem thus appears to be a rational approximation problem in the hyperbolic metric.

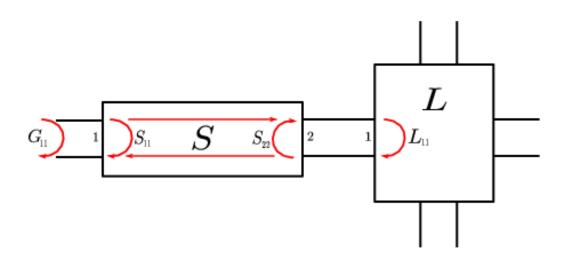


Figure 5. Filter plugged on a system with reflection coefficient  $L_{11}$ 

## 6.2.1. Multiplexer synthesis via interpolation and common junction design

Based on our work linking Nevanlinna-Pick interpolation and point-wise matching techniques [6] we tackled the synthesis of a multiplexer on the basis of frequency specifications relative to a triplexer furnished by CNES and deemed to be problematic. Theoretical results guaranty the existence in this case, under a strict contractivity hypothesis on the common junction, of a simultaneous pointwise matching solution of all three channel filters. This result is however not constructive as it relies on Brouwer's fixed point theorem, a purely topological argument. In the context of the PhD of D. Martinez, we developed a continuation algorithm, starting from a completely decoupling junction and ending up with the manifold junction of interest. When the junction decouples all the channels, the overall matching problem results in 3 independent Nevanlinna-Pick interpolation problems as described in [6]: this yield the starting point of our continuation approach. The manifold peaks have also been identified as crucial here: these are resonances taking place in the common junction of the multiplexer, at which transmission of energy becomes impossible between a given channel and the common port. These peaks have been mathematically characterized, and a systematic combinatorial algorithm designed for the synthesis of a "peak free" manifold junction. In particular it was proven, that an extremely compact junction is needed to fit the specifications furnished by CNES: when dispersive effects increase (and they do with the size of the junction) the appearance of manifold peaks has been proven inevitable. Using a continuation approach to compute the channel filters responses and a combinatorial procedure to design a peak-free junction, a complete triplexer has been synthesized that fits the CNES specifications. The synthesis was first considered in terms of circuits and eventually transformed in a real hardware realized in waveguide technology (see Figure.6). The latter is currently being manufactured at XLIM laboratories, where our colleague S. Bila is co-advising D. Martinez' PhD.

#### 6.2.2. Uniform matching and global optimality considerations

The interpolation procedure of [6] provides us with matching/rejecting filtering characteristics at a discrete set of frequencies. It can serve as a starting point for heavier optimization procedures, where the matching and rejection specifications are expressed uniformly over the bandwidth. Although the practical results thus obtained are quite convincing, we have no proof of their global optimality. This has led us to seek alternative approaches allowing us to assess, at least in simple cases, global optimality of the obtained response. By optimality of a response we mean, as in classical filtering, a best match of the response in the uniform norm on a given pass-band, while meeting given rejection constraints on a stop-band, and this for a given maximal

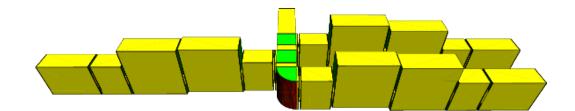


Figure 6. Full wave simulation of the realized triplexer, constituted of a very compact fishbone junction and three channel filters, each of order 6

degree  $n_c$  of the matching network. Following the approach of Fano and Youla, we considered the problem of designing a 2 × 2 loss-less frequency response, under the condition that a specified load can be "unchained" from one of its port. This classically amounts to set interpolation conditions on the response at the transmission zeros of the Darlington extension of the load. When the load admits a rational representation of degree  $n_a = 1$ , and if the transmission zeros of the overall system are fixed, we were able to show that the uniform matching problem over an interval, together with rejection constraints at other frequency locations, reduces to a convex minimization problem with convex constraints over the set of non-negative polynomials of given degree. When the load is of degree greater than 1, our approach is a convex relaxation of the original problem as the computed matching circuit has in general degree  $n_c + n_a - 1$ . This delivers lower bounds for the original matching problem, the first that are known of this problem under degree constraint.

The internal representation of our problem, relies on the use of a Pick matrix  $\mathcal{P}$  depending on a positive polynomial p, that needs to be positive in terms of matrices, that is  $\mathcal{P}(p) \succeq 0$ . Although we know for the convexity of our global formulation [17], the concavity of the matrix valued map  $\mathcal{P}$  is not evident at all. Using arguments of matrix valued Nevanlinna-Pick interpolation we were able to establish it this years, that is: for all pair of positive polynomials  $(p_1, p_2)$  the following holds,

$$\mathcal{P}(\alpha p_1 + (1 - \alpha)p_2) \succeq \alpha \mathcal{P}(p_1) + (1 - \alpha)\mathcal{P}(p_2).$$

This is an important result, as it justifies the use of Lagrangian relaxation for our problem that appears to be a non-linear, convex, semi-definite optimization program (NLSDP), the hardest class among current convex optimization. We plan to build on this result, in order to obtain a critical point equation to our problem, in terms of extremal points of the involved polynomials.

The software implementation developed within the PhD of D. Martinez, combining logarithmic barrier functions and Lagrangian relaxation techniques has been made available for practitioners as Matlab library called Puma 5.2. Results obtained thank to this tool, have been presented in [15], [18] and on a dedicated workshop at the conference IMS2018. Design of use cases, for antenna matching problems relevant in 5G and IOT applications are currently being analyzed with LEAT, within the context of G. Bose's PhD.

### 6.3. Stability assessment of microwave amplifiers and design of oscillators

**Participants:** Laurent Baratchart, Sylvain Chevillard, Martine Olivi, Fabien Seyfert, Sébastien Fueyo, Adam Cooman.

The goal is here to help design amplifiers, in particular to detect instability at an early stage of the design. This activity has gained momentum with the doctoral work of (S. Fueyo), co-advised with J.-B. Pomet (from the McTao Inria project-team) and the postdoctoral stay of (A. Cooman) that eventually resulted in substantial software developments. Application of our work to oscillator design methodologies started recently in collaboration with Smain Amari from the Royal Military College of Canada (Kingston, Canada).

As opposed to Filters and Antennas, Amplifiers and Oscillators are active components that intrinsically entail a non-linear functioning. The latter is due to the use of transistors governed by electric laws exhibiting saturation effects, and therefore inducing input/output characteristics that are no longer proportional to the magnitude of the input signal. Hence, they typically produce non-linear distortions. A central question arising in the design of amplifiers is to assess stability. The latter may be understood around a functioning point when no input but noise is considered, or else around a periodic trajectory when an input signal at a specified frequency is applied. For oscillators, a precise estimation of their oscillating frequency is crucial during the design process. As regards devices devised to operate at relative low frequencies, time domain simulations, based on the integration of the underlying non-linear dynamical system, answers these questions satisfactorily. For complex microwave amplifiers and oscillators, the situation is however drastically different: the time step necessary to integrate the transmission line's dynamical equations (which behave like simple electrical wire at low frequency) becomes so small that simulations are intractable in reasonable time. In addition to this problem, most linear components of these circuits are known through their frequency response, and require therefore a preliminary, numerically unstable step to obtain their impulse response, prior to any time domain simulation.

For all these reasons it is widely preferred to perform the analysis of such systems in the frequency domain. In the case of stability issues around a functioning point, where only small input signals are considered, the stability of the linearized system obtained by a first order approximation of each non-linear dynamic is considered. This is done by means of the analysis of transfer impedance functions computed at some ports of the circuit. We have shown, that under some realistic hypothesis on the building blocks of the circuit, these transfer functions are meromorphic functions of the frequency variable s, with at most a finite number of unstable poles in the right half-plane [19].

Dwelling on the unstable/stable decomposition in Hardy Spaces, we developed a procedure to assess the stability or instability of the transfer functions at hand, from their evaluation on a finite frequency grid [9], that we further improved in [16] to address the design of oscillators, in collaboration with Smain Amari. The evaluation of the admittance function of interest is furnished, on a finite frequency band, by a circuit simulator. Progress were made on the interpolation procedure and the determination of a filtering function that are used to obtain a functional representation of high order of the unstable part of the admittance function to be analyzed. The latter was tested on a time-delayed Chua oscillator circuit: the analytical model of this circuit is known in closed form, and using continuation techniques on the involved delay components it is possible to compute the exact unstable poles of this circuit: two being exactly at the oscillators frequency, while two others spurious poles at DC frequency are present and are usually hard to detect with classical methods. Our approximation based procedure, which was fed with incomplete frequency data estimation of the admittance, was able to recover all poles within a relative error of less than 0.01%. A real world example of an MMIC oscillator was also analyzed and confirmed the procedure's effectiveness. A complete software library called pisa (see Section 5.1) have been developed to render these techniques accessible for practitioners. Although these results are very satisfying in practice, we are aiming for a result that would link together, the width of the measurement band, the density of the measurement points with the precision with which a pole, located within a certain depth into the complex plan can be identified. Extensions of our procedure to the strong signal case, where linearization is considered around a periodic trajectory, yielding harmonic transfer functions is also being worked on.

When stability is studied around a periodic trajectory, which is determined in practice by Harmonic Balance algorithms, linearization yields a linear time varying dynamical system with periodic coefficients and a periodic trajectory thereof. While in finite dimension the stability of such systems is well understood via the Floquet theory, this is no longer the case in the infinite dimensional setting when delays are considered. Dwelling on the theory of retarded systems, S. Fueyo's PhD work showed in previous years that, for certain simple circuits with properly positioned resistors, the monodromy operator is a compact perturbation of a stable operator, and that only finitely many unstable point of its spectrum can occur. This year, we proved a similar result for general circuits, provided that they are passive at very high frequency. For this, we use Lyapunov functions for the transmission lines to establish exponential  $L^2$ -stability, and then rely on counting techniques and impulse response estimates to obtain  $L^{\infty}$  stability from the exponential  $L^2$ -stability. We are currently developing the link between the monodromy operators of a general circuit and the so-called Harmonic Transfer Function of the circuit. A practical application of this result will be to generalize the previously described techniques of stability assessment around a functioning point into a stability assessment technique around periodic trajectories. This can be recast in terms of the finiteness of the number of abscissas of unstable poles of the Harmonic Transfer functions of the circuit. It will be of great importance to generalize such considerations to more complex circuits, whose structure is less well understood at present.

## 6.4. The Hardy-Hodge decomposition

Participant: Laurent Baratchart.

(This is joint work with T. Qian and P. Dang from the university of Macao.) It was proven in previous year that on a smooth compact hypersurface  $\Sigma$  embedded in  $\mathbb{R}^n$ , a  $\mathbb{R}^n$ -valued vector field of  $L^p$  class decomposes as the sum of a harmonic gradient from inside  $\Sigma$ , a harmonic gradient from outside  $\Sigma$ , and a tangent divergence-free field. This year we extended this result to Lipschitz surfaces for  $2 - \varepsilon , where <math>\varepsilon$  and  $\varepsilon'$  depend on the Lipschitz constant of the surface. We also proved that the decomposition is valid for 1 $when <math>\Sigma$  is *VMO*-smooth (*i.e.*  $\Sigma$  is locally the graph of Lipschitz function with derivatives in *VMO*). By projection onto the tangent space, this gives a Helmholtz-Hodge decomposition for vector fields on a Lipschitz hypersurface, which is apparently new since existing results deal with smooth surfaces. In fact, the Helmholtz-Hodge decomposition is valid on surfaces (not just hypersurfaces), and an article is currently being written on this topic. The Hardy-Hodge decomposition generalizes the classical Plemelj formulas from complex analysis.

## 6.5. Imaging and modeling ancient materials

Participants: Vanna Lisa Coli, Juliette Leblond.

This is a very recent activity of the team, linked to images classification in archaeology in the framework of the project ToMaT, "Multiscale Tomography: imaging and modeling ancient materials, technical traditions and transfers" (see Section 8.1), and to the post-doctoral stay of V. L. Coli ; it is pursued in collaboration with L. Blanc-Féraud (project-team Morpheme, I3S-CNRS/Inria Sophia/iBV), D. Binder (CEPAM-CNRS, Nice), in particular.

The pottery style is classically used as the main cultural marker within Neolithic studies. Archaeological analyses focus on pottery technology, and particularly on the first stages of pottery manufacturing processes. These stages are the most demonstrative for identifying the technical traditions, as they are considered as crucial in apprenticeship processes. Until now, the identification of pottery manufacturing methods was based on macro-traces analysis, i.e. surface topography, breaks and discontinuities indicating the type of elements (coils, slabs...) and the way they were put together for building the pots. Overcoming the limitations inherent to the macroscopic pottery examination requires a complete access to the internal structure of the pots. Micro-computed tomography ( $\mu$ CT) has recently been used for exploring ancient materials microstructure. This non-invasive method provides quantitative data for a big set of proxies and is perfectly adapted to the analysis of Cultural heritage materials.

The main challenge of our current analyses aims to overcome the lack of existing protocols to apply in order to quantify observations. In order to characterize the manufacturing sequences, the mapping of the paste variability (distribution and composition of temper) and the discontinuities linked to different classes of pores, fabrics and/or organic inclusions appears promising. The totality of the acquired data composes a set of 2-D and 3-D surface and volume data at different resolutions and with specific physical characteristics related to each acquisition modality (multimodal and multi-scale data). Specific shape recognition methods need to be developed by application of robust imaging techniques and 3-D-shapes recognition algorithms.

In a first step, we devised a method to isolate pores from the 3-D data volumes; we are currently focusing our investigation on 2-D slices displaying pores locations and we considering several data processing treatments, such as multiresolution processing and Hough transform (derived from Radon transform), in order to evaluate their outcome when applied to these very particular images. Different possibilities of investigation will be analyzed as well, such as "a contrario" analysis and deep learning techniques.

## 6.6. Behavior of poles in meromorphic approximation

Participant: Laurent Baratchart.

We proved this year that if a function is holomorphic outside a disk of radius r < 1 in the complex plane, then its best approximant on the unit circle, in the uniform norm, by a meromorphic function having at most n poles in the unit disk has at most m poles of modulus greater than r, where m is independent of n. This is the first result on the behavior of singularities in meromorphic approximation to a function with 2-D singular set. We are currently working on analogs in a non-circular geometry and in rational rather than meromorphic approximation.

## 6.7. Tools for numerically guaranteed computations

Participant: Sylvain Chevillard.

The overall and long-term goal is to enhance the quality of numerical computations. The software tool Sollya (see Section 3.4.5), developed together with C. Lauter (Université Pierre et Marie Curie) intends to provide an interactive environment for performing numerically rigorous computations. It comes as a standalone tool and also as a C library that allows one to benefit from all the features of the tool in C programs.

In September 2018, we released version 7.0. Among other things, this release fixes some bugs and improves the way base functions are internally handled. Another important novelty of 2018 is that Sollya now comes with the companion pythonsollya<sup>0</sup> proposed by third-party developers to provide all the features of Sollya within Python. Some of the novelties in the API of the library version of Sollya 7.0, were made to ease the development of pythonsollya.

<sup>&</sup>lt;sup>0</sup>https://gitlab.com/metalibm-dev/pythonsollya/

## **MCTAO Project-Team**

# 7. New Results

## 7.1. Well posedness in Optimal Transport

**Participants:** Zeinab Badreddine, Ludovic Rifford, Robert Mccann [Univ of Toronto, Canada], Abbas Moameni [Carleton Univ, Ottawa, Canada].

Concerning the Kantorovitch problem, in continuation of the work by McCann and Rifford [67], Moameni and Rifford have studied (see [12]) some conditions on the cost which are sufficient for the uniqueness of optimal plans (provided that the measures are absolutely continuous with respect to the Lebesgue measure). As a by-product of their results, the authors show that the costs which are uniquely minimizing for the Kantorovitch problem are dense in the  $C^0$ -topology. Many others applications and examples are investigated.

Concerning the Monge problem in the sub-Riemannian setting, Zeinab Badreddine [2] obtained the first result of well-posedness in cases where singular minimizing curves may be present. This study is related to the so-called measure contraction property. In collaboration with Rifford [22], Badreddine obtained new classes of sub-Riemannian structures satisfying measure contraction properties.

## 7.2. Strong Sard conjecture for sub-Riemannian structures

**Participants:** Ludovic Rifford, André Belotto Da Silva [Université Aix-Marseille, France], Alessio Figalli [ETH, Swizerland], Adam Parusinski [Université Côte d'Azur, France].

In [25], we address the strong Sard conjecture for sub-Riemannian structures on 3-dimensional analytic manifolds. More precisely, given a totally non-holonomic analytic distribution of rank 2 on a 3-dimensional analytic manifold, we investigate the size of the set of points that can be reached by singular horizontal paths starting from a given point and prove that it has Hausdorff dimension at most 1. In fact, this set is a semi-analytic curve, provided that the lengths of the singular curves under consideration are bounded with respect to a given complete Riemannian metric. As a consequence, combining these techniques with recent developments on the regularity of sub-Riemannian minimizing geodesics, we prove that minimizing sub-Riemannian geodesics in 3-dimensional analytic manifolds are always of class C1, and actually are analytic outside of a finite set of points. This paper can be seen as a major step toward a proof of the Sard conjecture in any dimension.

This is a drastic improvement of the results published in [4] (appeared this year), that proved a slightly weaker property for a less general class of systems.

# 7.3. Optimal approximation of internal controls for a wave-type problem with fractional Laplacian using finite-difference method

Participants: Pierre Lissy, Ionel Roventa [University of Craiova, Romania].

In paper [30], a finite-difference semi-discrete scheme for the approximation of internal controls of a onedimensional evolution problem of hyperbolic type involving the spectral fractional Laplacian is considered. The continuous problem is controllable in arbitrary small time. However, the high frequency numerical spurious oscillations lead to a loss of the uniform (with respect to the mesh size) controllability property of the semi-discrete model in the natural setting. For all initial data in the natural energy space, if we filter the high frequencies of these initial data in an optimal way, the uniform controllability property in arbitrary small time is restored. The proof is mainly based on a (non-classic) moment method.

## 7.4. Singularities in minimum time control

**Participants:** Jean-Baptiste Caillau, Michaël Orieux, Jacques Féjoz [Univ. Paris Dauphine], Robert Roussarie [Univ. Bourgogne-Franche Comté].

We analyze singularities arising in minimum time systems. Consider a control affine system in dimension four with control on the disc such that the controlled fields together with their first order Lie brackets with the drift have full rank. There is a natural stratification of the codimension two singular set in the cotangent bundle leading to a local classification of extremals in terms of singular and bang arcs. This analysis was done in [56] using the nilpotent model, and extended in [35] by interpreting the singularities of the extremal flow as equilibrium points of a regularized dynamics to prove the continuity of the flow. After a suitable blow-up, one can actually treat these singularities as connections of pairs of normally hyperbolic invariant manifolds in order to find a suitable stratification of the flow and prove finer regularity properties. Another issue is to be able to give global bounds on the number of these heteroclinic connections. This can be done by means of *à la Sturm* estimations. This work is part of the PhD thesis of Michaël Orieux [1] and is described in the preprint [28]. In an ongoing work, we also investigate second order sufficient conditions for extremals with such singularities.

## 7.5. Software advances

**Participants:** Jean-Baptiste Caillau, Olivier Cots [Univ. Toulouse], Lamberto Dell'Elce, Thibaud Kloczko, Pierre Martinon [COMMANDS team], Jean-Baptiste Pomet.

McTAO and COMMANDS have been awarded an AMDT (Action Mutualisée de DéveloppemenT) funding of two years to develop a common interface for *Hampath* and BOCOP. This AMDT, coined ct for "Control tools" is to start in January 2019. Our midterm goal is to set the standard for the numerical resolution of optimal control problems. On the basis of the two well established codes BOCOP and *Hampath* from the optimal control community, thanks to this ADT we want to design a high-level modular architecture in order to:

- interoperate BOCOP and Hampath,
- offer a high-level common user interface for the two codes.

Another expected outcome of the ADT is to integrate state of the art processes into the development of the two solvers (collaborative dev tools, reliable repositories, continuous integration...)

## 7.6. Averaging optimal control problems with two frequencies

Participants: Jean-Baptiste Caillau, Lamberto Dell'Elce, Jean-Baptiste Pomet.

Averaging is a valuable technique to gain understanding in the long-term evolution of fast-oscillating dynamical systems. Recent contributions (pioneered by McTAO members in the framework of a long-standing project funded by CNES and Thales Alenia Space) proved that averaging can be applied to the extremal flow of optimal control problems. This study extends the aforementioned results by tackling averaging of time optimal systems with two fast variables with particular emphasis on the treatment of adjoint variables and on the understanding of resonance effects on their dynamics. The chapter [18] details part of this work, and a dedicated paper is in preparation [29].

## 7.7. Integrability properties of the controlled Kepler problem

**Participants:** Jean-Baptiste Caillau, Michaël Orieux, Jacques Féjoz [Univ. Paris Dauphine], Robert Roussarie [Univ. Bourgogne-Franche Comté].

We prove, using Moralès–Ramis theorem, that the minimum-time controlled Kepler problem is not meromorphically integrable in the Liouville sense on the Riemann surface of its Hamiltonian. The Kepler problem is a classical reduction of the two-body problem. We think of the Cartesian coordinate as being the position of a spacecraft, and of the attraction as the action of the Earth. We are interested in controlling the transfer of the spacecraft from one Keplerian orbit towards another one, in the plane. By virtue of Pontrjagin maximum principle, the minimum time dynamics is a Hamiltonian system. The controlled Kepler problem can be embedded in the two parameter family obtained when considering the control of the circular restricted three-body

problem. In the uncontrolled model, it is well known that the Kepler case is integrable and geodesic (there exists a Riemannian metric such that Keplerian curves are geodesics of this metric), while there are obstructions to integrability for positive ratio of masses. In the controlled case, the Kepler problem for the energy cost has been shown to be integrable (and geodesic) when suitably averaged. The aim of this work is to study the integrability properties of the Kepler problem for time minimization. The pioneering work of Ziglin in the 80s, followed by the modern formulation of differential Galois theory in the late 90s by Moralès, Ramis and Simó, have led to a very diverse literature on the integrability of Hamiltonian systems. According to Pontrjagin Maximum principle, one can turn general optimization problems with dynamical constraints into Hamiltonian systems, which are generally not everywhere differentiable. Optimal control theory thus provides an abundant class of dynamical systems for which integrability is a central question. Yet, differential Galois theory has not so often been applied in this context, in part because of the difficulty brought by the singularities. Notwithstanding theses singularities, we show how to apply these ideas to the Kepler system, and prove that it is not meromorphically integrable in the Liouville sense on the Riemann surface of its Hamiltonian. This work is also part of the PhD thesis of Michaël Orieux [1] and is described in the paper [11].

## 7.8. Quasi-satellite orbits in the proximity of Martian moons

**Participants:** Lamberto Dell'Elce, Nicola Baresi [JAXA, Japan], Josué Cardoso Dos Santos [Sao Paolo State University, Brasil], Yasuhiro Kawakatsu [JAXA, Japan].

The Martian Moons eXploration mission is currently under development at the Japan space agency (JAXA) and will be the first spacecraft mission to retrieve pristine samples from the surface of Phobos. In preparation for the sampling operations, MMX will collect observations of Phobos from stable retrograde relative trajectories, which are referred to as quasi-satellite orbits (QSOs). This study investigates the navigability of mid- and high-altitude QSOs in terms of relative orbit elements. After developing an analytical model for the long-term evolution of QSOs and a numerical map between mean and osculating (instantaneous) orbital elements, we use a Lyapunov control law for orbit maintenance purposes based on mean relative orbit element differences. These results were presented in [16] and they pave the way for a perspective collaboration between JAXA and McTAO.

## 7.9. The Copepod and Purcel swimmer

Participants: Bernard Bonnard, Jérémy Rouot, Piernicola Bettiol, Monique Chyba [U. Hawaii].

In the continuation to J. Rouot Phd thesis (2016), our results are presented in a series of papers [7], [5], [6]. The most efficient strokes are computed using geometric studies and numerical simulations, in relation with sub-Riemannian geometry and periodic optimal control algorithms. In the copepod case the model is validated by simulations and a copepod robot was constructed at Hawaii to mimic the copepod. The experiment was reproduced at EPF Troyes under the supervision of J. Rouot. The reference [21] gathers the results of MRI and swimmers in a unified setting combining geometric and numeric techniques developed in McTAO.

## 7.10. Multi-link vs flexible filament swimmers

**Participants:** Laetitia Giraldi, Clément Moreau, Jean-Baptiste Pomet, Hermes Gadhêla [Univ. of York, United Kingdom].

The inertialess fluid-structure interactions of active or passive inextensible filaments and slender-rods are ubiquitous in nature, from the dynamics of semi-flexible polymers and cytoskeletal filaments to cellular mechanics and flagella, or in artificial micro-swimmers (see Section 7.12).

For a microscopic inextensible elastic filament immersed into a fluid, even approximating the fluid-structure interaction by the Resistive Force Theory formulation, the system of PDEs resulting from elastohydrodynamical laws is structurally convoluted and demanding numerically. The N-link swimmer model, where the continuous filament is replaced by N segments with elasticity concentrated at the joints, can be seen as a coarse-graining formulation of the latter. In [10] (see also [31]), the N-link swimmer model is presented in this perspetive and it is demonstrated numerically how this system can be used as an alternative. It can be solved numerically with any ODE solver and overcomes well-known numerical instabilities when solving numerically the full PDE for the filament. Computations can be as much as a hundred times faster. Generalisations for more complex interactions are demonstrated on four examples commonly found in biological systems, a Matlab code is provided as a basis for further generalisations.

More theoretical study of this approximation property are under investigation, also in the framework of Clément Moreau's PhD.

#### 7.11. Energy-optimal strokes for multi-link micro-swimmers

**Participants:** Laetitia Giraldi, François Alouges [École Polytechnique], Antonio Desimone [SISSA Trieste, Italy], Yshar Or [Technion, Haifa, Israel], Oren Wiezel [Technion, Haifa, Israel].

In a common work that is presented in [33], submitted to *New Journal of Physics*, we consider a slender planar multi-link micro-swimmer (N links, see Section 7.10), where the time derivatives of the angles defining the shape are taken as controls, and we are mostly interested in small-amplitude undulations about its straight configuration.

Based only on the leading order dynamics in that vicinity, the optimal stroke to achieve a given prescribed displacement in a given time period is then obtained as the largest eigenvalue solution of a constrained optimal control problem. Remarkably, the optimal stroke is an ellipse lying within a two-dimensional plane in the (N-1)-dimensional space of joint angles, where N can be arbitrarily large. For large N, the optimal stroke is a traveling wave of bending, modulo edge effects.

We also solved, numerically, the fully non-linear optimal control problem for the cases N = 3 (Purcell's threelink swimmer) and N = 5 showing that, as the prescribed displacement becomes small, the optimal solutions obtained using the small-amplitude assumption are recovered. We also show that, when the prescribed displacements become large, the picture is different. For N = 3 we recover the non-convex planar loops already known from previous studies. For N = 5 we obtain non-planar loops, raising the question of characterizing the geometry of complex high-dimensional loops.

## 7.12. Swimming magnetic micro-robots

**Participants:** Luca Berti, Yacine El Alaoui-Faris, Laetitia Giraldi, Jean-Baptiste Pomet, Christophe Prud'Homme [Université de Strasbourg], Stéphane Régnier [UPMC - Sorbonne Universités].

We are in a collaboration with the Parisian robotics laboratory ISIR (Institut des Systèmes Intelligents et de Robotique) to enhance the control of artificial micro-swimmers that are actually built and implemented there. This involves building models and using them for control design. These robots are "magnetic micro-swimmers": part of them is magnetized and the control is an ambient magnetic field.

Yacine El Alaoui-Faris's PhD, co-advised with Stéphane Régnier, started October, 2017. It is centered on finite-dimensional models. The robots under consideration are made of a magnetic head and a flexible tail; the model is a 3-D counterpart of the planar "multi-link micro-swimmers" discussed in Section 7.10.

The validation of this nonlinear ODE model, with or without magnetic actuation, has been achieved this year, both against continuous models present in the literature and against experimental data at ISIR. This model has a definite interest by itself, and in the case of magnetic actuation, it allowed the numerical computation of periodic controls (magnetic field) that optimize the longitudinal velocity with prescribed maximum amplitude of the magnetic field oscillations. This process is described in a manuscript under preparation, to be submitted to *Physical Review Letters*.

These controls have very recently been tested in lab and a very significant efficiency gain over classical sinusoidal oscillations has been evidenced. This is a very encouraging experimental result.

Luca Berti's PhD, co-advised with Christophe Prud'homme, started this fall. It is focused on PDE models that are closer to the real physics but more intricate. His master's thesis was mostly a numerical project in the framework of Cemracs 2018 (http://smai.emath.fr/cemracs/cemracs18/), where we modeled the displacement of a deformable swimmer using a coupling between Stokes equations and hyper-elasticity equations. The PDEs was solved using the Feel++ finite elements library. We validated the fluid model using an exact solution for a rotating rigid body. The motion of a one-hinged swimmer (which obeys to the scallop theorem) was successfully simulated. The physical robots from ISIR are now considered in his PhD.

## 7.13. Necessary conditions for local controllability, motivated by the Two-link Magneto-elastic Micro-swimmer

Participants: Laetitia Giraldi, Pierre Lissy [Univ. Paris Dauphine], Clément Moreau, Jean-Baptiste Pomet.

After proving in [66] a local controllability for the 2-link magneto-elastic swimmer around its straight configuration and noting that this property is weaker than Small-Time Locally Controllable (STLC), we investigated "full" STLC for this system, and were able to show that, except for very specific values of the lengths and magnetizations, this system is *not* STLC. This is published in [9]. This lead us to necessary condition for STLC for more general classes of systems. This is part of Clément Moreau's doctoral research and a publication is under preparation, for classes of control-affine systems with two controls that are not micro-swimmer models, but stem from the observations in [9] and [66].

## 7.14. Numerical and Symbolic computations in MRI

Participants: Bernard Bonnard, Jérémy Rouot, Thibaut Verron, Olivier Cots [ENSEEIHT Toulouse].

Academic year 2016-17 with the two Postdoctoral position at Toulouse (J. Rouot at LAAS and T. Verron, Enseeith) was the opportunity to complete our investigations about the contrast and multi-saturation problem in MRI. This concerns numeric and symbolic computations using Hampath, Bocop, Gloptipoly and Maple software. The reference [27], to be published in MCRF, contains all the results and techniques about this project and is the final paper of this longstanding work in quantum theory.

## 7.15. Stability of nonlinear high frequency amplifiers

Participants: Laurent Baratchart [FACTAS project-team], Sébastien Fueyo, Jean-Baptiste Pomet, Gilles Lebeau.

Sébastien Fueyo's PhD is co-advised on this topic. The problem is presented in Section 4.4.

These amplifiers contain on the one hand nonlinear active components and on the other hand lines, that induce some sort of delays and make the system infinite-dimensional: they are, for each choice of a periodic input, a nonlinear infinite dimensional dynamical system. The Computer Aided Design tools mentioned in Section 4.4 provide a periodic solution under this periodic forcing and may also give the frequency response of the linearized system along this trajectory with some artificial "small" excitation. The goal is to deduce stability from these data.

It is an opportunity to build theoretical basis and justification to a stability analysis through harmonic identification; the latter is one of the specialties of FACTAS, we collaborate on the infinite-dimensional non-linear stability analysis for periodic solutions and how it works with the results of harmonic identification.

On academic examples of simple circuits, we have given full justification (with some possible obstructions) to the prediction of stability through transfer function identification. The theoretical interest is that the spectrum of the operator that gives stability is not as elementary as predicted in the literature, but stability can be predicted nonetheless. This was presented at a local conference, Université Côte d'Azur Complex Days in January, and a more complete publication is under preparation.

On more general structures, new results are available too, publications are in progress.

## 7.16. Optimal sampled-control with applications to Muscular Control

Participants: Bernard Bonnard, Toufik Bakir [L2I, Univ. de Bourgogne Franche Conté], Jérémy Rouot.

The study was initialized two years ago under the impulse of Toufik Bakir (LE2I-UBFC). Based on preliminary experimental studies, the chosen model to muscular control integrates the fatigue variables and is known as *Ding et al force-fatigue model* in the literature. It is a refinement of the historical Hill model (Medecine Nobel Prize 1922). Preliminary results lead to construct a nonlinear observer and the optimized pulses trains are computed using MPC methods [15]. More recently in collaboration with L. Bourdin (Limoges), optimal control techniques were introduced in the framework of sampled-control problems. Pontryagin type necessary conditions were obtained with preliminary numerical simulations. On these topics, paper [23] has been submitted to *JOTA*, October 2018; [3] is accepted for publication in *Networks and Heterogeneous Media*, 2018.

## 7.17. An Optimal Control Strategy Separating Two Species of Microalgae in Photobioreactors

Participants: Olivier Bernard [BIOCORE project-team], Walid Djema, Laetitia Giraldi.

We investigate a minimum time control problem in a chemostat continuous photobioreactor model that describes the dynamics of two distinct microalgae populations. Our objective is to optimize the time of selection – or separation – between two species of microalgae. In [17], we focus on Droop's model which takes into account the internal quota storage of each microalgae species. Using the Pontryagin's principle, we find a dilution-based control strategy that steers the model trajectories to a suitable target in minimal time. Our study reveals that singular arcs play a key role in the optimal synthesis. Using numerical simulations, we show that the optimal control strategy is mainly of type bang-singular. A numerical optimal synthesis is performed throughout the paper, thereby confirming the optimality of the provided feedback-control law.

## **NACHOS Project-Team**

## 6. New Results

## 6.1. Electromagnetic wave propagation

#### 6.1.1. POD-based reduced-order DGTD method

Participants: Stéphane Lanteri, Kun Li [UESTC, Chengdu, China], Liang Li [UESTC, Chengdu, China].

This study is concerned with reduced-order modeling for time-domain electromagnetics and nanophotonics. More precisely, we consider the applicability of the proper orthogonal decomposition (POD) technique for the system of 3D time-domain Maxwell equations, possibly coupled to a Drude dispersion model, which is employed to describe the interaction of light with nanometer scale metallic structures. We introduce a discontinuous Galerkin (DG) approach for the discretization of the problem in space based on an unstructured tetrahedral mesh. A reduced subspace with a significantly smaller dimension is constructed by a set of POD basis vectors extracted offline from snapshots that are obtained by the global DGTD scheme with a second order leap-frog method for time integration at a number of time levels. POD-based ROM is established by projecting (Galerkin projection) the global semi-discrete DG scheme onto the low-dimensional space. The stability of the POD-based ROM equipped with the second order leap-frog time scheme has been analysed through an energy method. Numerical experiments have allowed to verify the accuracy, and demonstrate the capabilities of the POD-based ROM. These very promising preliminary results are currently consolidated by assessing the efficiency of the proposed POD-based ROM when applied to the simulation of 3D nanophotonic problems.

#### 6.1.2. Numerical treatment of non-local dispersion for nanoplasmonics

**Participants:** Herbert de Gersem [TEMF, Technische Universität Darmstadt, Germany], Stéphane Lanteri, Antoine Moreau [Université Clermont Auvergne], Claire Scheid, Dimitrios Loukrezis [TEMF, Technische Universität Darmstadt, Germany], Serge Nicaise [Université de Valenciennes et du Hainaut-Cambresis], Armel Pitelet [Université Clermont Auvergne], Nikolai Schmitt, Jonathan Viquerat.

When metallic nanostructures have sub-wavelength sizes and the illuminating frequencies are in the regime of metal's plasma frequency, electron interaction with the exciting fields have to be taken into account. Due to these interactions, plasmonic surface waves (called plasmons) can be excited and cause extreme local field enhancements. Exploiting such field enhancements in applications of interest requires a detailed knowledge about the occurring fields which can generally not be obtained analytically. For the numerical modeling of light-matter interaction on the nanoscale, the choice of an appropriate model is a crucial point. Approaches that are adopted in a first instance are based on local (no interaction between electrons) dispersion models e.g. Drude or Drude-Lorentz. From the mathematical point of view, these models lead to an additional ordinary differential equation in time that is coupled to Maxwell's equations. When it comes to very small structures in a regime of 2 nm to 25 nm, non-local response due to electron collisions have to be taken into account. This leads to additional, in general non-linear, partial differential equations and is significantly more difficult to treat, though. The classical model is based on a hydrodynamical approach that takes non-local response of the electrons into account. We in particular focus our attention on the linearized version of this model called Linearized Hydrodynamical Drude model. We conducted numerical studies in 2D (published in 2016) and 3D on a linearized hydrodynamic model (published in 2018). However differences between local and nonlocal response are still small. Especially for today's fabrication precision, it remains a challenging task to find reliable structures where non-locality is dominant over e.g. geometrical errors. Motivated by trying to find experimental setups where non-locality is clearly distinguishable from other effects, we studied two promising structures, in close collaboration with physicists. First, in collaboration with A. Pitelet and A. Moreau from Université Clermont Auvergne, and D. Loukrezis and H. De Gersem from Technische Universität Darmstadt, we studied the impact of non-locality on gratings and showed that non-locality can affect surface plasmons propagating at the interface between a metal and a dielectric with a sufficiently high permittivity. We then design a grating coupler that should allow to experimentally observe this influence. Finally, we carefully set up a procedure to measure the signature of spatial dispersion precisely, paving the way for future experiments. Indeed, to ensure that the impact of non-locality exceeds geometric fabrication uncertainties, we proposed a post-fabrication characterization of the grating coupler. Based on the solution of inverse problems leading to the actually fabricated geometry and an uncertainty quantification (UQ) analysis, we conclude that non-locality should clearly be measurable in the grating coupler setting. This work has been submitted in a physics journal. Secondly in collaboration with A. Moreau we considered a nanocube setup that consists of an infinite gold ground layer plus a dielectric spacer of a given height above which a silver nanocube is chemically deposited. Due to this particular setting, the illumination of such a device is creating inside the gap between the nanocube and the ground layer (i.e. inside the dielectric layer) a gap plasmon that is very sensitive to non-locality. We proposed a surrogate-model based telemetry strategy in order to obtain the fabricated cube dimension (inverse problem). Based on this geometric characterization, we decreased the gap-size between the gold substrate and the silver cube and have compared local and non-local numerical simulations. We showed that the influence of non-locality exceeds the experimental error-bars for gap-sizes below 3.1 nm. Additionally, our nonlocal simulations are able to explain the discrepancy between the experiment and local simulations for very small gap-sizes. This project is still ongoing, since we are waiting for another set of experimental results.

On a theoretical side, we pursue the collaboration with S. Nicaise (Université de Valenciennes et du Hainaut-Cambresis) and proved well-posedness of the linearized non-local Drude model for various boundary conditions. We furthermore focused on establishing polynomial stability with optimal energy decay rate. We conducted a thorough study of energy stability for various numerical schemes and DG formulation using a general framework and finally numerically investigate the discrete polynomial stability. This work is almost finalized.

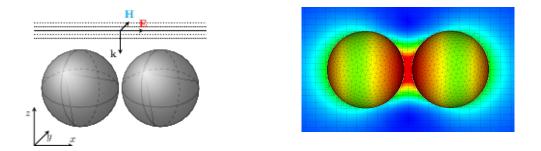


Figure 4. Nanosphere dimer system. Left figure sketches the dimer setup with an  $e_x$  polarized incident plane wave. Right figure shows the 3D field distribution of the electric field on the dimer surface and on a cutting plane and along the dimer axis (PhD thesis of Nikolai Schmitt).

## 6.1.3. Study of 3D periodic structures at oblique incidences

Participants: Claire Scheid, Nikolai Schmitt, Jonathan Viquerat.

In this work, we focus on the development of the use of periodic boundary conditions with sources at oblique incidence in a DGTD framework. Whereas in the context of the Finite Difference Time Domain (FDTD) methods, an abundant literature can be found, for DGTD, the amount of contributions reporting on such methods is remarkably low. In this work, we supplement the existing references using the field transform technique with an analysis of the continuous system using the method of characteristics and provide an energy estimate. Furthermore, we also study the numerical stability of the resulting DGTD scheme. After numerical validations, two realistic test problems have been considered in the context of nanophotonics with our DIOGENeS DGTD solver. This work is under review.

#### 6.1.4. Toward thermoplasmonics

Participants: Yves d'Angelo, Guillaume Baffou [Fresnel Institute, Marseille], Stéphane Lanteri, Claire Scheid.

Although losses in metal is viewed as a serious drawback in many plasmonics experiments, thermoplasmonics is the field of physics that tries to take advantage of the latter. Indeed, the strong field enhancement obtained in nanometallic structures lead to a localized raise of the temperature in its vicinity leading to interesting photothermal effects. Therefore, metallic nanoparticles may be used as heat sources that can be easily integrated in various environments. This is especially appealing in the field of nanomedecine and can for example be used for diagnosis purposes or nanosurgery to cite but just a few. This year, we initiated a preliminary work towards this new field in collaboration with Y. D'Angelo (Université Côte d'Azur) and G. Baffou (Fresnel Institute, Marseille) who is an expert in this field. Due to the various scales and phenomena that come into play, the numerical modeling present great challenges. The laser illumination first excite a plasmon oscillation (reaction of the electrons of the metal) that relaxes in a thermal equilibrium and in turn excite the metal lattice (phonons). The latter is then responsible for heating the environment. A relevant modeling approach thus consists in describing the electron-phonon coupling through the evolution of their respective temperature. Maxwell's equations is then coupled to a set of coupled nonlinear hyperbolic equations describing the evolution of the temperatures of electrons, phonons and environment. The nonlinearities and the different time scales at which each thermalization occurs make the numerical approximation of these equations quite challenging.

#### 6.1.4.1. Numerical modeling of metasurfaces

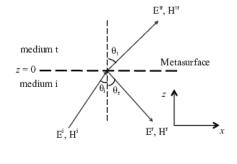
**Participants:** Loula Fezoui, Patrice Genevet [CRHEA laboratory, Sophia Antipolis], Stéphane Lanteri, Liang Li [UESTC, Chengdu, China], Ronan Perrussel [Laplace laboratory, Toulouse].

Metamaterials are composed of periodic subwavelength metal/dielectric structures that resonantly couple to the electric and/or magnetic components of the incident electromagnetic fields, exhibiting properties that are not found in nature. Planar metamaterials with subwavelength thickness, or metasurfaces, consisting of a layer of dielectric or plasmonic nanostructures, can be readily fabricated using lithography and nanoprinting methods, and the ultrathin thickness in the wave propagation direction can greatly suppress the undesirable losses. Metasurfaces enable a spatially varying optical response, mold optical wavefronts into shapes that can be designed at will, and facilitate the integration of functional materials to accomplish active control and greatly enhanced nonlinear response. Designing metasurfaces is generally a challenging inverse problem. A recently introduced synthesis techniques is based on so-called General Sheet Transition Conditions (GSTC) that can be leveraged to define the components of general bianisotropic surface susceptibility tensors characterizing the metasurface. A GSTC-based design technique has several advantages: 1) it is exact; 2) it is general, transforming arbitrary incident waves into arbitrary reflected and transmitted waves, 3) it often admits closed-form solutions, 4) it provides deep insight into the physics of the transformations, 5) it allows multiple (at least up to 4) simultaneous and independent transformations. We study the numerical treatment of GSTC in the time-domain and frequency-domain regimes in the DG and HDG settings respectively.

#### 6.1.4.2. Corner effects in nanoplasmonics

**Participants:** Camille Carvalho [Applied Mathematics Department, University of California Merced, USA], Patrick Ciarlet [ENSTA, POEMS project-team], Claire Scheid.

In this work, we study nanoplasmonic structures with corners (typically a diedral/triangular structure). This is the central subject considered in the PhD thesis of Camille Carvalho. In the latter, the focus is made on a lossles Drude dispersion model with a frequency-domain approach. Several well posedness problems arise due to the presence of corners and are addressed in the PhD thesis. A time-domain approach in this context is also relevant and we propose to use the techniques developed in the team in this prospect. Even if both approaches (time-domain and frequency-domain) represent similar physical phenomena, problems that arise are different. These two approaches appear as complementary; it is thus worth bridging the gap between the two frameworks. We are currently performing a thorough comparison in the case of theses 2D structures with corners and we especially focus on the amplitude principle limit that raises a lot of questions.



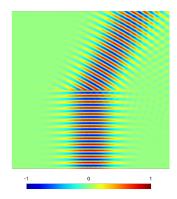


Figure 5. Simulation of a generalized refracting metasurface: problem formulation (left) and real part of  $H_y$ , refraction at  $\theta = \pi/6$  (right).

#### 6.1.4.3. MHM methods for the time-domain Maxwell equations

**Participants:** Alexis Gobé, Stéphane Lanteri, Diego Paredes Concha [Instituto de Matemáticas, Universidad Católica de Valparaiso, Chile], Claire Scheid, Frédéric Valentin [LNCC, Petropolis, Brazil].

Although the DGTD method has already been successfully applied to complex electromagnetic wave propagation problems, its accuracy may seriously deteriorate on coarse meshes when the solution presents multiscale or high contrast features. In other physical contexts, such an issue has led to the concept of multiscale basis functions as a way to overcome such a drawback and allow numerical methods to be accurate on coarse meshes. The present work, which is conducted in the context of the HOMAR Associate Team, is concerned with the study of a particular family of multiscale methods, named Multiscale Hybrid-Mixed (MHM) methods. Initially proposed for fluid flow problems, MHM methods are a consequence of a hybridization procedure which caracterize the unknowns as a direct sum of a coarse (global) solution and the solutions to (local) problems with Neumann boundary conditions driven by the purposely introduced hybrid (dual) variable. As a result, the MHM method becomes a strategy that naturally incorporates multiple scales while providing solutions with high order accuracy for the primal and dual variables. The completely independent local problems are embedded in the upscaling procedure, and computational approximations may be naturally obtained in a parallel computing environment. In this study, a family of MHM methods is proposed for the solution of the time-domain Maxwell equations where the local problems are discretized either with a continuous FE method or a DG method (that can be viewed as a multiscale DGTD method). Preliminary results have been obtained in the two-dimensional case.

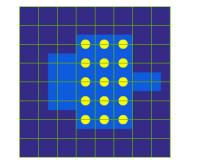
#### 6.1.4.4. MHM methods for the frequency-domain Maxwell equations

**Participants:** Théophile Chaumont-Frelet, Zakaria Kassali, Stéphane Lanteri, Frédéric Valentin [LNCC, Petropolis, Brazil].

We have initiated this year a study of MHM methods for the system of frequency-domain Maxwell equations based on very promising results recently obtained by T. Chaumont-Frelet and F. Valentin for the Helmholtz equation. The design principles are very similar to those underlying MHM methods for the system of time-domain Maxwell equations however we expect to achieve more convincing results for highly multiscale problems since we do not have to deal with the time dimension in the present case. Part of this study is conducted in the context of the PHOTOM (PHOTOvoltaic solar devices in Multiscale computational simulations) Math-Amsud project.

#### 6.1.4.5. HDG methods for the time-domain Maxwell equations

Participants: Stéphane Descombes, Stéphane Lanteri, Georges Nehmetallah.



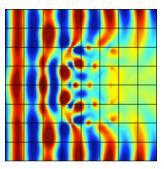


Figure 6. Light propagation in a photonic crystal structure using a MHM-DGTD method for solving the 2D Maxwell's equations. Left: quadrangular mesh. Right: contour lines of the amplitude of the electric field.

This study is concerned with the development of accurate and efficient solution strategies for the system of 3D time-domain Maxwell equations coupled to local dispersion models (e.g. Debye, Drude or Drude-Lorentz models) in the presence of locally refined meshes. Such meshes impose a constraint on the allowable time step for explicit time integration schemes that can be very restrictive for the simulation of 3D problems. We consider here the possibility of using an unconditionally stable implicit time or a locally implicit time integration scheme combined to a HDG discretization method. As a preliminary step, we have investigated a fully explicit HDG method generalizing the classical upwind flux-based DG method for the system of time-domain Maxwell equations. We have studied the stability of this new HDG method and in particular, the influence of the stabilization parameter on the CFL condition. We are now progressing toward the design of a new family of high order in time hybrid explicit-implicit HDG methods to deal efficiently with CFL restriction due to grid-induced stiffness.

#### 6.1.4.6. HDG methods for frequency-domain plasmonics

Participants: Stéphane Lanteri, Mostafa Javadzadeh Moghtader, Liang Li [UESTC, Chengdu, China].

HDG method is a new class of DG family with significantly less globally coupled unknowns, and can leverage a post-processing step to gain super-convergence. Its features make HDG a possible candidate for computational electromagnetics applications, especially in the frequency-domain. The HDG method introduces an hybrid variable, which represents an additional unknown on each face of the mesh, and leads to a sparse linear system in terms of the degrees of freedom of the hybrid variable only. Our HDG method had been first introduced for the system of 3D time-harmonic Maxwell's, combined to an iterative Schwarz domain decomposition (DD) algorithm to allow for an efficient parallel hybrid iterative-direct solver. The resulting DD-HDG solver has been applied to classical applications of electromagnetics in the microwave regime. In the present study we further focus on this particular physical context and propose a arbitrary high order HDG method for solving the system of 3D frequency-domain Maxwell equations coupled to a generalized model of physical dispersion in metallic nanostructures at optical frequencies. Such a generalized dispersion model unifies most common dispersion models, like Drude and Drude-Lorentz models, and it permits to fit large range of experimental data. The resulting DD-HDG solver is capable of using different element types and orders of approximation, hence enabling the possibilities of *p*-adaptivity and non-conforming meshing, and proves to have interesting potentials for modeling of complex nanophotonic and nanoplasmonic problems.

## 6.2. Elastodynamic wave propagation

#### 6.2.1. Multiscale DG methods for the time-domain elastodynamic equations

**Participants:** Marie-Hélène Lallemand, Claire Scheid, Weslley Da Silva Pereira [LNCC, Petropolis, Brazil], Frédéric Valentin [LNCC, Petropolis, Brazil].

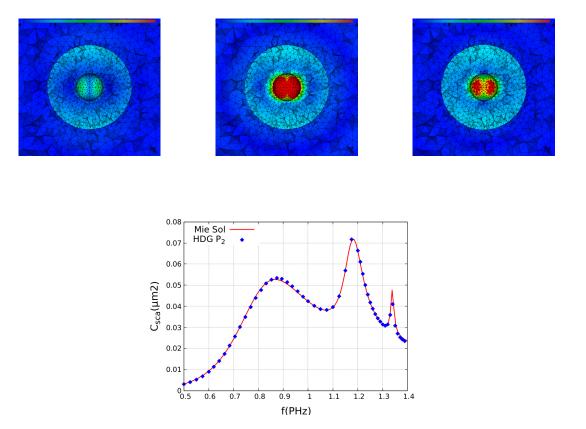


Figure 7. Top figures: scattering of a plane wave by a 50 nm gold nanosphere: magnitude of  $\mathbf{E}$  field at frequencies 1070 THz (left), 1185 THz (middle) and 1300 THz (right). Simulations based on a HDG- $\mathbb{P}_2$  method. Bottom figure: Scattering cross section.

In the context of the visit of Frédéric Valentin in the team, we have initiated a study aiming at the design of novel multiscale methods for the solution of the time-domain elastodynamic equations, in the spirit of MHM (Multiscale Hybrid-Mixed) methods previously proposed for fluid flow problems. Motivation in that direction naturally came when dealing with non homogeneous anisotropic elastic media as those encountered in geodynamics related applications, since multiple scales are naturally present when high contrast elasticity parameters define the propagation medium. Instead of solving the usual system expressed in terms of displacement or displacement velocity, and stress tensor variables, a hybrid mixed-form is derived in which an additional variable, the Lagrange multiplier, is sought as representing the (opposite) of the surface tension defined at each face of the elements of a given discretization mesh. We consider the velocity/stress formulation of the elastodynamic equations, and study a MHM method defined for a heterogeneous medium where each elastic material is considered as isotropic to begin with. If the source term (the applied given force on the medium) is time independent, and if we are given an arbitrarily coarse conforming mesh (triangulation in 2D, tetrahedrization in 3D), the proposed MHM method consists in first solving a series of fully decoupled (therefore parallelizable) local (element-wise) problems defining parts of the full solution variables which are directly related to the source term, followed by the solution of a global (coarse) problem, which yields the degrees of freedom of both the Lagrange multiplier dependent part of the full solution variables and the Lagrange multiplier itself. Finally, the updating of the full solution variables is obtained by adding each splitted solution variables, before going on the next time step of a leap-frog time integration scheme. Theoretical analysis and implementation of this MHM method where the local problems are discretized with a DG method, are underway.

## 6.3. High performance numerical computing

# 6.3.1. High order HDG schemes and domain decomposition solvers for frequency-domain electromagnetics

**Participants:** Emmanuel Agullo [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Cristobal Samaniego Alvarado [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Mathieu Faverge [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Matthieu Kuhn [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri, Grégoire Pichon [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Pierre Ramet [HIEPACS project-team, Inria Bordeaux - Sud-Ouest].

This work is undertaken in the context of PRACE 5IP (http://www.prace-ri.eu/prace-5ip/) project and aims at the development of scalable frequency-domain electromagnetic wave propagation solvers, in the framework of the HORSE simulation software. HORSE is based on a high order HDG scheme formulated on an unstructured tetrahedral grid for the discretization of the system of three-dimensional Maxwell equations in heterogeneous media, leading to the formulation of large sparse undefinite linear system for the hybrid variable unknowns. This system is solved with domain decomposition strategies that can be either a purely algebraic algorithm working at the matrix operator level (i.e. a black-box solver), or a tailored algorithm designed at the continuous PDE level (i.e. a PDE-based solver). In the former case, we collaborate with the HIEPACS project-team at Inria Bordeaux - Sud-Ouest in view of adapting and exploiting the MaPHyS (Massively Parallel Hybrid Solver - https://gitlab.inria.fr/solverstack/maphys) algebraic hybrid iterative-direct domain decomposition solver. More precisely, this collaboration is concerned with two topics: one one hand, the improvement of the iterative convergence of MaPHyS for the HDG hybrid variable linear system and, on the other hand, the leveraging of low rank compression techniques for reducing the memory footprint of the factorization of subdomain problems using the PaStiX (Parallel Sparse matriX package - http://pastix.gforge.inria.fr/) package.

# 6.3.2. High order HDG schemes and domain decomposition solvers for frequency-domain electromagnetics

**Participants:** Stéphane Lanteri, Laércio Lima Pilla [CORSE project-team, Inria Grenoble - Rhône Alpes], Jean-François Méhaut [CORSE project-team, Inria Grenoble - Rhône Alpes].

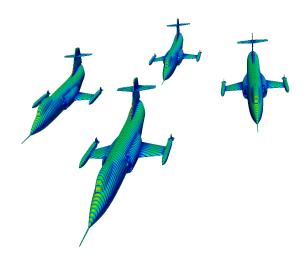


Figure 8. Scattering of a plane wave by a squadron Lockheed F-104 Starfighter. Contour lines of the amplitude of E field. Simulations are performed with a HDG scheme based on a cubic interpolation of the electric and magnetic field unknowns, combined with a PDE-based domain decomposition solver.

This work is undertaken in the context of PRACE 5IP (http://www.prace-ri.eu/prace-5ip/) project and aims at the development of a hybrid MPI/OpenMP parallellization of the DGTD solver of the DIOGENeS software suite. In practice, we concentrated our efforts on identifying and evaluating the best approaches for implementing fine grain parallism of the main DG numerical kernels, based on OpenMP features for loop-based parallelism on one hand, and task-based parallelism on the other hand.

## 6.4. Applications

#### 6.4.1. Gap-plasmon confinement with gold nanocubes

**Participants:** Stéphane Lanteri, Antoine Moreau [Institut Pascal, Université Blaise Pascal], Armel Pitelet [Institut Pascal, Université Blaise Pascal], Claire Scheid, Nikolai Schmitt, Jonathan Viquerat.

The propagation of light in a slit between metals is known to give rise to guided modes. When the slit is of nanometric size, plasmonic effects must be taken into account, since most of the mode propagates inside the metal. Indeed, light experiences an important slowing-down in the slit, the resulting mode being called *gap-plasmon*. Hence, a metallic structure presenting a nanometric slit can act as a light trap, i.e. light will accumulate in a reduced space and lead to very intense, localized fields. Recently, the chemical production of random arrangements of nanocubes on gold films at low cost was proved possible by Antoine Moreau and colleagues at Institut Pascal. Nanocubes are separated from the gold substrate by a dielectric spacer of variable thickness, thus forming a narrow slit under the cube. When excited from above, this configuration is able to support gap-plasmon modes which, once trapped, will keep bouncing back and forth inside the cavity. At visible frequencies, the lossy behavior of metals will cause the progressive absorption of the trapped electromagnetic field, turning the metallic nanocubes into efficient absorbers. The frequencies at which this absorption occurs can be tuned by adjusting the dimensions of the nanocube and the spacer. In collaboration with Antoine Moreau, we propose to study numerically the impact of the geometric parameters of the problem on the behaviour of a single nanocube placed over a metallic slab (see Fig. 9).

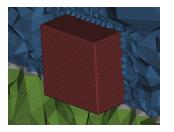




Figure 9. Meshes of rounded nanocubes with rounding radii ranging from 2 to 10 nm. Red cells correspond to the cube. The latter lies on the dielectric spacer (gray cells) and the metallic plate (green). Blue cells represent the air surrounding the device.

#### 6.4.2. Photovoltaics

The ultimate success of photovoltaic (PV) cell technology requires substantial progress in both cost reduction and efficiency improvement. An actively studied approach to simultaneously achieve these two objectives is to leverage *light trapping* schemes. Light trapping allows solar cells to absorb sunlight using an active material layer that is much thinner than the material's intrinsic absorption length. This then reduces the amount of materials used in PV cells, which cuts cell cost in general, and moreover facilitates mass production of PV cells that are based on less abundant materials. In addition, light trapping can improve cell efficiency, since thinner cells provide better collection of photo-generated charge carriers. Enhancing the light absorption in ultrathin film silicon solar cells is thus of paramount importance for improving efficiency and reducing cost. We are involved in several studies in collaboration with physicists that aim at simulating light trapping in complex solar cell structures using high order DG and HDG solvers developed in our core research activities.

#### 6.4.2.1. Light-trapping in texturized thin film solar cells

**Participants:** Urs Aeberhard [IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, German], Karsten Bittkau [IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, German], Alexis Gobé, Stéphane Lanteri.

This work is undertaken in the context of the EoCoE Center of Excellence in collaboration with researchers from IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, Germany. The objective is to design a scalable high order DGTD solver for the simulation of light trapping in a multi-layer solar cell with surface texture. For that purpose, we rely on the DIOGENeS software suite from which we extract a high order DGTD solver for the problem under consideration, taking into account its specificities (in particular, with regards to material models and boundary conditions). We also need to specify and develop a dedicated preprocessing tool for building topography conforming geometrical models. Simulations are performed on the Occigen PRACE system at CINES.

#### 6.4.2.2. Light-trapping in nanocone gratings

**Participants:** Stéphane Collin [Sunlit team, C2N-CNRS, Marcoussi], Alexis Gobé, Julie Goffard [Sunlit team, C2N-CNRS, Marcoussi], Stéphane Lanteri.

There is significant recent interest in designing ultrathin crystalline silicon solar cells with active layer thickness of a few micrometers. Efficient light absorption in such thin films requires both broadband antireflection coatings and effective light trapping techniques, which often have different design considerations. In collaboration with physicists from the Sunlit team at C2N-CNRS, we conduct a numerical study of solar cells based on nanocone gratings. Indeed, it has been previously shown that by employing a double-sided grating design, one can separately optimize the geometries for antireflection and light trapping purposes to achieve broadband light absorption enhancement [47]. In the present study, we adopt the nanocone grating considered in [47]. This structure contains a crystalline silicon thin film with nanocone gratings also made of silicon. The circular

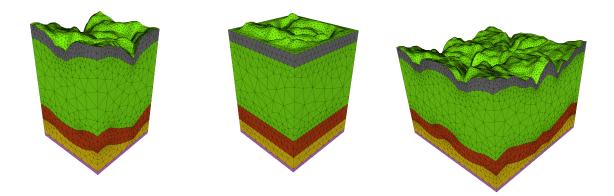


Figure 10. Simulation of light trapping in a multi-layer solar cell with surface texture using a high order DGTD fullwave solver and topography conforming geometrical models.

nanocones form two-dimensional square lattices on both the front and the back surfaces. The film is placed on a perfect electric conductor (PEC) mirror. The ultimate objective of this study is to devise a numerical optimization strategy to infer optimal values of the geometrical characteristics of the nanocone grating on each side of the crystalline silicon thin film. Absorption characteristics are here evaluated using the high order DGTD solver from the DIOGENeS software suite.

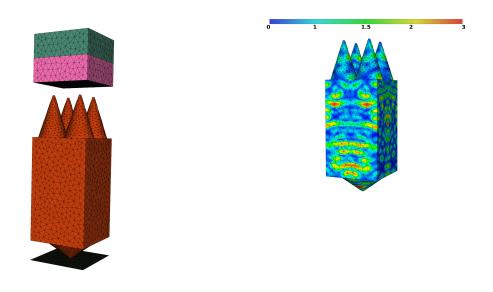


Figure 11. Simulation of light trapping in a solar cell based on nanocone gratings. Geometrical model (left) and contour lines of the module of the DFT of **E** for a wavelength  $\lambda = 857$  nm (right).

#### 6.4.3. Inver design of metasurfaces

**Participants:** Régis Duvigneau [ACUMES project-team, Inria Sophia Antipolis-Méditerranée], Mahmoud Elsawy, Patrice Genevet [CRHEA laboratory, Sophia Antipolis], Stéphane Lanteri.

Metasurfaces are flat surfaces consisting of sub-wavelength nanoresonators, made of plasmonic or high dielectric refractive index materials patterned in a specific way. These flat surfaces provide nearly full control of the light properties in a very short propagation distance with high resolution. By changing the dimensions, shapes, and orientation of these nanoresonators, different functionalities can be obtained. The complexity of the problem and the wide parameter space, make the direct modelling problem insufficient. Recently, several optimization techniques have been applied to the field of nanophotonics (including metasurfaces) by solving an inverse design problem. Generally speaking, there are two classes of optimization techniques that have been used in the metasurface designs; local and global techniques. The local methods depend on the initial guess and most of them require the computation of the gradient, which might be challenging. In addition, they are limited to small parameter space. On the other hand, global optimization techniques are suitable for optimizing several parameters moreover, they do not stuck in a local minima/maxima like the local methods. However, most of the global techniques used in the metasurface designs require costly simulations (for large parameter space), which make them inapplicable for modeling real-life designs that require 3D fullwave solvers. In this study conducted in collaboration with physicists at CRHEA, we use two efficient global optimization techniques based on statistical learning in order to overcome the disadvantageous of usual global optimization methods. The first one is the covariance matrix adaptation evolutionary strategy (CMA-ES). The CMA-ES has been gaining a lot of attention since it requires fewer cost function evaluations compared to the other evolutionary algorithms like genetic algorithms especially for 3D problems that require expensive simulations even with the high-performance computational resources. The second method is the Efficient Global Optimization (EGO) algorithm. The EGO algorithm is based on the surrogate modelling, that is to say, replacing the complex or costly evaluation process by a simpler and cheaper model to reduce dramatically the computational cost (number of calls for the electromagnetic simulations). Both techniques are offered by the Famosa library (http://famosa.gforge.inria.fr), which is developed by R. Duvigneau and colleagues in the ACUMES projectteam.

## **TOSCA Project-Team**

# 5. New Results

## 5.1. Probabilistic numerical methods, stochastic modelling and applications

**Participants:** Mireille Bossy, Nicolas Champagnat, Quentin Cormier, Madalina Deaconu, Olivier Faugeras, Coralie Fritsch, Pascal Helson, Antoine Lejay, Radu Maftei, Victor Martin Lac, Hector Olivero-Quinteros, Émilie Soret, Denis Talay, Etienne Tanré, Milica Tomasevic, Denis Villemonais.

#### 5.1.1. Published works and preprints

- M. Bossy, J. Fontbona (Universidad de Chile, Chile) and H. Olivero-Quinteros (CIMFAV, Valparaíso, Chile) analysed mathematical model for the collective behavior of a fully connected network of finitely many neurons. They obtained that the whole system synchronize, up to some error controlled by the channels noise level. The associated nonlinear McKean-Vlasov equation concentrates, as time goes to infinity, around the dynamics of a single Hodgkin-Huxley neuron with a chemical neurotransmitter channel [42].
- M. Bossy, A. Dupré, P. Drobinski, L. Violeau and C. Briard (Zephyr ENR) obtained advances in stochastic Lagrangian approach for atmospheric boundary layer simulation, on the analysis of an optimal rate of convergence for the particle approximation method, and on validation case with the simulation of a Zephyr ENR wind farm site of six turbines [36].
- M. Di Iorio (Marine Energy Research and Innovation Center, Santiago, Chile), M. Bossy, C. Mokrani (Marine Energy Research and Innovation Center, Santiago, Chile), and A. Rousseau obtained advances in stochastic Lagrangian approaches for the simulation of hydrokinetic turbines immersed in complex topography [33], [50].
- Together with M. Andrade-Restrepo (Univ. Paris Diderot) and R. Ferrière (Univ. Arizona and École Normale Supérieure), N. Champagnat studied deterministic and stochastic spatial eco-evolutionary dynamics along environmental gradients. This work focuses on numerical and analytical analysis of the clustering phenomenon in the population, and on the patterns of invasion fronts [40].
- N. Champagnat and J. Claisse (Ecole Polytechnique) studied the ergodic and infinite horizon controls of discrete population dynamics with almost sure extinction in finite time. This can either correspond to control problems in favor of survival or of extinction, depending on the cost function. They have proved that these two problems are related to the quasi-stationary distribution of the processes controled by Markov controls [16].
- N. Champagnat and B. Henry (Univ. Lille 1) studied a probabilistic approach for the Hamilton-Jacobi limit of non-local reaction-diffusion models of adaptive dynamics when mutations are small. They used a Feynman-Kac interpretation of the partial differential equation and large deviation estimates to obtain a variational characterization of the limit. They also studied in detail the case of finite phenotype space with exponentially rare mutations, where they were able to obtain uniqueness of the limit [17].
- N. Champagnat and D. Villemonais solved a general conjecture on the Fleming-Viot particle systems approximating quasi-stationary distributions (QSD): in cases where several quasi-stationary distributions exist, it is expected that the stationary distribution of the Fleming-Viot processes approaches a particular QSD, called minimal QSD. They proved that this holds true for general absorbed Markov processes with soft obstacles [48].
- N. Champagnat, K. Coulibaly-Pasquier (Univ. Lorraine) and D. Villemonais obtained general criteria for existence, uniqueness and exponential convergence in total variation to QSD for multidimensional diffusions in a domain absorbed at its boundary [37]. These results improve and simplify the existing results and methods.

- N. Champagnat and D. Villemonais obtained contraction properties in total variation of general penalized processes, including time-inhomogeneous Markov processes with absorption and Markov processes in varying environments [20]. Their method allows to improve significantly the former results of [62], [63].
- N. Champagnat and D. Villemonais studied with R. Schott (Univ. Lorraine) models of deadlocks in distributed systems. They use the approach developped recently by the first two authors to study quasi-stationary distributions in order to characterize and compute numerically the asymptotic behaviour of the deadlock time and the behaviour of the system before deadlock, both for discrete and for diffusion models [47].
- A. Lejay and A. Brault have followed their work on rough flow, which provides an unified framework to deal with the theory of rough paths from the points of view of flows. In particular, they have shown existence of flows even when the associated rough differential equations have multiple solutions [44], [45].
- A. Lejay and P. Pigato have provided an estimator of the diffusion and drift coefficients when they are discontinuous at a threshold. These estimators have been applied to financial data and exhibit leverage as well as mean-reversion effects on S&P 500 stocks' prices [57], [30]
- A. Lejay, L. Lenôtre and G. Pichot have proposed a new Monte Carlo method based on random exponential time steps to deal with discontinuous diffusions coefficients and drift [35], [56]
- A. Lejay, S. Haraketi and E. Haoula have shown how to construct a diffusion on the Sierpinski gasket lifted to the Heisenberg group [53].
- J. Bion-Nadal (Ecole Polytechnique) and D. Talay have pursued their work on a Wasserstein-type distance on the set of the probability distributions of strong solutions to stochastic differential equations. This new distance is defined by restricting the set of possible coupling measures and can be expressed in terms of the solution to a stochastic control problem, which allows one to deduce a priori estimates or to obtain numerical evaluations: cf. [41]. This solution is now shown to exist and be smooth even in cases where the infinitesimal generators of the considered diffusion processes are not strongly elliptic.

A notable application concerns the following modeling issue: given an exact diffusion model, how to select a simplified diffusion model within a class of admissible models under the constraint that the probability distribution of the exact model is preserved as much as possible? The objective being to select a model minimizing the above distance to a target model, the construction and analysis of an efficient stochastic algorithm are being in progress.

- In [60] D. Talay and M. Tomasevic have developed and analysed a new type of stochastic interpretation of the one-dimensional parabolic-parabolic Keller-Segel systems. It involves an original type of McKean-Vlasov interaction kernel. At the particle level, each particle interacts with all the past of each other particle. At the mean-field level studied here, the McKean-Vlasov limit process interacts with all the past time marginals of its probability distribution. In [12] M. Tomasevic has proven that the two-dimensional parabolic-parabolic Keller-Segel system in the whole Euclidean space and the corresponding McKean-Vlasov stochastic differential equation are well-posed under some explicit conditions on the parameters of the model.
- D. Talay and M. Tomasevic are studying the well-posedness and the propagation of chaos of the particle system related to the two-dimensional parabolic-parabolic Keller-Segel system. The singularity of the interaction kernel being more critical than in the one-dimensional case, the preceding analysis [26] cannot be extended and a fully new methodology needs to be developed.
- V. Martin Lac, D. Talay and M. Tomasevic have worked on theoretical and algorithmic questions related to the simulation of the Keller–Segel particle systems. A preliminary version of a library has been developed.
- H. Olivero (Inria, now University of Valparaiso, Chile) and D. Talay have constructed and analysed an hypothesis test which helps to detect when the probability distribution of complex stochastic

simulations has an heavy tail and thus possibly an infinite variance. This issue is notably important when simulating particle systems with complex and singular McKean-Vlasov interaction kernels whick make it extremely difficult to get a priori estimates on the probability laws of the mean-field limit, the related particle system, and their numerical approximations. In such situations the standard limit theorems do not lead to effective tests. In the simple case of independent and identically distributed sequences the procedure developed this year and its convergence analysis are based on deep tools coming from the statistics of semimartingales.

- V. Martin Lac, H. Olivero-Quinteros and D. Talay have worked on theoretical and algorithmic questions related to the simulation of large particle systems under singular interactions and to critical numerical issues related to the simulation of independent random variables with heavy tails. A preliminary version of a library has been developed.
- C. Graham (École Polytechnique) and D. Talay are ending and polishing the second volume of their series on Mathematical Foundation of Stochastic Simulation to be published by Springer.
- P-E. Jabin (University of Maryland) and D. Talay have ended their work on a mean-field game and shown the convergence of the joint density function of the controlled particle system. The construction of the limit has required the construction of suitable Sobolev spaces on sets of probability measures on Polish spaces.
- E. Tanré and Pierre Guiraud (Univ. of Valparaíso) have worked on the synchronization in a model of network of noisy biological neurons. Using a large deviation principle, they prove the stability of the synchronized state under stochastic perturbations. They also give a lower bound on the probability of synchronization for networks which are not initially synchronized. This bound shows the robustness of the emergence of synchronization in presence of small stochastic perturbations [25].
- E. Tanré, P. Grazieschi (Univ. Warwick), M. Leocata (Univ. Pisa), C. Mascart (Univ. Côte d'Azur), J. Chevallier (Univ. of Grenoble) and F. Delarue (Univ. Côte d'Azur) have extended the previous work [9] to sparse networks of interacting neurons. They have obtained a precise description of the limit behavior of the mean field limit according to the probability of (random) interactions between two individual LIF neurons [52].
- E. Tanré has worked with Nicolas Fournier (Sorbonne Université) and Romain Veltz (MATHNEURO Inria team) on a network of spiking networks with propagation of spikes along the dendrites. Consider a large number n of neurons randomly connected. When a neuron spikes at some rate depending on its electric potential, its membrane potential is set to a minimum value v<sub>min</sub>, and this makes start, after a small delay, two fronts on the dendrites of all the neurons to which it is connected. Fronts move at constant speed. When two fronts (on the dendrite of the same neuron) collide, they annihilate. When a front hits the soma of a neuron, its potential is increased by a small value w<sub>n</sub>. Between jumps, the potentials of the neurons are assumed to drift in [v<sub>min</sub>, ∞), according to some well-posed ODE. They prove the existence and uniqueness of a heuristically derived mean-field limit of the system when n → ∞ [51].
- E. Tanré has worked with Patricio Orio (CINV, Chile) and Alexandre Richard (Centrale-Supelec) on the modelling and measurement of long-range dependence in neuronal spike trains. They exhibit evidence of memory effect in genuine neuronal data and compared a fractional integrate-and-fire model with the existing Markovian models [31].
- Q. Cormier and E. Tanré studied with Romain Veltz (team MATHNEURO) the long time behavior of a McKean-Vlasov SDE modeling a large assembly of neurons. A convergence to the unique (in this case) invariant measure is obtained assuming that the interactions between the neurons are weak enough. The key quantity in this model is the "firing rate": it gives the average number of jumps per unit of times of the solution of the SDE. They derive a non-linear Voltera equation satisfied by this rate. They used methods from integral equation to control finely the long time behavior of this firing rate [49].

- D. Villemonais collaborates with the Gerontology Service of CHRU Nancy on statistics of time evolution of telomere lengths in human blood cells. This is a collaboration with Anne Gégout Petit (IECL, Inria BIGS), Simon Toupance (CHRU Nancy), Eliane Albuisson (CHRU Nancy), Athanasios Benetos (CHRU Nancy), Daphnée Germain (Ecole des Mines de Nancy). They proposed in [32] a telomeric signature for human beings, stable along age evolution. Lionel Lenôtre works as a post-doc on this topic within the project GEENAGE of LUE.
- D. Villemonais studied with C. Coron (Univ. Paris-Saclay) and S. Méléard (École Polytechnique) the extinction probability before fixation for multi-dimensional models of Wright-Fisher type with mutations [21].
- In collaboration with E. Horton and A. Kyprianou (University of Bath), D. Villemonais studied the large-time asymptotic behaviour of the neutron transport equation in a three-dimensional domain [55]. This work is motivated by the simulation of the flow of particles in a nuclear tank.
- D. Villemonais studied with C. Mailler (University of Bath) the asymptotic behaviour of generalized measure-valued Polya urn models taking values in non-compact sets, using techniques from the theory of stochastic algorithms [58].

## 5.1.2. Other works in progress

- N. Champagnat, C. Fritsch and S. Billiard (Univ. Lille) are working on food web modeling.
- N. Champagnat and D. Villemonais are working with M. Benaïm (Univ. Neuchatel) on the convergence of stochastic algorithms to the quasi-stationary distribution of diffusion processes absorbed at the boundary of a domain.
- N. Champagnat is working with S. Méléard (École Polytechnique) and C. Tran Viet (Univ. Lille 1) on evolutionary models of bacteria with horizontal transfer. They study a scaling of parameters taking into account the influence of negligible but non-extinct populations, allowing to study specific phenomena observed in these models (re-emergence of traits, cyclic evolutionary dynamics and evolutionary suicide).
- Q. Cormier is investigating new methods to explore the long time behavior of the McKean-Vlasov SDE of [49], to go beyond the weak interactions case. The long time behavior of such McKean-Vlasov equations can be intricate as there can be multiple invariant measures or stable oscillations of the law of the process. The objective of this work is to develop (numerical and theoretical) methods to check the local stability of a given invariant measure of this non-linear SDE.
- C. Fritsch is working with A. Gégout-Petit (Univ. Lorraine and EPI BIGS), B. Marçais (INRA, Nancy) and M. Grosdidier (INRA, Avignon) on a statistical analysis of a Chalara Fraxinea model [34].
- C. Fritsch is working with Marianne Clausel (Univ. Lorraine) and Julien Trombini (Two-I) on the modeling of emotions spreading in a crowd.
- A. Lejay and A. Brault (U. Paris Descartes) continue their work to extend the framework of rough flows.
- O. Faugeras (MATHNEURO Inria Research Team), É. Soret (joint postdoc with MATHNEURO Inria Research Team) and É. Tanré are working on Mean-Field description of thermodynamics limits of large population of neurons with random interactions. They study the asymptotic behaviour for an asymmetric neuronal dynamics in a network of linear Hopfield neurons. They obtain the convergence in law of each component to a Gaussian process. The limit object is not a Markov process.
- P. Helson, E. Tanré and R. Veltz (MATHNEURO Inria team), are working on a neural network model of memory. The aim is to propose a new retrieval criterion and its mathematical analysis.
- E. Tanré has worked with Alexandre Richard (Centrale-Supelec) and Soledad Torres (Universidad de Valparaíso, Chile) on a one-dimensional fractional SDE reflected on the line. The existence and uniqueness of this process is known in the case where the Hurst parameter *H* of the noise (fBM) is larger than 0.5. They have proved the existence of a penalization scheme (suited to numerical approximation) to approach this object.

## **ABS Project-Team**

## 5. New Results

## 5.1. Modeling interfaces and contacts

Keywords: docking, scoring, interfaces, protein complexes, Voronoi diagrams, arrangements of balls.

#### 5.1.1. Origin of Public Memory B Cell Clones in Fish After Antiviral Vaccination

Participants: F. Cazals, S. Marillet.

In collaboration with S. Magadan, L. Jouneau, S. Marillet, P. Boudinot (INRA, Virologie et Immunologie Moléculaires, Université Paris-Saclay, Jouy-en-Josas, France); M. Puelma Touzel, T. Mora, A. Walczak (Laboratoire de Physique Théorique, CNRS, Sorbonne Université, and Ecole Normale Supérieure (PSL), Paris, France); W. Chaara, A. Six (Sorbonne Université, INSERM, UMR S 959, Immunology-Immunopathology -Immunotherapy (I3), Paris, France); E. Quillet (INRA, Génétique Animale et Biologie Intégrative, Université Paris-Saclay, Jouy-en-Josas, France); O. Sunyer (Department of Pathobiology, School of Veterinary Medicine, University of Pennsylvania, Philadelphia, PA, United States); S. Fillatreau (INEM, INSERM U1151/CNRS UMR8253, Institut Necker-Enfants Malades, Faculté de Médecine Paris Descartes, Paris, France; Faculté de Médecine, Université Paris Descartes, Sorbonne Paris Cité, Paris, France; Assistance Publique des Hopitaux de Paris (AP-HP), Hopital Necker Enfants Malades, Paris, France).

Vaccination induces *public* antibody clonotypes common to all individuals of a species, that may mediate universal protection against pathogens. Only few studies tried to trace back the origin of these public B-cell clones. Here [16] we used Illumina sequencing and computational modeling to unveil the mechanisms shaping the structure of the fish memory antibody response against an attenuated Viral Hemorrhagic Septicemia rhabdovirus. After vaccination, a persistent memory response with a public VH5JH5 IgM component was composed of dominant antibodies shared among all individuals. The rearrangement model showed that these public junctions occurred with high probability indicating that they were already favored before vaccination due to the recombination process, as shown in mammals. In addition, these clonotypes were in the naive repertoire associated with larger similarity classes, composed of junctions differing only at one or two positions by amino acids with comparable properties. The model showed that this property was due to selective processes exerted between the recombination and the naive repertoire. Finally, our results showed that public clonotypes greatly expanded after vaccination displayed several VDJ junctions differing only by one or two amino acids with similar properties, highlighting a convergent response. The fish public memory antibody response to a virus is therefore shaped at three levels: by recombination biases, by selection acting on the formation of the pre-vaccination repertoire, and by convergent selection of functionally similar clonotypes during the response. We also show that naive repertoires of IgM and IgT have different structures and sharing between individuals, due to selection biases. In sum, our comparative approach identifies three conserved features of the antibody repertoire associated with public memory responses. These features were already present in the last common ancestors of fish and mammals, while other characteristics may represent speciesspecific solutions.

## 5.2. Modeling macro-molecular assemblies

**Keywords:** macro-molecular assembly, reconstruction by data integration, proteomics, mass spectrometry, modeling with uncertainties, connectivity inference.

5.2.1. Complexity Dichotomies for the Minimum F-Overlay Problem – Application for low resolution models of macro-molecular assemblies Participant: D. Mazauric. In collaboration with N. Cohen (CNRS, Laboratoire de Recherche en Informatique) and F. Havet (CNRS, Inria/I3S project-team Coati) and I. Sau (CNRS, Laboratoire d'Informatique de Robotique et de Microélectronique de Montpellier) and R. Watrigant (University Lyon I, Laboratoire de l'Informatique du Parallélisme).

In this article [14], we analyze a generalization of the minimum connectivity inference problem (MCI). MCI models the computation of low-resolution structures of macro-molecular assemblies, based on data obtained by native mass spectrometry. The generalization studied in this article, allows us to consider more refined constraints for the characterization of low resolution models of large assemblies. We model this problem by using hypergraphs: for a (possibly infinite) fixed family of graphs F, we say that a graph Goverlays F on a hypergraph H if V(H) is equal to V(G) and the subgraph of G induced by every hyperedge of H contains some member of F as a spanning subgraph. While it is easy to see that the complete graph on |V(H)| overlays F on a hypergraph H whenever the problem admits a solution, the Minimum F-Overlay problem asks for such a graph with at most k edges, for some given  $k \in \mathbb{N}$ . This problem allows to generalize some natural problems which may arise in practice. For instance, if the family F contains all connected graphs, then Minimum F-Overlay corresponds to the MCI problem. Our main contribution is a strong dichotomy result regarding the polynomial vs. NP-complete status with respect to the considered family F. Roughly speaking, we show that the easy cases one can think of (e.g. when edgeless graphs of the right sizes are in F, or if F contains only cliques) are the only families giving rise to a polynomial problem: all others are NP-complete. We then investigate the parameterized complexity of the problem and give similar sufficient conditions on F that give rise to W[1]-hard, W[2]-hard or FPT problems when the parameter is the size of the solution.

## 5.3. Modeling the flexibility of macro-molecules

Keywords: protein, flexibility, collective coordinate, conformational sampling dimensionality reduction.

# **5.3.1.** Characterizing molecular flexibility by combining *IRMSD* measures **Participants:** F. Cazals, R. Tetley.

The root mean square deviation (RMSD) and the least RMSD are two widely used similarity measures in structural bioinformatics. Yet, they stem from global comparisons, possibly obliterating locally conserved motifs. We correct these limitations with the so-called combined RMSD [26], which mixes independent IRMSD measures, each computed with its own rigid motion. The combined RMSD is relevant in two main scenarios, namely to compare (quaternary) structures based on motifs defined from the sequence (domains, SSE), and to compare structures based on structural motifs yielded by local structural alignment methods. We illustrate the benefits of combined RMSD over the usual RMSD on three problems, namely (i) the assignment of quaternary structures for hemoglobin (scenario #1), (ii) the calculation of structural phylogenies (case study: class II fusion proteins; scenario #1), and (iii) the analysis of conformational changes based on combined RMSD of rigid structural motifs (case study: one class II fusion protein; scenario #2). Using these, we argue that the combined RMSD is a tool a choice to perform positive and negative discrimination of degree of freedom, with applications to the design of move sets and collective coordinates. Combined RMSD are available within the Structural Bioinformatics Library (http://sbl.inria.fr).

#### 5.3.2. Multiscale analysis of structurally conserved motifs

Participants: F. Cazals, R. Tetley.

This work [25] develops a generic framework to perform a multiscale structural analysis of two structures (homologous proteins, conformations) undergoing conformational changes. Practically, given a seed structural alignment, we identify structural motifs with a hierarchical structure, characterized by three unique properties. First, the hierarchical structure sheds light on the trade-off between size and flexibility. Second, motifs can be combined to perform an overall comparison of the input structures in terms of combined RMSD, an improvement over the classical least RMSD. Third, motifs can be used to seed iterative aligners, and to design hybrid sequence-structure profile HMM characterizing protein families. From the methods standpoint, our framework is reminiscent from the bootstrap and combines concepts from rigidity analysis (distance difference matrices), graph theory, computational geometry (space filling diagrams), and topology (topological

persistence). On challenging cases (class II fusion proteins, flexible molecules) we illustrate the ability of our tools to localize conformational changes, shedding light of commonalities of structures which would otherwise appear as radically different. Our tools are available within the Structural Bioinformatics Library (http://sbl.inria.fr). We anticipate that they will be of interest to perform structural comparisons at large, and for remote homology detection.

# 5.3.3. Hybrid sequence-structure based HMM models leverage the identification of homologous proteins: the example of class II fusion proteins

Participants: F. Cazals, R. Tetley.

#### In collaboration with P. Guardado-Calvo, J. Fedry, and F. Rey (Inst. Pasteur Paris, France).

In [27], we present a sequence-structure based method characterizing a set of functionally related proteins exhibiting low sequence identity and loose structural conservation. Given a (small) set of structures, our method consists of three main steps. First, pairwise structural alignments are combined with multi-scale geometric analysis to produce structural motifs i.e. regions structurally more conserved than the whole structures. Second, the sub-sequences of the motifs are used to build profile hidden Markov models (HMM) biased towards the structurally conserved regions. Third, these HMM are used to retrieve from UniProtKB proteins harboring signatures compatible with the function studied, in a bootstrap fashion. We apply these hybrid HMM to investigate two questions related to class II fusion proteins, an especially challenging class since known structures exhibit low sequence identity (less than 15%) and loose structural similarity (of the order of 15A in IRMSD ). In a first step, we compare the performances of our hybrid HMM against those of sequence based HMM. Using various learning sets, we show that both classes of HMM retrieve unique species. The number of unique species reported by both classes of methods are comparable, stressing the novelty brought by our hybrid models. In a second step, we use our models to identify 17 plausible HAP2-GSC1 candidate sequences in 10 different drosophila melanogaster species. These models are not identified by the PFAM family HAP2-GCS1 (PF10699), stressing the ability of our structural motifs to capture signals more subtle than whole Pfam domains. In a more general setting, our method should be of interest for all cases functional families with low sequence identity and loose structural conservation. Our software tools are available from the FunChaT package of the Structural Bioinormatics Library (http://sbl.inria.fr).

# 5.3.4. Hamiltonian Monte Carlo with boundary reflections, and application to polytope volume calculations

#### Participants: F. Cazals, A. Chevallier.

#### In collaboration with S. Pion (Auctus, Inria Bordeaux).

This paper [23] studies HMC with reflections on the boundary of a domain, providing an enhanced alternative to Hit-and-run (HAR) to sample a target distribution in a bounded domain. We make three contributions. First, we provide a convergence bound, paving the way to more precise mixing time analysis. Second, we present a robust implementation based on multi-precision arithmetic – a mandatory ingredient to guarantee exact predicates and robust constructions. Third, we use our HMC random walk to perform polytope volume calculations, using it as an alternative to HAR within the volume algorithm by Cousins and Vempala. The tests, conducted up to dimension 50, show that the HMC RW outperforms HAR.

### 5.3.5. Wang-Landau Algorithm: an adapted random walk to boost convergence

Participants: F. Cazals, A. Chevallier.

The Wang-Landau (WL) algorithm is a recently developed stochastic algorithm computing densities of states of a physical system. Since its inception, it has been used on a variety of (bio-)physical systems, and in selected cases, its convergence has been proved. The convergence speed of the algorithm is tightly tied to the connectivity properties of the underlying random walk. As such, we propose in [22] an efficient random walk that uses geometrical information to circumvent the following inherent difficulties: avoiding overstepping strata, toning down concentration phenomena in high-dimensional spaces, and accommodating multidimensional distribution. Experiments on various models stress the importance of these improvements to

make WL effective in challenging cases. Altogether, these improvements make it possible to compute density of states for regions of the phase space of small biomolecules.

## **5.4. Algorithmic foundations**

Keywords: Computational geometry, computational topology, optimization, data analysis.

Making a stride towards a better understanding of the biophysical questions discussed in the previous sections requires various methodological developments discussed below.

### 5.4.1. A Sequential non-parametric multivariate two-sample test

Participant: F. Cazals.

In collaboration with A. Lhéritier (Amadeus, France).

Given samples from two distributions, a nonparametric two-sample test aims at determining whether the two distributions are equal or not, based on a test statistic. Classically, this statistic is computed on the whole dataset, or is computed on a subset of the dataset by a function trained on its complement. We consider methods in a third tier [15], so as to deal with large (possibly infinite) datasets, and to automatically determine the most relevant scales to work at, making two contributions. First, we develop a generic sequential nonparametric testing framework, in which the sample size need not be fixed in advance. This makes our test a truly sequential nonparametric multivariate two-sample test. Under information theoretic conditions qualifying the difference between the tested distributions, consistency of the two-sample test is established. Second, we instantiate our framework using nearest neighbor regressors, and show how the power of the resulting two-sample test can be improved using Bayesian mixtures and switch distributions. This combination of techniques yields automatic scale selection, and experiments performed on challenging datasets show that our sequential tests exhibit comparable performances to those of state-of-the-art nonsequential tests.

#### 5.4.2. Comparing two clusterings using matchings between clusters of clusters

Participants: F. Cazals, D. Mazauric, R. Tetley.

In collaboration with R. Watrigant (University Lyon I, Laboratoire de l'Informatique du Parallélisme, France).

Clustering is a fundamental problem in data science, yet, the variety of clustering methods and their sensitivity to parameters make clustering hard. To analyze the stability of a given clustering algorithm while varying its parameters, and to compare clusters yielded by different algorithms, several comparison schemes based on matchings, information theory and various indices (Rand, Jaccard) have been developed. We go beyond these by providing a novel class of methods computing meta-clusters within each clustering-a meta-cluster is a group of clusters, together with a matching between these. Let the intersection graph of two clusterings be the edge-weighted bipartite graph in which the nodes represent the clusters, the edges represent the non empty intersection between two clusters, and the weight of an edge is the number of common items. We introduce the so-called D-family-matching problem on intersection graphs, with D the upper-bound on the diameter of the graph induced by the clusters of any meta-cluster. First we prove NP-completeness and APX-hardness results, and unbounded approximation ratio of simple strategies. Second, we design exact polynomial time dynamic programming algorithms for some classes of graphs (in particular trees). Then, we prove spanning-tree based efficient algorithms for general graphs. Our experiments illustrate the role of D as a scale parameter providing information on the relationship between clusters within a clustering and in-between two clusterings. They also show the advantages of our built-in mapping over classical cluster comparison measures such as the variation of information (VI).

# 5.4.3. How long does it take for all users in a social network to choose their communities? Participant: D. Mazauric.

In collaboration with J.-C. Bermond (Inria/I3S project-team Coati) and A. Chaintreau (Columbia University in the city of New York) and G. Ducoffe (National Institute for Research and Development in Informatics and Research Institute of the University of Bucharest). We consider a community formation problem in social networks, where the users are either friends or enemies. The users are partitioned into conflict-free groups (*i.e.*, independent sets in the *conflict graphG<sup>-</sup>* = (V, E) that represents the enmities between users). The dynamics goes on as long as there exists any set of at most k users, k being any fixed parameter, that can change their current groups in the partition *simultaneously*, in such a way that they all strictly increase their utilities (number of friends *i.e.*, the cardinality of their respective groups minus one). Previously, the best-known upper-bounds on the maximum time of convergence were  $O(|V|\alpha(G^-))$  for  $k \leq 2$  and  $O(|V|^3)$  for k = 3, with  $\alpha(G^-)$  being the independence number of  $G^-$ . Our first contribution in this paper consists in reinterpreting the initial problem as the study of a dominance ordering over the vectors of integer partitions. With this approach, we obtain for  $k \leq 2$  the tight upper-bound  $O(|V|\min\{\alpha(G^-), \sqrt{|V|}\})$  and, when  $G^-$  is the empty graph, the exact value of order  $\frac{(2|V|)^{3/2}}{3}$ . The time of convergence, for any fixed  $k \geq 4$ , was conjectured to be polynomial [35], [41]. In this paper we disprove this. Specifically, we prove that for any  $k \geq 4$ , the maximum time of convergence is an  $\Omega(|V|^{\Theta(\log |V|)})$ .

# See [19] for details.

#### 5.4.4. Sequential metric dimension

#### Participant: D. Mazauric.

In collaboration with J. Bensmail (13S, Inria/13S project-team Coati) and F. Mc Inerney (Inria/13S projectteam Coati) and N. Nisse (Inria, Inria/13S project-team Coati) and S. Pérennes (CNRS, Inria/13S project-team Coati).

In the localization game, introduced by Seager in 2013, an invisible and immobile target is hidden at some vertex of a graph G. At every step, one vertex v of G can be probed which results in the knowledge of the distance between v and the secret location of the target. The objective of the game is to minimize the number of steps needed to locate the target whatever be its location.

We address the generalization of this game where  $k \ge 1$  vertices can be probed at every step. Our game also generalizes the notion of the *metric dimension* of a graph. Precisely, given a graph G and two integers  $k, \ell \ge 1$ , the *localization* problem asks whether there exists a strategy to locate a target hidden in G in at most  $\ell$  steps and probing at most k vertices per step. We first show that, in general, this problem is NP-complete for every fixed  $k \ge 1$  (resp.,  $\ell \ge 1$ ). We then focus on the class of trees. On the negative side, we prove that the localization problem is NP-complete in trees when k and  $\ell$  are part of the input. On the positive side, we design a (+1)-approximation for the problem in n-node trees, *i.e.*, an algorithm that computes in time  $O(n \log n)$  (independent of k) a strategy to locate the target in at most one more step than an optimal strategy. This algorithm can be used to solve the localization problem in trees in polynomial time if k is fixed.

We also consider some of these questions in the context where, upon probing the vertices, the relative distances to the target are retrieved. This variant of the problem generalizes the notion of the *centroidal dimension* of a graph.

See [17], [18], [21] for details.

# **ATHENA Project-Team**

# 6. New Results

## 6.1. Computational Diffusion MRI

### 6.1.1. Reducing the Number of Samples in Spatio-Temporal dMRI Acquisition Design

**Participants:** Patryk Filipiak, Rutger Fick [TheraPanacea, Paris], Alexandra Petiet [ICM, CENIR, Paris], Mathieu Santin [ICM, CENIR, Paris], Anne-Charlotte Philippe [ICM, CENIR, Paris], Stéphane Lehericy [ICM, CENIR, Paris], Philippe Ciuciu [CEA, Université Paris-Saclay], Demian Wassermann [Inria Parietal], Rachid Deriche.

Acquisition time is a major limitation in recovering brain white matter microstructure with diffusion magnetic resonance imaging. The aim of this work is to bridge the gap between growing demands on spatiotemporal resolution of diffusion signal and the real-world time limitations. We introduce an acquisition scheme that reduces the number of samples under adjustable quality loss. Finding a sampling scheme that maximizes signal quality and satisfies given time constraints is NP-hard. Therefore, a heuristic method based on a genetic algorithm is proposed in order to find suboptimal solutions in acceptable time. The analyzed diffusion signal representation is defined in the  $q\tau$  space, so that it captures both spatial and temporal phenomena. The experiments on synthetic data and in vivo diffusion images of the C57Bl6 wild-type mouse corpus callosum reveal superiority of the proposed approach over random sampling and even distribution in the  $q\tau$  space.

This work has been published in [12].

# 6.1.2. Dmipy, a Diffusion Microstructure Imaging toolbox in Python to improve research reproducibility

**Participants:** Abib Olushola Yessouffou Alimi, Rutger Fick [TheraPanacea, Paris], Demian Wassermann [Inria Parietal], Rachid Deriche.

The recovery of microstructure-related features of the brain's white matter is a current challenge in diffusion MRI (dMRI). In particular, multi-compartment (MC)-based models have been a popular approach to estimate these features. However, the usage of MC-models is often limited to those hard-coded in publicly available toolboxes.

In this work, we present Diffusion Microstructure Imaging in Python (Dmipy), a diffusion MRI toolbox which allows accessing any multi-compartment-based model and robustly estimates these important features from single-shell, multi-shell, and multi-diffusion time, and multi-TE data. Dmipy follows a *building block*-based philosophy to microstructure imaging, meaning an MC-model can be constructed and fitted to dMRI data using any combination of underlying tissue models, axon dispersion or diameter distributions, and optimization algorithms.using less than 10 lines of code, thus helps improve research reproducibility. In describing the toolbox, we show how Dmipy enables to easily design microstructure models and offers to the users the freedom to choose among different optimization strategies.We finally present three advanced examples of highly complex modeling approaches which are made easy using Dmipy.

This work has been published in [21], [30].

### 6.1.3. Non-parametric graphnet-regularized representation of dMRI in space and time

**Participants:** Rutger Fick [TheraPanacea, Paris], Alexandra Petiet [ICM, CENIR, Paris], Mathieu Santin [ICM, CENIR, Paris], Anne-Charlotte Philippe [ICM, CENIR, Paris], Stéphane Lehericy [ICM, CENIR, Paris], Demian Wassermann [Inria Parietal], Rachid Deriche.

Effective representation of the four-dimensional diffusion MRI signal-varying over three-dimensional q-space and diffusion time  $\tau$  – is a sought-after and still unsolved challenge in diffusion MRI (dMRI). We propose a functional basis approach that is specifically designed to represent the dMRI signal in this q $\tau$ -space. Following recent terminology, we refer to our q $\tau$ -functional basis as  $q\tau$ -dMRI. q $\tau$ -dMRI can be seen as a time-dependent realization of q-space imaging by Paul Callaghan and colleagues. We use GraphNet regularization - imposing both signal smoothness and sparsity – to drastically reduce the number of diffusion-weighted images (DWIs) that is needed to represent the dMRI signal in the q $\tau$ -space. As the main contribution, q $\tau$ -dMRI provides the framework to – without making biophysical assumptions - represent the q $\tau$ -space signal and estimate timedependent q-space indices (q $\tau$ -indices), providing a new means for studying diffusion in nervous tissue. We validate our method on both in-silico generated data using Monte–Carlo simulations and an in-vivo test-retest study of two C57Bl6 wild-type mice, where we found good reproducibility of estimated q $\tau$ -index values and trends. In the hope of opening up new  $\tau$ -dependent venues of studying nervous tissues, q $\tau$ -dMRI is the first of its kind in being specifically designed to provide open interpretation of the q $\tau$ -diffusion signal.

This work has been published in [11].

# 6.1.4. Resolving the crossing/kissing fiber ambiguity using functionallyCOMMIT ( Convex Optimization Modeling for Microstructure Informed Tractography)

Participants: Matteo Frigo, Isa Costantini, Samuel Deslauriers-Gauthier, Rachid Deriche.

The architecture of the white matter is endowed with kissing and crossing bundles configurations. When these white matter tracts are reconstructed using diffusion MRI tractography, this systematically induces the reconstruction of many fiber tracts that are not coherent with the structure of the brain. The question on how to discriminate between true positive connections and false positive connections is the one addressed in this work. State-of-the-art techniques provide a partial solution to this problem by considering anatomical priors in the false positives detection process. We propose a novel model that tackles the same issue but takes into account both structural and functional information by combining them in a convex optimization problem. We validate it on two toy phantoms that reproduce the kissing and the crossing bundles configurations, showing that, through this approach, we are able to correctly distinguish true positives and false positives.

This work has been published in [25].

# 6.1.5. Reducing false positive connection in tractograms using joint structure-function filtering

**Participants:** Matteo Frigo, Guillermo Gallardo Diez, Isa Costantini, Alessandro Daducci [EPFL, Lausanne], Demian Wassermann [Inria Parietal], Samuel Deslauriers-Gauthier, Rachid Deriche.

Due to its ill-posed nature, tractography generates a significant number of false positive connections between brain regions. To reduce the number of false positives, Daducci et al. proposed the COMMIT framework, which has the goal of re-establishing the link between tractography and tissue microstructure. In this framework, the diffusion MRI signal is modeled as a linear combination of local models associated with streamlines where the weights are identified by solving a convex optimization problem. Streamlines with a weight of zero do not contribute to the diffusion MRI data and are assumed to be false positives. Removing these false positives yields a subset of streamlines supporting the anatomical data. However, COMMIT does not make use of the link between structure and function and thus weights all bundles equally. In this work, we propose a new strategy that enhances the COMMIT framework by injecting the functional information provided by functional MRI. The result is an enhanced tractogram filtering strategy that considers both functional and structural data.

This work has been published in [31].

# 6.1.6. Combining Improved Euler and Runge-Kutta 4th order for Tractography in Diffusion-Weighted MRI

**Participants:** Cherifi Dalila [IEEE University of Boumerdes, Algeria], Boudjada Messaoud [IEEE University of Boumerdes, Algeria], Morsli Abdelatif [IEEE University of Boumerdes, Algeria], Girard Gabriel [EPFL, Lausanne], Rachid Deriche.

In this work, we develop a general, deterministic tractography algorithm (CIERTE), which is a combination of Improved Euler and Range-Kutta fourth-order algorithm and test it on synthetic and real data. The proposed tractography method is validated using seven metrics of the tractometer evaluation system and positively compared to state-of-the-art tractography algorithms.

This work has been published in [9].

# 6.1.7. Fiber orientation distribution function from non-negative sparse recovery with quantitative analysis of local fiber orientations and tractography using DW-MRI datasets

**Participants:** Thinhinane Megherbi [USTHB, Algiers], Gabriel Girard [EPFL, Lausanne], Ghosh Aurobrata [AI Innovation Lab, Verisk Analytics], Fatima Oulebsir-Boumghar [USTHB, Algiers], Rachid Deriche.

In this work, we propose, evaluate and validate a new Diffusion Weighted MRI method to model and recover high quality tractograms even with multiple fiber populations in a voxel and from a limited number of acquisitions.

Our method relies on the estimation of the Fiber Orientation Distribution (FOD) function, parameterized as a non-negative sum of rank-1 tensors and the use of a non-negative sparse recovery scheme to efficiently recover the tensors, and their number. Each fiber population of a voxel is characterized by the orientation and the weight of a rank-1 tensor.

Using both deterministic and probabilistic tractography algorithms, we show that our method is able to accurately reconstruct narrow crossing fibers and obtain a high quality connectivity reconstruction even from a limited number of acquisitions. To this end, a validation scheme based on the connectivity recovered from tractography is developed to quantitatively evaluate and analyze the performance of our method. The tractometer tool is used to quantify the tractography obtained from a simulated DW-MRI dataset including a high angular resolution dataset of 60 gradient directions and a dataset of 30 gradient directions, each of them corrupted with Rician noise of SNR 10 and 20. The performance of our FOD model and its impact on the tractography results are also demonstrated and illustrated on in vivo DW-MRI datasets with high and low angular resolutions.

This work has been published in [15].

### 6.1.8. Solving the Cross-Subject Parcel Matching Problem Using Optimal Transport

**Participants:** Guillermo Gallardo Diez, Nathalie Gayraud, Maureen Clerc, Demian Wassermann [Inria Parietal], Samuel Deslauriers-Gauthier, Rachid Deriche.

Matching structural parcels across different subjects is an open problem in neuroscience. Even when produced by the same technique, parcellations tend to differ in the number, shape, and spatial localization of parcels across subjects. In this work, we propose a parcel matching method based on Optimal Transport. We test its performance by matching parcels of the Desikan atlas, parcels based on a functional criteria and structural parcels. We compare our technique against three other ways to match parcels which are based on the Euclidean distance, the cosine similarity, and the Kullback-Leibler divergence. Our results show that our method achieves the highest number of correct matches.

This work has been published in [32], [26].

## 6.1.9. A Closed-Form Solution of Rotation Invariant Spherical Harmonic Features in Diffusion MRI

Participants: Mauro Zucchelli, Samuel Deslauriers-Gauthier, Rachid Deriche.

Rotation invariant features are an indispensable tool for characterizing diffusion Magnetic Resonance Imaging (MRI) and in particular for brain tissue microstructure estimation. In this work, we propose a new mathematical framework for efficiently calculating a complete set of such invariants from any spherical function. Specifically, our method is based on the spherical harmonics series expansion of a given function of any order and can be applied directly to the resulting coefficients by performing a simple integral operation analytically. This enable us to derive a general closed-form equation for the invariants. We test our invariants on the diffusion MRI fiber orientation distribution function obtained from the diffusion signal both in-vivo and in synthetic data. Results show how it is possible to use these invariants for characterizing the white matter using a small but complete set of features.

This work has been published in [29].

#### 6.1.10. Rational invariants of ternary forms under the orthogonal group

**Participants:** Paul Görlach [MPI for Mathematics in the Sciences], Evelyne Hubert [Inria, AROMATH], Théodore Papadopoulo, Rachid Deriche.

In [68], [69], [81] we started to explore the theory of tensor invariants as a mathematical framework for computing new biomarkers for HARDI. We pursued this work and, in collaboration with the projectteam GALAAD/AROMATH, we succeeded to develop a complete set of rational invariants for ternary quartics [39]. Being rational, they are very close to the polynomial invariants developed in [69] but they constitute a complete set of invariants. They are also good tools to understand better the algebraic invariants of [81] and some others based on spherical harmonics decomposition [55]. We determined a generating set of rational invariants of minimal cardinality for the action of the orthogonal group O(3) on the space  $R[x, y, z]_{2d}$  of ternary forms of even degree 2d. The construction relies on two key ingredients. On one hand, the Slice Lemma allows us to reduce the problem to dermining the invariants for the action on a subspace of the finite subgroup B(3) of signed permutations. On the other hand, our construction relies in a fundamental way on specific bases of harmonic polynomials. These bases provide maps with prescribed B(3)-equivariance properties. Our explicit construction of these bases should be relevant well beyond the scope of this work. The expression of the B(3)-invariants can then be given in a compact form as the composition of two equivariant maps. Instead of providing (cumbersome) explicit expressions for the O(3)-invariants, we provide efficient algorithms for their evaluation and rewriting. We also use the constructed B(3)-invariants to determine the O(3)-orbit locus and provide an algorithm for the inverse problem of finding an element in  $R[x, y, z]_{2d}$  with prescribed values for its invariants. These are the computational issues relevant in brain imaging.

This work has been sumitted and is currently under review. A preprint is available in [39].

#### 6.1.11. Edema-informed anatomically constrained particle filter tractography

**Participants:** Samuel Deslauriers-Gauthier, Drew Parker [UPenn, USA], François Rheault [SCIL, Sherbrooke University, CA], Steven Brem [UPenn, USA], Maxime Descoteaux [SCIL, Sherbrooke University, CA], Ragini Verma [UPenn, USA], Rachid Deriche.

In this work, we propose an edema-informed anatomically constrained tractography paradigm that enables reconstructing larger spatial extent of white matter bundles as well as increased cortical coverage in the presence of edema. These improvements will help surgeons to maximize the extent of the resection while minimizing the risk of cognitive deficits. The new paradigm is based on a segmentation of the brain into gray matter, white matter, corticospinal fluid, edema and tumor regions which utilizes a tumor growth model. Using this segmentation, a valid tracking domain is generated and, in combination with anatomically constrained particle filter tractography, allows streamlines to cross the edema region and reach the cortex. Using subjects with brain tumors, we show that our edema-informed anatomically constrained tractography paradigm increases the cortico-cortical connections that cross edema-contaminated regions when compared to traditional fractional anisotropy thresholded tracking.

This work has been published in [24].

#### 6.1.12. Towards the assessment of myelination using time-dependent diffusion MRI indices

**Participants:** Abib Olushola Yessouffou Alimi, Alexandra Petiet [ICM, CENIR, Paris], Mathieu Santin [ICM, CENIR, Paris], Anne-Charlotte Philippe [ICM, CENIR, Paris], Stéphane Lehericy [ICM, CENIR, Paris], Demian Wassermann [Inria Parietal], Rachid Deriche.

In this work, we study the sensitivity of time-dependent diffusion MRI indices or  $q\tau$ -indices to demyelination in the mouse brain. For this, we acquire in vivo four-dimentional diffusion-weighted images-varying over gradient strength, direction and diffusion time-and estimate the  $q\tau$ -indices from the corpus callosum. First order Taylor approximation of each index gives fitting coefficients  $\alpha$  and  $\beta$  whose variance we investigate. Results indicate that, cuprizone intoxication affects mainly index coefficient  $\beta$  by introducing inequality of variances between the two mice groups, most significantly in the splenium and that MSD increases and RTOP decreases over diffusion time  $\tau$ .

This work has been published in [35].

### 6.1.13. An Analytical Fiber ODF Reconstruction in 3D Polarized Light Imaging

**Participants:** Abib Olushola Yessouffou Alimi, Yves Usson [UMR5525 TIMC-IMAG CNRS], Pierre-Simon Jouk [CHU Grenoble-Alpes], Gabrielle Michalowicz [CHU Grenoble-Alpes], Rachid Deriche.

Three dimensional polarized light imaging (3D-PLI) utilizes the birefringence in postmortem tissue to map its spatial fiber structure at a submillimeter resolution. In this work, we propose an analytical method to compute the fiber orientation distribution function (ODF) from high-resolution vector data provided by 3D-PLI. This strategy enables the bridging of high resolution 3D-PLI to diffusion magnetic resonance imaging with relatively low spatial resolution. First, the fiber ODF is modeled as a sum of K orientations on the unit sphere and expanded with a high order spherical harmonics series. Then, the coefficients of the spherical harmonics are derived directly with the spherical Fourier transform. We quantitatively validate the accuracy of the reconstruction against synthetic data and show that we can recover complex fiber configurations in the human heart at different scales.

This work has been published in [22].

# 6.1.14. fMRI Deconvolution via Temporal Regularization using a LASSO model and the LARS algorithm

**Participants:** Isa Costantini, Patryk Filipiak, Kostiantyn Maksymenko, Samuel Deslauriers-Gauthier, Rachid Deriche.

In the context of functional MRI (fMRI), methods based on the deconvolution of the blood oxygenated level dependent (BOLD) signal have been developed to investigate the brain activity, without a need of a priori knowledge about activations occurrence. In this work, we propose a novel temporal regularized deconvolution of the BOLD signal using the Least Absolute Shrinkage and Selection Operator (LASSO) model, solved by means of the Least-Angle Regression (LARS) algorithm. In this way, we were able to recover the underlying neurons activations and their dynamics.

This work has been published in [23], [37].

### 6.1.15. A Second Order Multi-Stencil Fast Marching Method with a Non-Constant Local Cost Model

**Participants:** Susana Merino-Caviedes [Universidad de Valladolid], Lucilio Cordero-Grande [King's College London], Maria Tereza Perez [Universidad de Valladolid], Pablo Casaseca-de-La-Higuera [Universidad de Valladolid], Marcos Martín-Fernández [Universidad de Valladolid], Carlos Alberola-Lopez [Universidad de Valladolid], Rachid Deriche.

The Fast Marching method is widely employed in several fields of image processing. Some years ago a Multi-Stencil version (MSFM) was introduced to improve its accuracy by solving the Eikonal equation for a set of stencils and choosing the best solution at each considered node. The following work proposes a modified numerical scheme for MSFM to take into account the variation of the local cost, which has proven to be second order. The influence of the stencil set choice on the algorithm outcome with respect to stencil orthogonality and axis swapping is also explored, where stencils are taken from neighborhoods of varying radius. The experimental results show that the proposed schemes improve the accuracy of their original counterparts, and that the use of permutation-invariant stencil sets provides robustness against shifted vector coordinates in the stencil set.

This work has been published in [16].

# 6.2. Unveiling brain activity using M/EEG

# 6.2.1. Data-driven cortical clustering to provide a family of plausible solutions to the M/EEG inverse problem

Participants: Maureen Clerc, Kostiantyn Maksymenko, Théodore Papadopoulo.

The Magneto/Electroencephalography (M/EEG) inverse problem consists in reconstructing cortical activity from M/EEG measurements. It is an ill-posed problem. Hence prior hypotheses are needed to constrain the solution space. In this work, we consider that the brain activity which generates the M/EEG signals is supported by single or multiple connected cortical regions. As opposed to methods based on convex optimization, which are forced to select one possible solution, we propose a cortical clustering based approach, which is able to find several candidate regions. These regions are different in term of their sizes and/or positions but fit the data with similar accuracy. We first show that even under the hypothesis of a single active region, several source configurations can similarly explain the data. We then use a multiple signal classification (MUSIC) approach to recover multiple active regions with our method. We validate our method on simulated and measured MEG data. Our results show that our method provides a family of plausible solutions which both accord with the priors and similarly fit the measurements.

This work is published in [41].

# 6.2.2. Fast approximation of EEG forward problem and application to tissue conductivity estimation

Participants: Maureen Clerc, Kostiantyn Maksymenko, Théodore Papadopoulo.

Bioelectric source analysis in the human brain from scalp electroencephalography (EEG) signals is sensitive to the conductivity of the different head tissues. Conductivity values are subject dependent, so non-invasive methods for conductivity estimation are necessary to suitably tune the EEG models. To do so, the EEG forward problem solution (so-called lead field matrix) must be computed for a large number of conductivity configurations. Computing one lead field requires a matrix inversion which is computationally intensive for realistic head models. Thus, the required time for computing a large number of lead fields can become impractical. In this work, we propose to approximate the lead field matrix for a set of conductivity configurations, using the exact solution only for a small set of basis points in the conductivity space. Our approach accelerates the computing time, while controlling the approximation error. Our method is tested for brain and skull conductivity estimation, with simulated and measured EEG data, corresponding to evoked somato-sensory potentials. This test demonstrates that the used approximation does not introduce any bias and runs significantly faster than if exact lead field were to be computed.

This work has been submitted to a journal and is available as a preprint [40].

# 6.2.3. Model based optimal multipolar stimulation without a priori knowledge of nerve structure

**Participants:** Maureen Clerc, Mélissa Dali [Inria Camin], David Guiraud [Inria Camin], Jérémy Laforêt [Inria Camin], Olivier Rossel [Inria Camin].

Multipolar cuff electrode can selectively stimulate areas of peripheral nerves and therefore enable to control independent functions. However, the branching and fascicularization are known for a limited set of nerves and the specific organization remains subject-dependent. This work presents general modeling and optimization methods in the context of multipolar stimulation using a cuff electrode without a priori knowledge of the nerve structure. Vagus nerve stimulation experiments based on the optimization results were then investigated.

The model consisted of two independent components: a lead field matrix representing the transfer function from the applied current to the extracellular voltage present on the nodes of Ranvier along each axon, and a linear activation model. The optimization process consisted in finding the best current repartition (ratios) to reach activation of a targeted area depending on three criteria: selectivity, efficiency and robustness.

The results showed that state-of-the-art configurations (tripolar transverse, tripolar longitudinal) were part of the optimized solutions but new ones could emerge depending on the trade-off between the three criteria and the targeted area. Besides, the choice of appropriate current ratios was more important than the choice of the stimulation amplitude for a stimulation without a priori knowledge of the nerve structure. We successfully assessed the solutions in vivo to selectively induce a decrease in cardiac rhythm through vagus nerve stimulation while limiting side effects. Compared to the standard whole ring configuration, a selective solution found by simulation provided on average 2.6 less adverse effects.

The preliminary results showed the correctness of the simulation, using a generic nerve geometry. It suggested that this approach will have broader applications that would benefit from multicontact cuff electrodes to elicit selective responses. In the context of the vagus nerve stimulation for heart failure therapy, we show that the simulation results were confirmed and improved the therapy while decreasing the side effects.

This work has been published in [10].

## 6.3. Combined M/EEG and dMRI

# 6.3.1. Linking resting-state functional connectivity and the structural connectome – investigation of an eigen-structure model

Participants: Rebecca Bonham-Carter, Samuel Deslauriers-Gauthier, Rachid Deriche.

Resting-state functional connectivity (rs-FC) dynamics are not random but rather structured with common dominant patterns called resting-state networks (RSNs). These dynamics are influenced by the underlying network of white-matter connections. Specifically, temporal correlations in resting-state BOLD fMRI signals have been correlated with the structural network determined via diffusion weighted imaging (DWI). The literature on this structure-function relationship encompasses generative non-linear models and a variety of linear models. The objective of this study is to provide new validation and understanding of two linear models. Both models enforce that the structural network Laplacian and rs-FC share a common eigen-structure. In contrast to previous work, in this work two linear models of resting-state functional connectivity (rs-FC), developed by Abdelnour et al., are validated on simulated BOLD fMRI data generated using The Virtual Brain18 (TVB) and 49 HCP subjects real structural connectomes. Both consider rs-FC as a diffusion process on the structural network. The mean correlations between rs-FC matrices we obtain 0.699 $\pm$ 0.086 and 0.518 $\pm$ 0.095, and between rs-FC eigenvalues 0.981 $\pm$ 0.013, agree with the original model implementations on empirical data. Using The Virtual Brain simulator together with real structural data is shown to offer a new and efficient test and validation framework for approaches predicting rs-FC from structure.

This work is under review.

#### 6.3.2. White Matter Information Flow Mapping from Diffusion MRI and EEG

**Participants:** Samuel Deslauriers-Gauthier, Jean-Marc Lina [Ecole de Technologie Supérieure, Montréal, CA], Russel Butler [Sherbrooke University, CA], Kevin Whittingstall [Sherbrooke University, CA], Pierre-Michel Bernier [Sherbrooke University, CA], Maxime Descoteaux [SCIL, Sherbrooke University, CA], Rachid Deriche.

The human brain can be described as a network of specialized and spatially distributed regions. The activity of individual regions can be estimated using electroencephalography and the structure of the network can be measured using diffusion magnetic resonance imaging. However, the communication between the different cortical regions occurring through the white matter, coined information flow, cannot be observed by either modalities independently. Here, we present a new method to infer information flow in the white matter of the brain from joint diffusion MRI and EEG measurements. This is made possible by the millisecond resolution of EEG which makes the transfer of information from one region to another observable. A subject specific Bayesian network is built which captures the possible interactions between brain regions at different times. This network encodes the connections between brain regions detected using diffusion MRI tractography derived white matter bundles and their associated delays. By injecting the EEG measurements as evidence into this model, we are able to estimate the directed dynamical functional connectivity whose delays are supported by the diffusion MRI derived structural connectivity. We present our results in the form of information flow diagrams that trace transient communication between cortical regions over a functional data window. The performance of our algorithm under different noise levels is assessed using receiver operating characteristic curves on simulated data. In addition, using the well-characterized visual motor network as grounds to test our model, we present the information flow obtained during a reaching task following left or right visual stimuli. These promising results present the transfer of information from the eyes to the primary motor cortex. The information flow obtained using our technique can also be projected back to the anatomy and animated to produce videos of the information path through the white matter, opening a new window into multi-modal dynamic brain connectivity.

This work is under review.

## 6.3.3. Bridging Brain Structure and Function by Correlating Structural Connectivity and Cortico-Cortical Transmission

**Participants:** Fabien Almairac [CHU Nice], Patryk Filipiak, Lavinia Slabu, Maureen Clerc, Théodore Papadopoulo, Denys Fontaine [CHU Nice], Lydiane Mondot [CHU Nice], Stéphan Chanalet [CHU Nice], Demian Wassermann [Inria Parietal], Rachid Deriche.

Elucidating the structure-function relationship of the brain is one of the main open questions in neuroscience. The capabilities of diffusion MRI-based (dMRI) techniques to quantify the connectivity strength between brain areas, namely structural connectivity, in combination with modalities such as electrocorticography (ECoG) to quantify brain function have enabled advances in this field. In this work, we aim to establish a relationship between: i) dMRI structural connectivity measures, ii) direct measures of electrical properties of the human brain cortex obtained with ECoG, iii) response elicited by direct electrostimulation of the brain (DES).

The results of this multi-modal approach combining structure and function explorations of the brain should: i) help to elucidate the relationship between non-invasive (dMRI) structural connectivity measures and corticocortical transmission properties (delays, transfer functions), ii) help in understanding the organization of the brain for cognitive functions as well as neurosurgical planning for resection of brain tumors and drug-resistant epilepsy

This work has been presented in [36].

# 6.4. Brain Computer Interfaces

### 6.4.1. Online enhancement of visuospatial attention performance

Participants: Maureen Clerc, Thomas Brochier [Institut des Neurosciences de la Timone], Romain Trachel.

This study on real-time decoding of visuospatial attention has two objectives: first, to reliably decode selfdirected shifts of attention from electroencephalography (EEG) data, and second, to analyze whether this information can be used to enhance visuospatial performance. Visuospatial performance was measured in a target orientation discrimination task, in terms of reaction time, and error rate. Our experiment extends the Posner paradigm by introducing a new type of ambiguous cues to indicate upcoming target location. The cues are designed so that their ambiguity is imperceptible to the user. This entails endogenous shifts of attention which are truly self-directed. Two protocols were implemented to exploit the decoding of attention shifts. The first 'adaptive' protocol uses the decoded locus to display the target. In the second 'warning' protocol, the target position is defined in advance, but a warning is flashed when the target mismatches the decoded locus. Both protocols were tested in an online experiment involving ten subjects. The reaction time improved in both the adaptive and the warning protocol. The error rate was improved in the adaptive protocol only. This proof of concept study brings evidence that visuospatial brain–computer interfaces (BCIs) can be used to enhance improving human–machine interaction in situations where humans must react to off-center events in the visual field.

This work has been published in [8].

# 6.4.2. Review of classification methods for EEG-based Brain-Computer Interfaces: A 10-year update

**Participants:** Maureen Clerc, Laurent Bougrain [Neurosys, Inria Nancy], Fabien Lotte [Potioc, Inria Bordeaux], Alain Rakotomamonjy [Université de Rouen].

Most current Electroencephalography (EEG)-based Brain-Computer Interfaces (BCIs) are based on machine learning algorithms. There is a large diversity of classifier types that are used in this field, as described in the 2007 review paper [75]. Now, approximately 10 years after this review publication, many new algorithms have been developed and tested to classify EEG signals in BCIs. The time is therefore ripe for an updated review of EEG classification algorithms for BCIs. We surveyed the BCI and machine learning literature from 2007 to 2017 to identify the new classification approaches that have been investigated to design BCIs. We synthesize these studies in order to present such algorithms, to report how they were used for BCIs, what were the outcomes, and to identify their pros and cons. We found that the recently designed classification algorithms for EEG-based BCIs can be divided into four main categories: adaptive classifiers, matrix and tensor classifiers, transfer learning and deep learning, plus a few other miscellaneous classifiers. Among these, adaptive classifiers were demonstrated to be generally superior to static ones, even with unsupervised adaptation. Transfer learning can also prove useful although the benefits of transfer learning remain unpredictable. Riemannian geometry-based methods have reached state-of-the-art performances on multiple BCI problems and deserve to be explored more thoroughly, along with tensor-based methods. Shrinkage linear discriminant analysis and random forests also appear particularly useful for small training samples settings. On the other hand, deep learning methods have not yet shown convincing improvement over state-of-the-art BCI methods. This paper provides a comprehensive overview of the modern classification algorithms used in EEG-based BCIs, presents the principles of these Review of Classification Algorithms for EEG-based BCI 2 methods and guidelines on when and how to use them. It also identifies a number of challenges to further advance EEG classification in BCI.

This work has been published in [14].

### 6.4.3. Automatizing calibration

Participants: Maureen Clerc, Federica Turi, Nathalie Gayraud.

Brain Computer Interfaces (BCIs) based on visual evoked potentials (VEP) allow for spelling from a keyboard of flashing characters. Among VEP BCIs, code-modulated visual evoked potentials (c-VEPs) are designed for high-speed communication. In c-VEPs, all characters flash simultaneously. In particular, each character flashes according to a predefined 63-bit binary sequence (m-sequence), circular-shifted by a different time lag. For a given character, the m-sequence evokes a VEP in the electroencephalogram (EEG) of the subject, which can be used as a template. This template is obtained during a calibration phase at the beginning of each session. Then, the system outputs the desired character after a predefined number of repetitions by estimating its time lag with respect to the template. Our work avoids the calibration phase, by extracting from the VEP relative lags between successive characters, and predicting the full word using a dictionary.

This work has been published in [28].

# **BIOCORE** Project-Team

# 7. New Results

## 7.1. Mathematical methods and methodological approach to biology

### 7.1.1. Mathematical analysis of biogical models

7.1.1.1. Model reduction and sensitivity analysis

Participants: Suzanne Touzeau, Jean-Luc Gouzé, Valentina Baldazzi.

Analysis and reduction of biochemical models. Dynamic models representing complex biological systems with numerous interactions can reach high dimensions and include complex nonlinearities. A model reduction method based on process weighing and pruning was developed and implemented on various models. A global sensitivity analysis was performed to check the method robustness against parameter uncertainty and variability ([16]). This work was part of Stefano Casagranda's PhD thesis (2017), and is also a collaboration with Bayer (Sophia Antipolis).

#### 7.1.1.2. Estimation and control

#### Participants: Suzanne Touzeau, Jean-Luc Gouzé.

*Parameter identification in compartmental systems.* In collaboration with F. Dayan (Startup Exactcure), we work on practical problems of identifiability of parameters in linear pharmacokinetic models. This was the subject of the internship of Jean-Baptiste Excoffier.

*Parameter identification in complex systems*. In complex biological systems, especially when data are scarce, identifying the model parameters is a challenge and raises identifiability issues. To fit a within-host immuno-logical model to a large data set of individual viremia profiles, we developed an ABC-like method, less computationally expensive than standard Bayesian fitting procedures. Rather than reproducing individual profiles, we ientified several parameter sets compatible with the data and reflecting the variability among individuals [59], [26]. This work was part of Natacha Go's post-doctorate, supported by the ANR MIHMES project, in collaboration with the Roslin Institute, Edinburgh, UK. It benefited from the resources and support of NEF computation cluster.

#### 7.1.1.3. Mathematical study of ecological models

**Participants:** Frédéric Grognard, Ludovic Mailleret, Pierre Bernhard, Nicolas Bajeux, Suzanne Touzeau, Israël Tankam Chedjou, Samuel Nilusmas.

Semi-discrete models have shown their relevance in the modeling of biological phenomena whose nature presents abrupt changes over the course of their evolution [85]. We used such models and analyzed their properties in several practical situations that are developed in Section 7.2.3, some of them requiring such a modeling to describe external perturbations of natural systems, and others to take seasonality into account [11]. External perturbations of interacting populations occur when some individuals are introduced or removed from a natural system, which occurs frequently in pest control applications, either through the direct removal of pests, through the introduction of artificial habitats for the predators or through the introduction of biological control agents in deterministic or stochastic fashion [72].

Seasonality is an important property of most agricultural systems in temperate environments since the year is divided into a cropping season and a 'winter' season; it gives the reference time for crop rotation between resistant and sensitive strains in a multi-seasonal optimization of root-knot nematodes control [56]. However, it can also arise in tropical environments where, in the absence of weather-related season, time is divided into cropping and fallow seasons, and where the duration of the latter can for example be used as a control method against phytopathogenic nematodes of the plantain plant [46], [58].

#### 7.1.1.4. Analysis of periodic behavior with hybrid models Participants: Jean-Luc Gouzé, Madalena Chaves.

*Periodic orbits in non monotonic negative feedback circuits.* In [91], we studied the occurrence of periodic solutions in an n-dimensional class of negative feedback systems defined by smooth vector fields with a window of not necessarily monotonic activity. We have now [36] further established uniqueness and stability of the periodic solution under some conditions on the parameters.

*Analysis tools for interconnection of Boolean networks.* Following the work in [96] and [78], we have generalized the method for computation of the asymptotic graph. In [22], a quantitative dimension is added to the asymptotic graph, through the computation of relative probabilities for each final attractor. In [19], we have extended this methodology for the case of Boolean networks with synchronous updates, in a collaboration with D. Figueiredo and M.A. Martins from the University of Aveiro, Portugal (project PHC Pessoa).

#### 7.1.1.5. Dynamics of complex feedback architectures

Participants: Jean-Luc Gouzé, Madalena Chaves.

To analyze the closed-loop dynamics of metabolic pathways under gene regulation, we propose a method to construct a state transition graph for a given regulatory architecture consisting of a pathway of arbitrary length, with any number of genetic regulators, and under any combination of positive and negative feedback loops [20]. Using this formalism, we analyze a "metabolator"-like mechanism (a pathway with two metabolites and three enzymes) and prove the existence of two co-existing oscillatory behaviors: damped oscillations towards a fixed point or sustained oscillations along a periodic orbit [21].

#### 7.1.2. Metabolic and genomic models

**Participants:** Jean-Luc Gouzé, Olivier Bernard, Valentina Baldazzi, Claudia Lopez Zazueta, Lucie Chambon, Agustin Yabo.

*Transcription and translation models in bacteria.* We study detailed models of transcription and translation for genes in a bacterium, in particular the model of gene expression of RNA polymerase [12]. This is part of the PhD thesis of Stefano Casagranda (2017), and done in collaboration with Inria IBIS project-team, in particular with D. Ropers.

Analysis and reduction of a model of sugar metabolism in peach fruit. Predicting genotype-to-phenotype relationships is a big challenge for plant biology and breeding. A model of sugar metabolism in peach fruit has been recently developed and applied to 10 peach varieties [25]. A reduction pipeline combining serveral strategies is currently developed to reduce both model size and nonlinearity and allow for further application to virtual breeding (collaboration with B. Quilot-Turion and Mohamed Memmah (INRA Avignon) as part of the PhD thesis of Hussein Kanso).

*Analysis of an integrated cell division-endoreduplication and expansion model.* The development of a new organ depends on cell-cyle progression and cell expansion, but the interaction and coordination between these processes, under different environments, is still unclear [29]. An integrated model of fruit development has been developed and used to test different interaction schemes, by comparing simulation results to observed cell ditribution data in tomato fruit [65], [47].

#### 7.1.2.1. Estimation and control

*Optimal allocation of resources in a bacterium.* We study by techniques of optimal control the optimal allocation between metabolism and gene expression during growth of bacteria, in collaboration with Inria IBIS project-team. We showed that a good suboptimal control solution could be implemented in the cell by ppGpp (a small molecule involved in the regulation of ribosomes) [80]. We developed different versions of the problem [40], and consider a new problem where the aim is to optimize the production of a product [39],(ANR projects Reset and Maximic, new PhD thesis of A. Yabo, collaboration with McTao Team). We also study variations of the model, including energy (ATP and ADP).

*Control of a model of synthesis of a virulence factor.* In collaboration with J.-A. Sepulchre (INLN Nice), we model the production of a virulence factor by a bacterium in a continuous stirred tank reactor. The production of this enzyme is genetically regulated, and degrades a polymeric external substrate into monomers. A nonlinear control is built [94], [38].

*Hybrid control of genetic networks.* We design control strategies based on the measurement and control of a unique gene within positive or negative loops of genetic networks, in order to stabilize the system around its unstable fixed point. The quantized nature of genetic measurements and the new synthetic control approaches available in biology encourage the use of piecewise constant control laws. A specific partitioning of the state space and the study of successive repulsive regions allow to show global convergence and global stability for the resulting system [48]. This is part of the thesis of L. Chambon.

#### 7.1.2.2. Slow-Fast analysis of metabolic models

Metabolic modeling generally assumes balanced growth, *i.e.* that there is no accumulation of intermediate compound, and that the metabolism is rapidly at quasi steady state. We go beyond this hypothesis by considering that some metabolic reactions are slow, while other are fast. Then we analyse the differential system using Tikhonov's Theorem. We compare the results obtained using the Drum approach [2], and show that Drum is a reasonable approximation, provided that growth rate stays low. This is part of the PhD thesis of Claudia Lopez Zazueta [31], [30], [54], [55].

7.1.2.3. Large scale metabolic modeling

Metabolic modeling generally assumes balanced growth, *i.e.* that there is no accumulation of intermediate compound, and that the metabolism is rapidly at quasi steady state. We have proposed a new approach called DRUM where this hypothesis is relaxed by splitting the metabolic network into subnetworks and assuming that some compounds can accumulate between the subnetworks [2], [73]. This approach was successfully applied to several cases where the variations in light or nutrient resources induce a strong accumulation in the microalgal cells which could not be represented by the state of the art approaches [74]. More recently we have expended this approach to identify the genomic regulations explaining the change in metabolism especially when considering nitrogen starvation under a light/dark regime.

### 7.1.3. Biochemical and signaling models

#### 7.1.3.1. Analysis and coupling of biological oscillators

**Participants:** Sofia Almeida, Madalena Chaves, Eleni Firippi.

*Modeling, analysis and coupling of the mammalian cell cycle and clock.* Each biological oscillator was modeled by a system of non-linear ordinary differential equations and its parameters calibrated against experimental data (both from the literature and from F. Delaunay's lab). The interactions between the two oscillators are investigated under uni- or bi-directional coupling schemes. Numerical simulations replicate the oscillators' period-lock response and recover observed clock to cell cycle period ratios such as 1:1, 3:2 and 5:4 (as observed in experiments, F. Delaunay's lab) mycitePhD:almeida. This work is in collaboration with F. Delaunay (ANR ICycle) and part of the PhD thesis of Sofia Almeida.

*Improving the design of a synthetic oscillator.* We analyse a two-variable model (the "Smolen" oscillator) using both numerical simulations and theoretical analysis through a piecewise affine approximation. Our objective is to investigate the existence of oscillatory behaviour and, in particular, to characterize and increase the region of parameters which admits sustained oscillations. This work is part of the PhD thesis of Eleni Firippi (ANR ICycle).

#### 7.1.3.2. Modeling the apoptotic signaling pathway

Participants: Madalena Chaves, Luis Gomes Pereira, Jérémie Roux.

The goal is to study the origins of cell-to-cell variability in response to anticancer drugs and provide a link between complex cell signatures and cell response phenotype. To do this, we have been analysing models of the apoptosis pathway to compare the effects of different sources of variability at the transcriptional, translational and receptor levels [57] (collaboration with J. Roux, for the PhD thesis of Luis Pereira; project Imodrez).

# 7.2. Fields of application

#### 7.2.1. Bioenergy

**Participants:** Olivier Bernard, Antoine Sciandra, Walid Djema, Ignacio Lopez Munoz, Ouassim Bara, Jean-Philippe Steyer.

#### 7.2.1.1. Modeling microalgae production

#### Experimental developments

*Running experiments in controlled dynamical environments.* The experimental platform made of continuous photobioreactors driven by a set of automaton controlled by the ODIN software is a powerful and unique tool which gave rise to a quantity of very original experiments. Such platform improved knowledge of several biological processes such as lipid accumulation or cell cycle under light fluctuation, etc.

This experimental platform was used to control the long term stress applied to a population of microalgae. This Darwinian selection procedure generated two new strains after more than 6 months in the so called selectiostats.

Other experiments were carried out to reproduce the light signal percept by a cell in a raceway pond [24], derived from Lagrangian hydrodynamical computations. The experiments show that pigments content of the microalgae is highly related to the experimented hydrodynamic regime.

On top of this, we carried out outdoor pilot experiments with solar light. We tested the impact of various temperatures, resulting from different shadowing configurations on microalgal growth rate. This is the topic of Bruno Assis Pessi's master thesis. The impact of process configuration on  $CO_2$  transfer rate has also been tested and quantified [17].

These works have been carried out in collaboration with A. Talec and E. Pruvost (CNRS/Sorbonne Université -Oceanographic Laboratory of Villefranche-sur-Mer LOV).

*Metabolism of carbon storage and lipid production.* A metabolic model has been set up and validated for the microalgae *Isochrysis luthea*, on the basis of the DRUM framework, in order to simulate autotophic, heterotropic and mixotrophic growth, and to determine how to reduce substrate inhibition. The model was extended for other substrates such as glucose or glycerol. A simplified model was developed by I. Lopez to represent the dynamics of polar lipids, especially when faced to higher oxygen concentration.

*Modeling the coupling between hydrodynamics and biology.* In collaboration with the Inria ANGE team, a model coupling the hydrodynamics of the raceway (based on an original multilayer discretisation of Navier-Stokes equations) with microalgae growth was developed [75]. This model is supported by the work of ANGE aiming at improving the discretization scheme of the Navier-Stokes equations and eventually to more accurately represent the hydrodynamics of the raceway and reconstruct Lagrangian trajectories. The accurate reconstruction of the trajectories is verified by a statistical analysis of the probability densities. As a consequence, more relevant experimental protocols have been proposed to more realistically design simplified light signal for experiments [24].

*Modeling photosynthetic biofilms.* Several models have been developed to represent the growth of microalgae within a biofilm. A first structured physiological model uses mixture theory to represent the microalgae growth, based on the consideration of intracellular reserves triggering the processes of growth, respiration and excretion. We consider separately the intracellular storage carbon (lipids and carbohydrates) and the functional part of microalgae [92]. Another approach accounts for the dynamics of the light harvesting systems when cells are submitted to rapid successions of light and dark phases. A simpler model was developed and used to identify the optimal working mode of a process based on photosynthetic biofilm growing on a conveyor belt [41].

*Modeling microalgae production processes.* The integration of different models developed within BIOCORE [76] was performed to represent the dynamics of microalgae growth and lipid production in raceway systems. The model was validated at industrial scale with cultivation of the microalgae Dunaliella salina [15].

This model was then used to predict productivity in raceway systems, depending on climatic conditions. A Model Predictive Control strategy was developed to on-line adapt influent flow rate and water depth to temperature and light.

We have shown in [87] that a control strategy based on shadowing with solar panel can significantly improve productivity, especially during the early growth stage of the culture.

*Modeling thermal adaptation in microalgae.* We have studied and compared several models of microalgae growth to different temperatures [82]. Experiments have been carried out in collaboration with A.-C. Baudoux (Biological Station of Roscoff) in order to study growth of various species of the microalgae genus *Micromonas* at different temperatures. After calibration of our models, we have shown that the pattern of temperature response is strongly related to the site where cells were isolated. We derived a relationship to extrapolate the growth response from isolation location. With this approach, we proved that the oceanwide diversity of *Micromonas* species is very similar to the oceanwide diversity of the phytoplankton. We have used Adaptive Dynamics theory to understand how temperature drives evolution in microalgae. We could then predict the evolution of this biodiversity in a warming ocean and show that phytoplankton must be able to adapt within 1000 generation to avoid a drastic reduction in biodiversity [23].

*Modeling viral infection in microalgae.* Experiments have been carried out in collaboration with A.-C. Baudoux (Biological Station of Roscoff) in order to study the impact of viral infections on the development of populations of *Micromonas* at different temperatures. This work revealed a qualitative change in viral infection when temperature increases. A model was developed to account for the infection of a *Micromonas* population, with population of susceptible, infected and also free viruses. The model turned out to accurately reproduce the infection experiments at various temperatures, and the reduction of virus production above a certain temperature [79].

#### 7.2.1.2. Control and Optimization of microalgae production

*Optimization of the bioenergy production systems.* A model predictive control algorithm was run based on simple microalgae models coupled with physical models where culture depth influences thermal inertia. Optimal operation in continuous mode for outdoor cultivation was determined when allowing variable culture depth. Assuming known weather forecasts considerably improved the control efficiency.

*Interactions between species.* We have proposed an optimal control strategy to select the microalgal strain with the lowest pigment content. The control takes benefit from photoinhibition to compute light stresses penalizing the strains with a higher pigment content and finally select microalgae with lower chlorophyll content. This characteristic is of particular interest for maximizing biomass production in dense cultures. The strategy has been carried out at the LOV and eventually the productivity of *Tisochrysis lutea* was improved by 75%.

Finaly, optimal strategies when selecting the strain of interest within two species competing for the same substrate has been proposed, when dynamics is represented by a Droop model [42].

### 7.2.2. Biological depollution

#### 7.2.2.1. Control and optimization of bioprocesses for depollution

Participants: Olivier Bernard, Carlos Martinez Von Dossow, Jean-Luc Gouzé.

We consider artificial ecosystems including microalgae, cyanobacteria and bacteria in interaction. The objective is to more efficiently remove inorganic nitrogen and phosphorus from wastewater, while producing a microalgal biomass which can be used for biofuel or bioplastic production. Models have been developed including predators grazing the microalgae. Experiments with nitrogen fixing cyanobacteria were carried out, and simple models of the ecosystem where developed to assess the potential of such organisms to support the nitrogen need of microalgae [18].

#### 7.2.2.2. Coupling microalgae to anaerobic digestion

**Participants:** Olivier Bernard, Antoine Sciandra, Jean-Philippe Steyer, Frédéric Grognard, Carlos Martinez Von Dossow.

The coupling between a microalgal pond and an anaerobic digester is a promising alternative for sustainable energy production and wastewater treatment by transforming carbon dioxide into methane using light energy. The ANR Phycover project is aiming at evaluating the potential of this process [95].

We have proposed several models to account for the biodiversity in the microalgal pond and for the interaction between the various species. These models were validated with data from the Saur company. More specifically, we have included in the miroalgae model the impact of the strong turbidity, and derived a theory to better understand the photolimitation dynamics especially when accounting for the photo-inhibition in the illuminated periphery of the reactor [33]. Optimal control strategies playing with the dilution rate, shadowing or modifying depth were then studied [32].

#### 7.2.2.3. Life Cycle Assessment

Participants: Olivier Bernard, Jean-Philippe Steyer, Marjorie Alejandra Morales Arancibia.

*Environmental impact assessment.* In the sequel of the pioneering life cycle assessment (LCA) work of [83], we continued to identify the obstacles and limitations which should receive specific research efforts to make microalgae production environmentally sustainable [62].

In the Purple Sun ANR-project, we studied a new paradigm to improve the energy balance by combining biofuel production with photovoltaic electricity. The LCA of a greenhouse with, at the same time, photovoltaic panels and low emissivity glasses is studied. Depending on the period of the year, changing the species can both improve productivity and reduce environmental footprint.

This work is the result of a collaboration with Arnaud Helias of INRA-LBE (Laboratory of Environmental Biotechnology, Narbonne) and Pierre Collet (IFPEN).

### 7.2.3. Design of ecologically friendly plant production systems

#### 7.2.3.1. Controlling plant arthropod pests

Participants: Frédéric Grognard, Ludovic Mailleret, Suzanne Touzeau, Nicolas Bajeux, Yves Fotso Fotso.

*Optimization of introduction processes.* The question of how many and how frequently natural enemies should be introduced into crops to most efficiently fight a pest species is an important issue of integrated pest management. The topic of optimization of natural enemies introductions has been investigated for several years [84], [90] [71], and was one of the key features of L. Mailleret's HDR thesis [11]. A central theoretical result concerns the unveiling of the crucial influence of within-predator density dependent processes. To evaluate this theoretical prediction in a more realistic, stochastic and spatially explicit setting, a stochastic individual based model has been built on the multi-agent programmable modeling environment Netlogo. Extensive simulatory experiments were performed to assess the effects of density dependent processes as well as spatial structure and stochasticity on augmentative biological control performance and variability [67], [68].

In a more general setting, we studied the impact on the introduction success of a population of the interplay of Allee effects, stochasticity in introduction sizes, and occurrence of catastrophes that temporarily wipe out the population. The mean first passage time (MFPT) for a population to reach a viable size was used as a measure of establishment success for the introduction processes [72].

*Characteristics of space and the behavior and population dynamics of parasitoids.* We studied the influence of the spatial structure and characteristics of the environment on the establishment and spread of biological control agents through computer simulations and laboratory experiments on parasitoids of the genus Trichogramma. This was the topic of Thibaut Morel Journel [89] and is the topic of Marjorie Haond's PhD thesis (ISA, 2015-). The two last articles associated with Thibaut Morel Journel's Thesis appeared this year. In the first one [34], we investigated the effect of habitat fragmentation on the establishment and early spread of an introduced population. We showed that by increasing the risks of dispersal from the introduction site to unfavourable habitat early during the invasion, fragmentation decreased establishment success. However, by decreasing the distance between favourable habitat patches, it also improved the subsequent spread of introduced species over larger areas. In the second paper [35], we explored the influence of different characteristics of the structural connectivity of an invaded habitat on the invading population. We demonstrated how spread

was hindered by habitat clusters and accelerated by the presence of hubs. These results highlight the importance of considering the structure of the invaded area to predict the outcome of invasions. In a different study stemming from Marjorie Haond Thesis, we showed how habitat richness [27] as represented by its local carrying capacity can positively influence the spreading speeed of an expanding population. This work is being performed in collaboration with Elodie Vercken (ISA) and Lionel Roques (BioSP, Avignon).

In a metapopulation context, we studied the invasion success into an environment where part of the patches are sources (favourable environments) and the others are sinks; a criterion has been obtained predicting invasion success when the number of sources is larger than some threshold [70].

*Modeling and control of coffee berry borers.* We developed a model describing the coffee berry borer dynamics based on the insect life-cycle and the berry availability during a single cropping season. An optimal control problem was formulated by implementing chemical control (insecticides) and/or biological control (entomopathogenic fungi such as *Beauveria bassiana*, microbial parasitoids, traps). The aim was to maximise the yield at the end of the cropping season, while minimising the borer population for the next cropping season and the control costs. The existence of an optimal solution was shown and the problem was solved numerically [49], [44]. This ODE model was extended to integrate the berry maturation age. The well-posedness of the resulting PDE model was shown and an asymptotic analysis was conducted. This research pertains to Yves Fotso Fotso's PhD thesis, who visited BIOCORE during 5 months in 2018 through the EPITAG associate team.

#### 7.2.3.2. Controlling plant pathogens

Participants: Frédéric Grognard, Ludovic Mailleret, Suzanne Touzeau, Pauline Clin.

*Sustainable management of plant resistance.* We studied other plant protection methods dedicated to fight plant pathogens. One such method is the introduction of plant strains that are resistant to one pathogen. This often leads to the appearance of virulent pathogenic strains that are capable of infecting the resistant plants.

Experiments were conducted in INRA Avignon for Potato Virus Y on pepper plants to evaluate the effect of four traits influencing evolutionary forces leading to resistance breakdown: virus effective population sizes, either at plant inoculation or during infection, virus accumulation and differential selection during infection. A generalized linear model showed a strong impact of the second and third one while a positive interection between differential selection and virus accumulation was identified [37]. Also, a stochastic model was developed to help determine the efficiency of pyramiding qualitative resistance and quantitative resistance narrowing population bottlenecks exerted on viruses, the latter aiming at slowing down virus adaptation to the qualitative resistance. It showed the efficiency of pyramiding when the fitness cost of RB virus variants in susceptible plants is intermediate [93]. These studies provide a framework to select plants with appropriate virus-evolution-related traits to avoid or delay resistance breakdown. This was done in collaboration with Frédéric Fabre (INRA Bordeaux) and Benoît Moury (INRA Avignon).

We pursued the calibration of the (spatio-)temporal epidemiological model of the phoma stem canker of oilseed rape, using field data on resistance deployment and virulence of phoma populations. Ongoing work includes the development of a simulation tool designed for researchers as well as non academic partners from technical institutes and agriculture cooperatives, who interact through the MoGeR project. It benefits from the resources and support of NEF computation cluster.

Taking advantage of plant diversity and immunity to minimize disease prevalence. An epidemiological model of gene-for-gene interaction considering a mechanism related to the specific defense response of plants, the systemic acquired resistance (SAR) was developed. SAR provides a sort of immunity to virulent pathogens for resistant plants having undergone an infection attempt by an avirulent pathogen. This model showed that there exists an optimal host mixture that ensures the lowest plant disease prevalence, so as to optimize the crop yield. It is especially efficient for pathogens with a low or intermediate basic reproduction rate and hosts with a high SAR efficiency [51], [52]. This was the topic of Pauline Clin's master thesis and was done in collaboration with Frédéric Hamelin (Agrocampus Ouest).

#### 7.2.3.3. Plant-nematode interactions.

**Participants:** Valentina Baldazzi, Frédéric Grognard, Ludovic Mailleret, Suzanne Touzeau, Israël Tankam Chedjou, Samuel Nilusmas.

Phytophagous nematodes are small little-mobile worms that feed and reproduce on plant roots, generating considerable losses in numerous crops all over the world. Most eco-friendly plant protection strategies are based on the use of resistant crops, but agricultural practices also contribute to nematode control.

We developed a first physiological model of plant-nematode interactions, explicitly describing resource (water and carbon) allocation between roots and shoots. Indeed, nematodes draw on root carbon pool and reduce plant water uptake from the soil. The consequences on plant growth were analyzed as a function of plant physiological characteristics. In parallel, an experiment was conducted on pepper and tomato plants to monitor plant growth with or without nematodes. Data will be used to calibrate the model. This work was the topic of Thomas Brenière [77] and was done in collaboration with Caroline Djian-Caporalino (ISA, INRA Sophia Antipolis).

We studied the stability of the hybrid interaction model between nematodes and plantain roots [46]. An optimisation problem was formulated to determine the duration between cropping seasons (fallow period) that maximises the farmer's cumulated yield, which is affected by the nematode population, while minimising the costs of nematode control and nursery-bought pest-free suckers, on a fixed time horizon that lasts several cropping seasons. We first considered that the farmer buys and plants pest-free suckers at the beginning of each cropping season. This allows for a fallow period which reduces the nematode population in the soil, as these pests need roots to feed on and reproduce. Two cases were considered: a fixed or a variable fallow period. In the first case, the existence of an optimal solution was proven and its location was computed for small infestations. In the second case, the existence of an optimal strategy was proven and was numerically computed [58]. This research pertains to Israël Tankam Chedjou's PhD thesis, who visited BIOCORE during 5 months in 2018 through the EPITAG associate team.

We studied the resistance-based nematode control. As virulent nematodes exhibit a reduced fitness on susceptible crops, combining both resistant and susceptible plants can help increase the efficacy and sustainability of such control methods. In the *Solanaceae* family, there are two major resistance genes: the first one induces an early reaction when the nematode enters in the root system and the second one induces a late reaction when the nematode creates its feeding site. We used a semi-discrete model describing the plant-nematode interactions within and between cropping season to implement the action of both resistance genes. We computed and compared the optimal deployment strategies of both resistant crops [56]. This research pertains to Samuel Nilusmas' PhD thesis (2016–).

#### 7.2.3.4. Optimality/games in population dynamics

Participants: Frédéric Grognard, Ludovic Mailleret, Pierre Bernhard.

*Optimal resource allocation.* Mycelium growth and sporulation are considered for phytopathogenic fungi. For biotrophic fungi, a flow of resource is uptaken by the fungus without killing its host; in that case, life history traits (latency-sporulation strategy) have been computed based on a simple model considering a single spore initiating the mycelium, several spores in competition and applying optimal resource allocation, and several spores in competition through a dynamic game through the analytico-numerical solution of the Hamilton-Jacobi-Bellman-Isaacs equation [97]. The solution of this dynamic game has been shown to be the equilibrium of two-trait adaptive dynamics [50]. This work, in the framework of the ANR Funfit project, is done with Fabien Halkett of INRA Nancy.

*Optimal foraging and residence times variations.* In this work, we built on our re-analysis of the Marginal Value Theorem (MVT) [4] to study the effect on the optimal foraging strategy of habitat conversion, whereby patches are converted from one existing type to another, hence changing the frequency of each type in the environment. We studied how realized fitness and the average rate of movement should respond to changes in the frequency distribution of patch-types, and how they should covary. We found that the initial pattern of patch-exploitation in a habitat can help predict the qualitative responses of fitness and movement rate following habitat conversion. We conclude that taking into account behavioral responses may help better understand the

ecological consequences of habitat conversion. This work was published through the novel preprint reviewing system of Peer Community In Ecology [66].

# **BIOVISION Project-Team**

# 6. New Results

### 6.1. High tech vision aid-systems for low-vision patients

### 6.1.1. Improving social interaction through augmented reality

**Participants:** Josselin Gautier, Pierre Kornprobst, Nicolas Chleq, Frédéric Dosière [Bosch Visiontec (Sophia Antipolis, France)], David Coupé [Bosch Visiontec (Sophia Antipolis, France)].

Today's visual enhancement systems for low-vision people consist of dedicated augmented reality hardware allowing to magnify or enhance the overall scene, independently of the image content or patient needs. For example, for patients with central vision loss, interacting with others may become a painful activity when faces and expressions can hardly be recognized. In [17], we introduce a new augmented reality system allowing to selectively enhance faces, using two image processing techniques [44], [50]. Our system is based on a Fove 0 head-mounted display (FOVE Inc, San Mateo, CA, USA). It has the capacity to adjust the enhancement to the detected faces' size and distance, hence maintaining a constant boost in the critical range of spatial frequency. It offers a binocular and large Field-of-View and performs at near real-time with a modest laptop computer using multithreading. Preliminary experiments with three patients with central vision loss suggest that the enhancements chosen strongly depends on each patient's condition and lead to improved recognition abilities when patients find their optimal settings.

This work is presented in [17].

### 6.1.2. Text auto-illustration for improving reading accessibility to low-vision people

**Participants:** Paula Pawlowski, Pierre Kornprobst, Elena Cabrio [Inria, EPI WIMMICS], Marco Benzi [Université Côte d'Azur (France)].

We have started to explore how to make reading more efficient and more enjoyable for low-vision patients through text auto-illustration. Text auto-illustration consists in automatically extracting images from the web which are related to a given text, using natural language processing methods.

# 6.2. Human vision understanding through joint experimental and modeling studies, for normal and distrophic vision

### 6.2.1. Retinal waves

**Participants:** Dora Karvouniari, Lionel Gil [Institut Non Linéaire de Nice - Institut de Physique de Nice (INLN, Université Côte d'Azur (France), France)], Olivier Marre [Institut de la Vision (Paris, France)], Serge Picaud [Institut de la Vision (Paris, France)], Bruno Cessac.

Retinal waves are bursts of activity occurring spontaneously in the developing retina of vertebrate species, contributing to the shaping of the visual system organization: retina circuitry shaping, retinotopy, eye segregation [51], [36], [46], [37]. They stop a few weeks after birth. Wave activity begins in the early development, long before the retina is responsive to light. It was recently found that they can be reinitiated pharmacologically in the adult mammalian retina [35]. This could have deep consequences on therapy for several degenerative retinal diseases. The mechanism of their generation, in developing, or adult retinas, remains however incompletely understood [52]. We have proposed a model for stage II retinal waves - induced by bursting Starburst Amacrine Cells (SACs) coupled by acetylcholine - with two objectives: (i) being sufficiently close to biophysics to explain and propose experiments and (ii) affording a mathematical analysis. From a bifurcations analysis we have highlighted several relevant biophysical parameters controlling waves generation, mainly regulating potassium and calcium dynamics. We thus explain how SACs in different species exhibit a large variability in their bursting periods with a common mechanism. We have proposed a testable experimental prediction providing a possible link of the evolution of voltage-dependent potassium channels along development with their role on the excitability properties of SACs. We have reproduced experimental findings (statistical characteristics of waves size, duration and frequency of appearance) and analysed how the evolution of cholinergic conductance due to the maturation of nicotinic receptors dramatically changes the retinal wave characteristics. We have also shown that the nonlinear dynamics generates heterogeneous local spatial structures inside which retinal waves propagate. This induces a wide variability in waves characteristics even though the network is perfectly homogeneous.

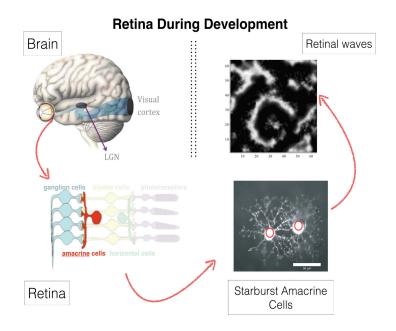


Figure 1. Multiscale dynamics of retinal waves

This work has been presented in [11], [13], [14], [16], [20], [12], [24].

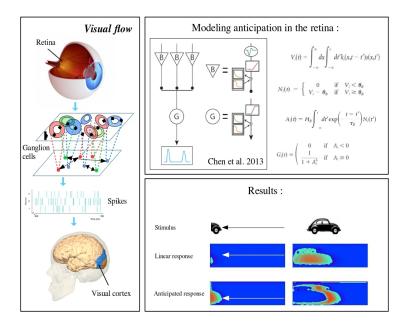
#### 6.2.2. Trajectory anticipation, from retina to V1

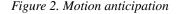
Participants: Bruno Cessac, Selma Souihel, Frédéric Chavane, Alain Destexhe, Matteo Di Volo, Olivier Marre.

Global motion processing is a major computational task of biological visual systems. When an object moves across the visual field, the sequence of visited positions is strongly correlated in space and time, forming a trajectory. These correlated images generate a sequence of local activation of the feedforward stream. At the present stage of knowledge, it is still unclear how the early visual system processes motion trajectories. Motion integration, anticipation and prediction would be jointly achieved through the interactions between feed-forward, lateral and feedback propagations within a common spatial reference frame, the retinotopic maps. Addressing this problem is particularly challenging, as it requires to probe these sequences of events

at multiple scales (from individual cells to large networks) and multiple stages (retina, primary visual cortex V1).

In the context of the ANR Trajectory, we are working on such an integrated approach. We aim at modelling the population responses at two key stages of visual motion encoding: the retina and V1 based on simultaneous micro- and mesoscopic recordings made by our partners Institut de Neurosciences de la Timone (CNRS and Aix-Marseille Université, France), Institut de la Vision (Paris, France) and Unité de Neurosciences Information et Complexité, Gif sur Yvette, France. We are designing a simulator of retinal output + V1, reproducing both the retinal anticipation and the cortical response measured by optical imaging. We are also analyzing the effects of lateral connectivity in the retina, via amacrine cells, in processing motion. This lateral connectivity is accountable for the correlated activity of RGCs in experimental data. We are measuring these correlations to add further biological plausibility to our model. This study is a step toward understanding mechanisms of motion coding and anticipation with strong impact on our understanding of the visual system.





These results have been presented in [26], [27]

# 6.2.3. Dimensionality reduction in spatio-temporal MaxEnt models and analysis of retinal ganglion cell spiking activity in experiments

**Participants:** Rubén Herzog [Centro Interdisciplinario de Neurociencia de Valparaíso (CINV, Valparaíso, Chile)], Rodrigo Cofré [Centro Interdisciplinario de Neurociencia de Valparaíso (CINV, Valparaíso, Chile)], Maria-Jose Escobar [Universidad Tecnico Federico Santa María (Electronics Engineering Department, Valparaíso, Chile)], Adrian Palacios [Centro Interdisciplinario de Neurociencia de Valparaíso (CINV, Valparaíso, Chile)], Bruno Cessac.

Retinal spike response to stimuli is constrained, on one hand by short range correlations (receptive field overlap) and on the other hand by lateral connectivity (cells connectivity). This last effect is difficult to handle from statistics because it requires to consider spatio-temporal correlations with a time delay long enough to take into account the time of propagation along synapses. Although MaxEnt models are useful to fit optimal model (maximizing entropy) under the constraints of reproducing observed correlations, they do address spatio-temporal correlations in their classical form (Ising or higher order interactions but without time delay). Binning in such models somewhat integrates propagation effects, but in an implicit form, and increasing binning severely bias data. To resolve this issue we have considered spatio-temporal MaxEnt model formerly developed e.g. by Vasquez et al. [49]. The price to pay, however is a huge set of parameters that must be fitted to experimental data to explain the observed spiking patterns statistics. There is no a priori knowledge of which parameters are relevant and which ones are contributing to overfitting. We propose here a method of dimension reduction, i.e. a projection on a relevant subset of parameters, relying on the so-called Susceptibility matrix closely related to the Fisher information. In contrast to standard methods in information geometry though, this matrix handles space and time correlations. We have applied this method for retina data obtained in a diurnal rodent (Octodon degus, having 30% of cones photoreceptors) and a 252-MEA system. Three types of stimuli were used: spatio-temporal uniform light, white noise and a natural movie. We show the role played by timedelayed pairwise interactions in the neural response to stimuli both for close and distant cells. Our conclusion is that, to explain the population spiking statistics we need both short-distance interactions as well as longdistance interactions, meaning that the relevant functional correlations are mediated not only by common input (i.e. receptive field overlap, electrical coupling; spillover) but also by long range connections.

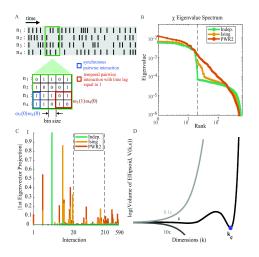


Figure 3. Dimension reduction method

This work has been submitted to Plos Comp Bio [22].

#### 6.2.4. Linear response for spiking neuronal networks with unbounded memory

**Participants:** Bruno Cessac, Rodrigo Cofré [Centro Interdisciplinario de Neurociencia de Valparaíso (CINV, Valparaíso, Chile)].

The activity of a neuronal network, characterized by action potentials (spikes), is constrained by the intrinsic properties of neurons and their interactions. When a neuronal network is submitted to external stimuli, the statistics of spikes changes, and it is difficult to disentangle the influence of the stimuli from the intrinsic dynamics. We have established a general linear response relation for spiking neuronal networks, based on

chains with unbounded memory. This relation allows quantifying the influence of a weak amplitude external stimuli on spatio-temporal spike correlations, in a general context where the memory in spike dynamics can go arbitrarily far in the past. With this approach, we show how linear response is explicitly related to neuron dynamics with an example, the gIF model, introduced by M. Rudolph and A. Destexhe [91]. This illustrates the effect of the stimuli, intrinsic neuronal dynamics, and network connectivity on spike statistics.

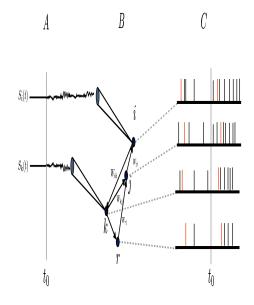


Figure 4. Linear response. The excitation of some neurons in a network will induce a variation in spike correlations between all connected neurons, even those which are not excited. We have computed this effect in [19].

This work has been submitted to Journal of Mathematical Neurosciences [19].

# **CAMIN Team**

# 6. New Results

# 6.1. A sensor fusion approach for inertial sensors based 3D kinematics and pathological gait assessments

Participants: Benoît Sijobert, Christine Azevedo, Jérôme Froger, Francois Feuvrier.

Pathological gait assessment and assistive control based on functional electrical stimulation (FES) in poststroke individuals, brings out a common need to robustly quantify kinematics facing multiple constraints.

Through an experimental study(Figure 5), we proposed a novel approach using inertial sensors to compute dorsiflexion angles and spatio-temporal parameters, in order to be later used as inputs for online close-loop control of FES. 26 post-stroke subjects were asked to walk on a pressure mat (GaitRite®) equipped with inertial measurement units (IMU) and passive reflective markers (Vicon®). A total of 930 strides were individually analyzed and results between IMU-based algorithms and reference systems compared. The novel methods integrated two aspects: 1) robust stance phase detection based on acceleration and angular rate combination and 2) estimation of joint angles based on an Attitude and Heading Reference System (non linear observer) algorithm and gravity cancellation for reconstructing 3D trajectory of individual steps. Mean absolute (MA) errors of dorsiflexion angles were found to be less than 4°, while stride lengths were robustly segmented and estimated with a MA error less than 10 cm [30]. These results open new doors to rehabilitation using adaptive FES closed-loop control strategies.

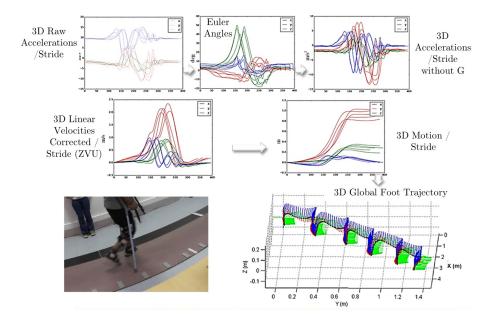


Figure 5. Illustration of the global approach needed to obtain gait trajectories from raw magneto-inertial data of a foot-mounted Inertial Measurement Unit to assess a circumduction gait.

# 6.2. FES-based online closed-loop control of knee joint to reduce stance phase asymmetry in post-stroke gait

Participants: Benoît Sijobert, Christine Azevedo, Charles Fattal.

Numerous stimulation strategies have been investigated over the past thirty years to assist or restore gait (Figure 6). The studies using FES to restore gait have been mostly conducted in post-stroke individuals and focused on correcting the drop foot syndrome by supplementing the absence of dorsiflexion. The state-of-the-art reflects a real lack of interest in using FES to improve the paretic knee rehabilitation, which however plays a key role in post-stroke gait recovery.

An experimental protocol (#RCB 2017-A03611-52, CRF La Chataigneraie, Menucourt, France) was designed with the main purpose of proposing a novel approach using a FES-based control of knee joint to reduce stance phase asymmetry and study the feasibility of using such FES systems in clinical rehabilitation, compared to classical knee orthosis. Secondary objectives aimed at improving gait quality, walking range and comfortable speed using the same modality. The main hypothesis was to determine if using FES to real-time control the paretic knee angle could reduce the time needed to recover a normal balance while providing a secure stance phase. To monitor weight bearing and stance time asymmetry the participants were equipped with instrumented insoles. The subjects were also equipped with 2 inertial measurement units located on the thigh and the tibia, wired to a Raspberry Pi3. Each IMU embedded a high speed based processor and a Kalman Filter directly providing quaternion estimation needed to compute knee angles. One IMU was installed in the back of the participants at the second sacral vertebra level to estimate vertical trunk displacement. Stimulation was sent via a two-channel wireless stimulator to the quadriceps and hamstrings via surface electrodes. A specific hardware architecture has been developed for this protocol. When required and depending on the participant's gait pattern, a "pre-stance" stimulation could be triggered either via an online detection of peak knee flexion or when the sagittal angular speed recorded via the gyroscope crossed zero. In stance phase, stimulation was triggered either to quadriceps or hamstrings, depending on the paretic knee angle (PKA) estimation relatively to the knee angle setpoint (KAS) defined by the practitioner as the optimal flexion during stance phase (around 5°). A proportional (P) controller adjusted the pulse width depending on the error  $\epsilon$  between PKA and KAS. Equipped with their usual technical aids (cane, ankle foot orthosis...) participants were asked to perform a 10mpath walking at a self-selected pace. An oral instruction was given at the beginning of each trial to encourage the participants to transfer their weight onto the paretic leg. This experiment is an ongoing experiment but preliminary tests have already validated the technical feasibility of the approach.

# 6.3. IMU-based FES cycling in individuals with SCI

**Participants:** Benoît Sijobert, Christine Azevedo, Ronan Le Guillou, Charles Fattal, Emerson Fachin Martin, Henrique Resende.

It has been shown that FES-cycling of subjects with Spinal Cord Injuries (SCI) results in physiological and psychological positive effects such as cardiovascular training, decrease in pressure sores occurrence and self-esteem improvements. However, the use of this technology has often remained restricted to indoor and stationary ergometers in clinical contexts, partly due to the small amount (10–25 W) of power produced and the requirement of experimented users to finely tuned the stimulation patterns needed to stimulate lower limb muscles with an adequate modality. In order to promote the research around this topic and more broadly the development of assistive technology for people with physical disabilities, we participated to the first Cybathlon in October 2016 (FreeWheels project), using a stimulation pattern based on crank angle. Taking part to this event highlighted the need for a simpler automated stimulation pattern generator, able to adapt the stimulation to the environment, to the muscle fatigue or to the individual (e.g. position on the bike, number of stimulable muscles, etc...). In order to further investigate control solutions, we first needed to be able to accurately quantify the influence of each parameter preliminarily used (stimulation pattern, stimulation parameters, fixed-wheel or free-wheel, individualized quadriceps, pilot position, etc...) on power produced and endurance and observe if other variables could be used as an input instead of the crank angle. The decision was made to develop an instrumented home trainer specifically designed to record a weak power (<200 W) while ensuring

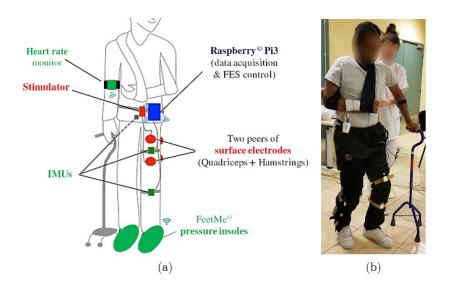


Figure 6. Experimental setup diagram (a) and picture (b). The participants are equipped with Bluetooth pressure insoles, 2 wired IMU on the leg and 1 wireless IMU in the back. A Raspberry records and processes the sensors data to send an appropriate command to a wireless stimulator to stimulate the quadriceps and hamstrings via surface electrodes

a minimum accuracy of 0.5 %: a rotating torquemeter (Scaime TSR 2300) was installed between the rear wheel and a flywheel thanks to a mechanical assembly built in collaboration with the National Engineering School of Saint-Étienne (ENISE, Loire, France)(Figure 7). The software part was developed as part of ADT STIMBIO.

Instead of using the crank angle, undergoing researches have also investigated the ability of using inertial sensors to automatically design a stimulation pattern on the bike depending on the knee angles. Based on the joint angle computation presented in section 6.1 and experimentally validated, a similar control modality have been studied and implemented. Using the online peak knee flexion algorithm developed in the study presented in section 6.2 to continuously detect this event, we developed a novel approach in order to trigger the quadriceps stimulation at the beginning of the pushing phase. This would enable to take into account a possible sliding in seat position without requiring an accurate placement of the IMUs or a geometrical model of the individual. A study has been initiated with the University of Brasilia (UnB, District Federal, Brazil) as part of the CACAO collaboration, to explore advanced control approaches [31]. Experimental data have been recorded and are investigated in order to compare the different control approaches (Figure 8).

### 6.4. Respiratory detection and monitoring

**Participants:** Xinyue Lu, Christine Azevedo, David Guiraud, Serge Renaux [Neuroresp], Thomas Similowski [Groupe Hospitalier Pitié-Salpêtrière].

This work is conducted within a CIFRE phd thesis. The general subject is the respiration induced by implanted stimulation for the tetraplegic and syndrome of Ondine. In France, every year, there is approximately 90 new spinal cord injuries who have a ventilatory dependence due to a high cervical involvement. The prevalence of syndrome of Ondine (central sleep apnea) would be 25.5 per million inhabitants. Because of many disadvantages of mechanical ventilation, the technique of implanted electrical stimulation to restore the respiratory function of the patients can be proposed. But existing systems are based on open-loop controllers,



Figure 7. Experimental setup using IMUs to record joint angles and a specifically designed home trainer to monitor power output.

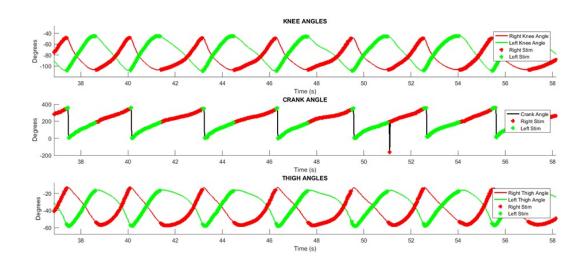


Figure 8. Comparison of stimulation patterns between crank angle and joint angle based triggering method.

ie the phrenic nerve is stimulated with the same intensity, at the same frequency for the whole time, even when the patients can breathe spontaneously. The principle aim of the work is to develop a respiratory detection/monitoring module in this context.

A solution based on tracheal sounds analysis has been developed. Tracheal sounds are recorded by microphone which is inserted into a support and stuck on the neck of subject like showed in Figure 9 .i. All the materials are showed in Figure 9 .ii: microphones (yellow), analog ampli-filtering card (red), the acquisition machine POWERLAB (green), the numeric development card NUCLEO (blue).

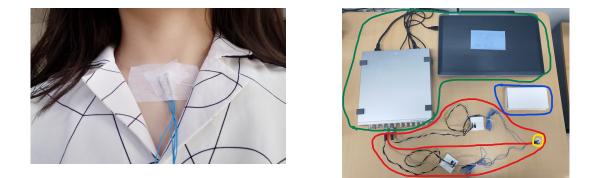


Figure 9. i)The placement of microphone ii)Recording materials

The signal is processed in its envelop (temporal domain) and frequency power (frequency domain). A threshold detection applied to detect respiration. An example of detection result is illustrated in Figure 10. Heart beating sounds can also be extracted to calculate cardiac rhythm.

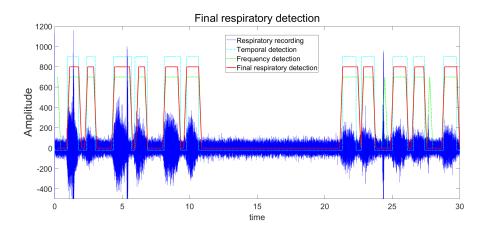


Figure 10. The detection result

Preliminary recordings on healthy individuals have been performed. Recordings on patients are in planning. Publications for conferences and journals are in preparation. The variation of cardiac amplitude will also be analyzed to give a secondary breathing detection. Advance signal processing techniques are now under study.

# 6.5. Attenuation and delay of remote potentials evoked by direct electrical stimulation during brain surgery.

**Participants:** Anthony Boyer, Sofiane Ramdani [LIRMM], Hugues Duffau [CHU Montpellier], David Guiraud, François Bonnetblanc.

Direct electrical stimulation (DES) is used during awake brain surgery for functional mapping as it generates transient behavioural disturbances, allowing the identification of both cortical areas and subcortical white matter pathways which are essential to the function. However, the electrophysiological effects of DES remain by far unknown. DES may be coupled with the measurement of Evoked Potentials (EPs) to study the conductive and integrative properties of activated neural ensembles and probe the spatiotemporal dynamics of short- and long- range networks. We recorded ECoG signals on two patients undergoing awake brain surgery and measured EPs on functional sites after cortical stimulations, using combinations of stimulation parameters (Figure 11). We were more particularly interested in the generation of evoked potentials (EPs) triggered by both close and remote stimulations. Obtained EPs were very similar in shape, suggesting a stereotyped electrophysiological response, but delayed in time and attenuated in amplitude when elicited from a different gyrus or remotely from the recording site. We were also able to observe the bidirectional nature of the arcuate fasciculus triggering EPs on 2 anatomically connected sites. We propose different activation and electrophysiological propagation mechanisms following DES based on recruited neural elements. The variations in amplitude and delay of EPs are most likely due to different propagation mechanisms, which can be intra- or sub- cortical, and correspond to commonly described DCRs and CCEPs.

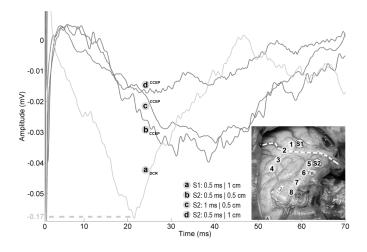


Figure 11. Differential recordings between electrodes 2 and 3 while stimulating S1 and S2. The picture illustrates the stimulation sites (S1, S2) and ECoG positioning with respect to the initial 60 Hz cortical brain mapping. Experimental DES was applied on: (1) the Wernicke's area (S1), associated with complete anomia; (2) the ventral premotor cortex (S2), which led to movement and counting interruptions. Tumor was about 164 cm3. The Sylvian fissure is highlighted by a thick dashed line.

# 6.6. High Frequency stimulation used for efficient and fiber type selective stimulation

Participants: David Guiraud, Mélissa Dali, Olivier Rossel, Thomas Guiho, Pawel Maciejasz.

In neural electrical stimulation, limiting the charge delivered during a stimulus pulse is essential to avoid nerve tissue damage and to save power. Previous experimental and modeling studies indicated that waveforms such as nonrectangular continuous pulses or rectangular chopped pulse were able to improve stimulation efficiency. The goal of this study is to evaluate if non-rectangular chopped pulses such as quarter sine and ramp are more charge efficient than rectangular chopped pulse. We performed in vivo study on 17 lumbricus terrestris and compared the charge per stimulating phase needed to activate lateral giant fibers (LGF) and medial giant fiber (MGF) using chopped non-rectangular chopped pulses and rectangular pulse, varying stimulation duration parameters. Results indicated that non rectangular chopped pulses activated MGF and LGF with less charge than rectangular chopped pulses. For MGF (respectively LGF), the gain of charge was up to 33.9% (resp. 17.8%) using chopped ramp, and up to 22.8% (resp. 18.1%) using chopped quarter sine.

## 6.7. Early detection of stroke during the accute phase

Participants: Victor Vagné, David Guiraud, Vincent Costalat, Emmanuelle Le Bars, Stéphane Perrey.

Cerebral infarctions can now be treated with new techniques using intravenous thrombolysis and thrombectomy. Their proven efficacy is directly correlated to the time lapse between the start of symptoms and the initiation of treatment. Currently, a definitive diagnosis can only be made once the patient has performed a radiological imaging (CT scan or MRI) on a medical center equipped with these expensive devices, thus enabling the medical team to initiate the appropriate treatment. Transit times during the pre-hospitalization phase before diagnosis are therefore often longer and have the greatest negative impact on the patient's prognosis. In collaboration with the interventional neuroradiology department of Gui de Chauliac Hospital, I2FH and Euromov, the EleVANT project is aiming to prospectively evaluate new techniques to assess a diagnosis of acute cerebral ischaemia. This low cost technology could be used in a mobile way for the very early diagnosis of cerebral infarction and thus reduce treatment delays, opening the way to a new generation of diagnostic tools. The concept consist on evaluating the cerebral near-infrared spectroscopy (NIRS) response to different stimulus, and to evaluate its lateralization. Recently, we tested our device on healthy volunteers. Method: Left and right hemisphere reactivity index are recorded by NIRS and normalized (Figure 12). Result: The experiments present a suitable feasibility and repeatability. In healthy subjects, a good response to the stimulus is recorded, and no significant differences between hemispheres are observed. The confidence level is acceptable since the amplitude response in above the standard deviation level.

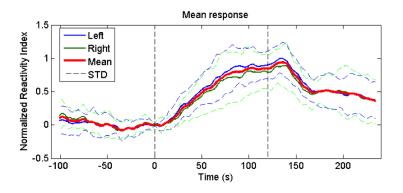


Figure 12. NIRS reactivity Index in response to a stimulus (bounded by the dashed lines)

Discussion: The approach reveal interesting results on healthy subject group. We expect a discriminant difference between hemispheric signals in acute cerebral ischemia.

## **6.8. Real-time simulation of stimulation systems**

Participant: Daniel Simon.

RT-STIM (Real-time FES simulation) is a C/C++ framework able to carry out realistic simulations of a fully featured functional electro-stimulation system. It allows for the temporally consistent co-simulation of both the continuous model of skeletal joints and muscles on one hand, and of numerical resources such as control tasks, schedulers and communication protocols on the other hand (Figure 13). Initial software-in-the-loop simulations can be seamlessly extended towards hardware-in-the-loop simulation by a progressive integration of real components such as a Raspberry portable control board or gateways towards Vivaltis stimulators and HiKoB sensors.

It is intended to be a support for the design and implementation of safe stimulation feedback controllers in the team. Hence, the simulation software is designed around the bio-mechanical models of joints and muscles excited using electro-stimulation developed in the Demar and Camin teams during the past years. To cope with the objectives of the team which targets the restoration of grasping for tetraplegia, a model of a human hand, currently using 23 joints and 23 muscles, has been integrated. It is expected to be a central tool for the Agilis project starting in 2019.

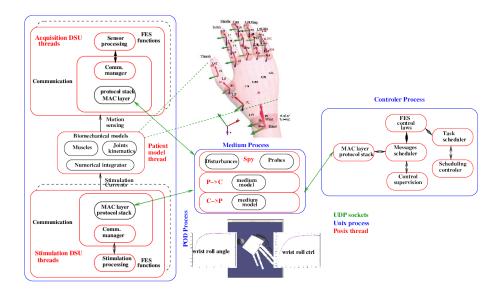


Figure 13. Simulation of a hand under FES

## 6.9. Real-time control for distributed stimulation systems

Participants: Daniel Simon, Ashwini Patil, Ronan Le Guillou.

Feedback control is needed to control complex movement, such as precise grasping, involving several muscles and nerves. Moreover, the components of the control loops (i.e., sensors, electrodes and micro-controllers) are distributed over communication links which induce data delivery scheduling, delays, and occasional data loss. A new approach gathering control and computation related design and implementation constraints was developed during the past years. From the feedback provided by experiments in real-time robot control,

Considering the non-linear and time varying models, simple controllers cannot provide reliable and robust solutions. the approach is developed along two main directions, control aware computing, e.g., using feedback schedulers, and real-time aware control, e.g. using feedback controllers designed to be robust and/or adaptive w.r.t. timing deviations [32].

Beyond simple control loops, a Model Predictive Control approach for FES using an adaptive horizon is under evaluation. Even if no conclusion about the control approach can be currently carried out, it was an occasion to positively evaluate the Julia programming language as an alternative to others high level languages for control design and real-time implementation.

A software control structure, primarily implemented and evaluated on a portable Rasperry3 micro-controller, is currently documented to become the root of a generic real-time control software template, usable even by non-specialists in the Camin team.

# **CASTOR Project-Team**

# 7. New Results

### 7.1. Block-structured meshes

Participants: Hervé Guillard, Alexis Loyer, Jalal Lakhlili [IPP Garching], Ahmed Ratnani [IPP Garching].

Due to the highly anisotropic character of strongly magnetized plasmas, a crucial point for numerical simulations is the construction of meshes that are aligned on the magnetic flux surfaces computed by Grad-Shafranov equilibrium solvers. This work has studied an original method for the construction of flux aligned grids that respect the magnetic equilibrium topology and that can be applied to block-structured meshes using  $C^1$  finite element methods (Hermite-Bézier/Cubic spline). The method relies on the analysis of the singularities of the magnetic flux function and the construction of the Reeb graph that allows the segmentation of the physical domain into sub-domains that can be mapped to a reference square domain. Once this domain decomposition has been done, the mapping of the sub-domain to reference patches can be done using integration along the streamlines of the flux function [16]. This work was performed in the framework of the EoCoE European project (see section 8.2.1.1).

### 7.2. Unstructured triangular meshes for tokamaks

Participants: Hervé Guillard, Alexis Loyer, Adrien Loseille [Gamma3 team, Inria Saclay].

The construction of block-structured flux aligned grids that respect the magnetic equilibrium topology experiences difficulties in the SOL region of the tokamaks where the flux lines cross the material walls. As an alternative to the use of block structured meshes, we have studied the construction of unstructured triangular meshes using constrained anisotropic Delaunay mesh generation [16]. This work was also performed in the framework of the EoCoE European project (see section 8.2.1.1).

### 7.3. Simulations of hydraulic jumps with a turbulent Shallow Water model

**Participants:** Hervé Guillard, Argiris Delis [Technical University of Crete, Greece], Yih-Chin Tai [National Cheng Kung University, Taiwan].

We have pursued the work realized in 2017, on a new model designed for the computation of turbulent hydraulic jumps. This model is able to describe the oscillatory nature of turbulent hydraulic jumps and as such corrects the deficiency of the classical shallow water equations. The comparisons with experiments performed at Tainan University are very satisfactory given the simplicity of the model. A journal paper [3] on this subject have been published and these results have been presented at the ETAMM2018 (Emerging Trends in Applied Mathematics and Mechanics 2018) conference.

# **7.4. 2D** $C^1$ triangular elements

Participants: Hervé Guillard, Ali Elarif, Boniface Nkonga.

In order to avoid some mesh singularities that arise when using quadrangular elements for complex geometries and flux aligned meshes, the use of triangular elements is a possible option that we have studied in the past years. In particular, we have developped the geometric tools necessary for the construction of Powell-Sabin splines and have applied these methods for the approximation of some simple hyperbolic PDE systems (namely the Euler equation of fluid dynamics [6]). The PhD thesis of Ali Elarif that has begun in october 2017 is devoted to the study of the applicability of these methods to more complex PDE models encountered in plasma physics and to an extension towards other triangular  $C^1$  elements (Clough-Tocher elements). The work realized this year has allowed to apply these finite element spaces to the approximation of elliptic equations and to design penalization methods to enforce non-homogeneous Dirichlet boundary conditions. In particular, the use of reduced Clough-Tocher elements has been applied to obtain solution of the free-boundary non-linear Grad-Shafranov equation. The results show that the use of these  $C^1$  elements produce results that are smoother than the ones obtained with low order P1 elements.

## 7.5. Equilibrium reconstruction at JET using Stokes model for polarimetry

Participant: Blaise Faugeras.

This paper presents the first application to real JET data of the new equilibrium code NICE which enables the consistent resolution of the inverse equilibrium reconstruction problem in the framework of non-linear free-boundary equilibrium coupled to the Stokes model equation for polarimetry. The conducted numerical experiments enable first of all to validate NICE by comparing it to the well-established EFIT code on 4 selected high performance shots. Secondly the results indicate that the fit to polarimetry measurements clearly benefits from the use of Stokes vector measurements compared to the classical case of Faraday measurements, and that the reconstructed p' and ff' profiles are better constrained with smaller error bars and are closer to the profiles reconstructed by EFTM, the EFIT JET code using internal MSE constraints.

## 7.6. Operational plasma boundary reconstruction with the NICE-VacTH code on WEST Tokamak

Participant: Blaise Faugeras.

A new regularization term has been proposed for the inverse problem of plasma boundary reconstruction using an expansion of the poloidal flux in toroidal harmonics. It has been implemented in the VacTH code and is used successfully on the WEST Tokamak.

## 7.7. Equilibrium reconstruction with NICE at WEST and within the framework of the European Integrated Tokamak Modelling WPCD project

Participant: Blaise Faugeras.

The adaptation of NICE to IMAS (the ITER standard using IDS as data type) has been carried on. Equilibrium reconstructions using IMAS have been performed on real JET measurements and are now performed routinely at WEST.

## 7.8. Equilibrium reconstruction with Equinox at JET

Participant: Blaise Faugeras.

The adaptation of NICE to IMAS the ITER standard using IDS as data type has been carried on. Equilibrium reconstructions using IMAS have been performed on real JET measurements and are now performed routineley at WEST.

### 7.9. Evolutive mode and iron model in NICE

Participants: Blaise Faugeras, Jacques Blum, Cédric Boulbe.

The capabilities of the equilbirum code NICE have been extended. The evolutive direct model and the iron model of the free boundary equilibrium code CEDRES++ have been ported in NICE.

## 7.10. Coupling CEDRES++ - WEST controller in IMAS

Participants: Cédric Boulbe, Jakub Urban [IPP Prague].

The free boundary equilibrium code has been fully adapted to IMAS and has been coupled to the magnetic controller of WEST. The code CEDRES++ simulate the plant and the controller provide the voltages applied to the PF supplies. This coupling has enabled to develop a tool in Python to interface easily Simulink controllers with IMAS. With that tool, it is possible to run a controller installed on a distant computer and to run it from IMAS. As a test case, the WEST controller has been interfaced with IMAS and coupled to CEDRES++ using an IMAS python workflow.

## 7.11. Spectral Element method for high order partial differential equations

Participants: Sebastian Minjeaud, Richard Pasquetti.

The Korteweg-de Vries equation has been addressed as an interesting model of high order partial differential equation. In [9] it is shown that it is possible to develop reliable and effective schemes, in terms of accuracy, computational efficiency, simplicity of implementation and, if required, conservation of the lower invariants, on the basis of a (only)  $H^1$ -conformal Galerkin approximation, namely the Spectral Element Method. The proposed approach is *a priori* easily extensible to other partial differential equations and to multidimensional problems.

## 7.12. Recent advances in Spectral element methods on simplicial meshes

Participants: Richard Pasquetti, Francesca Rapetti.

R. Pasquetti and F. Rapetti have investigated the cubature points based triangular spectral element method. Using cubature points, both for interpolations and quadratures, shows the advantage of yielding a diagonal mass matrix. Accuracy results are provided in [10], for elliptic problems in non polygonal domains, using various isoparametric mappings. The capabilities of the method are here again clearly confirmed.

### 7.13. Full-MHD with Jorek

Participants: Boniface Nkonga, Ashish Bhole.

In the context of A. Bohle PhD, we have developped a strategy to improve the formulation of finite element space in the context of iso-parametric finite elements with singular parametrization. This result in a set of constraints to be applied in the numerical formulation to fit in the well defined approximated space. Applied to interpolations, we recover the optimal order of convergence of the numerical approximation. Next step is applications to the resolution of reduced-MHD and then full-MHD.

# 7.14. A discontinuous Galerkin method for a two dimensional resistive MHD model

Participants: Ashish Bhole, Boniface Nkonga, Praveen Chandrashekar.

We consider the numerical approximation of two dimensional incompressible magnetohydrodynamics equations with vorticity and current as the dynamical variables. We construct a discontinuous Galerkin (DG) method for the MHD model written in symmetric form. The numerical flux is based on a Riemann solver and the scalar fluxes of velocity and magnetic field are computed using a Galerkin method. The performance of the method is demonstrated on some standard instability problems relevant to magnetically confined fusion reactors.

# 7.15. Fluctuation splitting Riemann solver for a non-conservative shear shallow water flow

Participants: Ashish Bhole, Boniface Nkonga, Sergey Gavrilyuk.

We propose a fluctuation splitting finite volume scheme for a non-conservative modeling of shear shallow water flow (SSWF). This model was originally proposed by Teshukov and was extended to include modeling of friction by Gavrilyuk (2018). We develop a cell-centered finite volume code to validate the proposed scheme with the help of some numerical tests. As expected, the scheme shows first order convergence. The numerical simulation of 1D roll waves shows a good agreement with the experimental results. The numerical simulations of 2D roll waves show similar transverse wave structures as observed by Gavrilyuk (Paper in revision at JCP).

## 7.16. Automating the design of Tokamak experiment scenarios

Participants: Jacques Blum, Holger Heumann, Xiao Song.

The real-time control of plasma position, shape and current in a tokamak has to be ensured by a number of electrical circuits consisting of voltage suppliers and axisymmetric coils. Finding good target voltages/currents for the control systems is a very laborious, non-trivial task due to non-linear effects of plasma evolution. We introduce here an optimal control formulation to tackle this task and present in detail the main ingredients for finding numerical solutions: the finite element discretization, accurate linearizations and Sequential Quadratic Programming. Case studies for the tokamaks WEST and HL2M highlight the exibility and broad scope of the proposed optimal control formulation.

## 7.17. Multiscales scheme for the MHD model in a tokamak

Participants: Hervé Guillard, Afeintou Sangam.

Recently, in [21], it is proven that the Reduced MHD equations are a singular limit of the Full MHD system when the inverse ratio parameter goes to zero. In this limit, the toroidal dynamics is almost entirely decoupled from the incompressible poloidal dynamics. From a numerical point of view, in this limit, the propagation of fast magnetosonic waves severely constraints the time step in explicit schemes. A possible remedy is therefore to design a semi-implicit time stepping strategy allowing an implicit handling of the fast waves but retaining an explicit treatment of the slow ones. In this work, we have derived a linear simplified model in two dimensions that retains the main characteristics of the formal passage from the Full MHD equations to the Reduced MHD system. A semi-implicit numerical scheme free of time step restrictions based on the fast wave velocity has been constructed for this model. The extension of this numerical scheme to the Full MHD model is under investigation.

# 7.18. Asymptotic Transport Models for heat and mass transport in reactive porious media

Participants: Bruno Dubroca, Afeintou Sangam.

*Charrier* and *Dubroca* in [20], have suggested an approach to derive rigously a family of models of mass and heat transfer in reactive porous media. At a microscopic level they proposed a model coupling the Boltzmann equation in the gas phase, the heat equation and appropriate interface conditions, including adsorption-deposition reactions. Then an asymptotic expansion mixing homogenization and fluid limit leads to a system of coupled diffusion equations where the effective diffusion tensors are defined from the microscopic geometry of the material. Open questions paved their work. We solve one of them, consisting in setting adequate conditions on interest models that ensure the uniqueness of solutions of the first order expansion. They are based on the concept of thermodynamically closed in average system.

## **COFFEE Project-Team**

## 7. New Results

### 7.1. A few words on the results of the year

- Face based discretization of two-phase Darcy flows in fractured porous medium with matrix fracture interface local nonlinear solver. Application to the simulation of the desaturation by suction in nuclear waster storages [20], [17].
- Convergence analysis of the gradient discretization of a two-phase Darcy flow model in fractured porous media with nonlinear transmission conditions [10].
- Numerical method for non-isothermal compositional Darcy flows combining face based and nodal based discretizations on hybrid meshes [22].
- We introduced and analyzed a novel Hybrid High-Order method for the steady incompressible Navier-Stokes equations. We showed under general assumptions the existence of a discrete solution, we proved convergence of the sequence of discrete solutions to minimal regularity exact solutions for general data and we proved optimal convergence rates for the velocity and the pressure [9].
- We proposed a nonlinear Discrete Duality Finite Volume scheme to approximate the solutions of drift diffusion equations. The scheme is built to preserve at the discrete level even on severely distorted meshes the energy / energy dissipation relation [7].
- We studied a Discrete Duality Finite Volume scheme for the unsteady incompressible Navier-Stokes problem with outflow boundary conditions [24].
- We introduced a new non-overlapping optimized Schwarz method for anisotropic diffusion problems. We studied the new method at the continuous level, proved its convergence using energy estimates, and also derived convergence factors to determine the optimal choice of parameters in the transmission conditions, and presented a discretization of the algorithm using discrete duality finite volumes [23].
- We consider a non-local traffic model involving a convolution product. Unlike other studies, the considered kernel is discontinuous on ℝ. We prove Sobolev estimates and prove the convergence of approximate solutions solving a viscous and regularized non-local equation. It leads to weak,  $C([0,T], L^2(\mathbb{R}))$  and  $C([0,T], L^2(\mathbb{R}))$ , and smooth,  $W^{2,2N}([0,T] \times \mathbb{R})$  and  $W^{2,2N}([0,T] \times \mathbb{R})$ , solutions for the non-local traffic model [4].
- We proposed a new closure for Geometrical Shock Dynamics taking into account the effect of transverse Mach variation for the fast propagation of shocks. The model has been tested using a Lagrangian solver [28].
- We proposed a new explicit pseudo-energy conserving time-integration scheme for separated Hamiltonian systems. We proved the second-order accuracy and conditional stability of the scheme. In addition, the scheme can be adapted into an asynchronous version while retaining its properties, which is adapted to slow-fast splitting strategies [14].
- We proposed a well-balanced scheme for the modified Lifschitz-Slyozov-Wagner system with diffusion, which models Ostwald ripening. The scheme outperforms a standard advection-diffusion scheme for long time dynamics [25].
- We investigate several models describing interacting particles, either motivated form physics or population dynamics.

## **EPIONE Project-Team**

## 6. New Results

## 6.1. Medical Image Analysis

#### 6.1.1. Learning a Probabilistic Model for Diffeomorphic Registration

**Participants:** Julian Krebs [Correspondant], Hervé Delingette, Tommaso Mansi [Siemens Healthineers, Princeton, NJ, USA], Nicholas Ayache.

This work is funded by Siemens Healthineers, Princeton, NJ, USA

deformable registration, probabilistic modeling, deep learning, latent variable model, deformation transport, disease clustering

We developed a probabilistic approach for deformable image registration in 3-D using deep learning methods [30]. This method includes:

- A probabilistic formulation of the registration problem through unsupervised learning of an encoded deformation model (Fig. 4).
- A differentiable exponentiation layer and an user-adjustable smoothness layer that ensure the outputs of neural networks to be regular and diffeomorphic.
- An analysis of size and structure of a latent variable space for registration.
- Experiments on deformation transport and disease clustering.

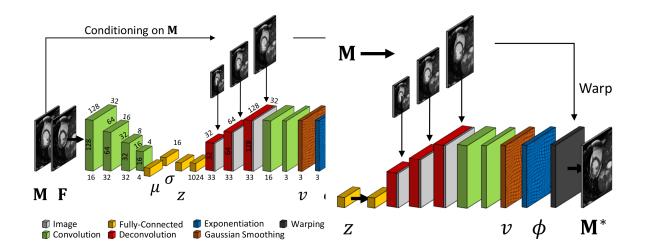


Figure 4. (Left) Probabilistic registration network including a diffeomorphic layer (exponentiation). Deformations are encoded in z from which velocities are decoded while being conditioned on the moving image. (Right) Decoder network for sampling and deformation transport: Apply z-code conditioned on any new image M.

#### 6.1.2. Learning Myelin Content in Multiple Sclerosis from Multimodal MRI

Participants: Wen Wei [Correspondent], Nicholas Ayache, Olivier Colliot [ARAMIS].

This work is done in collaboration with the Aramis-Project team of Inria in Paris and the researchers at the Brain and Spinal Cord Institute (ICM) located in Paris.

Multiple Sclerosis, MRI, PET, GANs

- We predict myelin content from multiparametric MRI [36].
- We design an adaptive loss and a sketch-refinement process for GANs, decomposing the problem into anatomy/physiology and myelin content prediction (Fig. 5).
- We show similar results to the PET-derived gold standard.

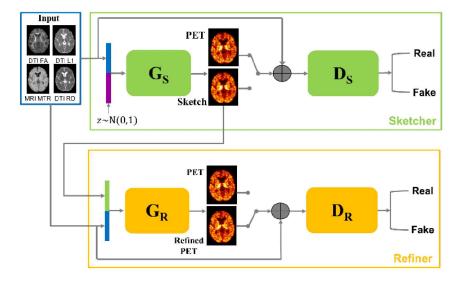


Figure 5. The sketcher receives MR images and generates the preliminary anatomy and physiology information. The refiner receives MR images IM and the sketch IS. Then it refines and generates PET images.

#### 6.1.3. Consistent and Robust Segmentation of Cardiac Images with Propagation

Participants: Qiao Zheng [Correspondant], Hervé Delingette, Nicolas Duchateau, Nicholas Ayache.

This project is funded by European Research Council (MedYMA ERC-AdG-2011-291080).

Cardiac segmentation, deep learning, neural network, 3D consistency, spatial propagation

We propose a method based on deep learning to perform cardiac segmentation on short axis MRI image stacks iteratively from the top slice (around the base) to the bottom slice (around the apex) [26][62]. At each iteration, a novel variant of U-net is applied to propagate the segmentation of a slice to the adjacent slice below it (Fig. 6).

- 3D-consistency is hence explicitly enforced.
- Robustness and generalization ability to unseen cases are demonstrated.
- Results comparable or even better than the state-of-the-art are achieved.

The corresponding open source software, CardiacSegmentationPropagation, is available in https://team.inria. fr/epione/en/software/.

#### 6.1.4. Deep Learning for Tumor Segmentation

**Participants:** Pawel Mlynarski [Correspondant], Nicholas Ayache, Hervé Delingette, Antonio Criminisi [MSR].

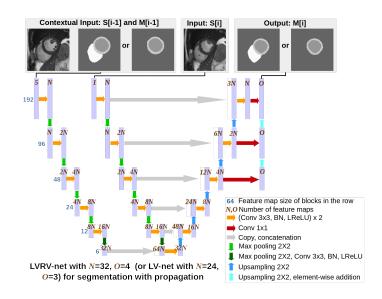


Figure 6. Propagation of cardiac segmentation by a neural network.

This work is funded by Inria-Microsoft Joint Center and is done in cooperation with Microsoft Research in Cambridge.

deep learning, semi-supervised learning, segmentation, MRI, tumors

- We proposed a model for tumor segmentation which is able to analyze a very large spatial context by combining 2D and 3D CNNs [56] (Fig. 7). Top-3 performance was obtained on BRATS 2017 challenge.
- We proposed an approach to train CNNs for tumor segmentation with a mixed level of supervision [55]. Our approach significantly improves segmentation accuracy compared to standard supervised learning.
- We designed a system for segmentation of organs at risk for protontherapy. Promising preliminary results were obtained.

## 6.2. Imaging & Phenomics, Biostatistics

#### 6.2.1. Radiomic analysis to improve diagnosis and therapy in oncology

**Participants:** Fanny Orlhac [Correspondant], Nicholas Ayache, Charles Bouveyron, Jacques Darcourt [CAL], Hervé Delingette, Olivier Humbert [CAL], Pierre-Alexandre Mattei [Copenhague University], Thierry Pourcher [CEA], Fanny Vandenbos [CHU Nice].

Inria postdoctoral fellowship for 16 months

Radiomics, Statistical learning, Metabolomics

- We proposed a modeling which extends the High-Dimensional Discriminant Analysis (HDDA) model by incorporating a sparsity pattern for each class, called sparse HDDA (sHDDA) [21].
- We demonstrated its efficacy in identifying lung lesions based on CT radiomic features (see Figure 8) [21] or triple-negative breast lesions from PET radiomic features and metabolomic data [34], [32], [33]. Thanks to the class-specific variable selection, the final model can be easily interpreted by physicians.
- We also demonstrated the capacity of the ComBat method to harmonize radiomic features extracted from PET images acquired with different imaging protocols [40], [39].

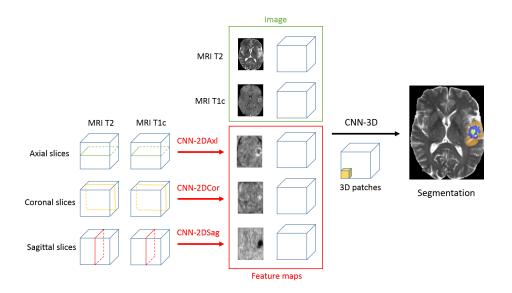


Figure 7. Illustration of our 2D-3D model for brain tumor segmentation.

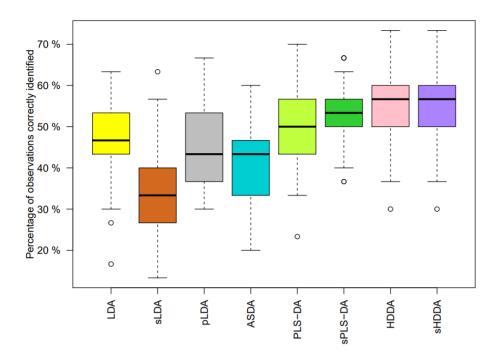


Figure 8. Classification accuracy of the eight statistical methods, including HDDA in pink and sHDDA in purple, to identifying lung lesions based on radiomic features extracted from CT images.

# 6.2.2. Statistical learning on large databases of heterogeneous imaging, cognitive and behavioral data

**Participants:** Luigi Antelmi [Correspondent], Marco Lorenzi, Valeria Manera, Philippe Robert, Nicholas Ayache.

Supported by the French government, through the UCA<sup>JEDI</sup> Investments in the Future project managed by the National Research Agency (ANR) ref. num. ANR-15-IDEX-01, our research is within the MNC3 initiative (Médecine Numérique: Cerveau, Cognition, Comportement), in collaboration with the Institut Claude Pompidou (CHU of Nice). Computational facilities are funded by the grant AAP Santé 06 2017-260 DGA-DSH, and by the Inria Sophia Antipolis - Méditerranée, "NEF" computation cluster.

statistical learning, joint analysis, neuroimaging

The aim of our work is to build scalable learning models for the joint analysis of heterogeneous biomedical data, to be applied to the investigation of neurological and neuropsychiatric disorders from collections of brain imaging, body sensors, biological and clinical data available in current large-scale databases such as ADNI<sup>0</sup> and local clinical cohorts.

We developed a computationally efficient formulation of probabilistic latent variable models [37]. This approach is capable to highlight meaningful relationships among biomarkers in the context of Alzheimer's disease (Figure 9) that can be used to develop optimal strategies for disease quantification and prediction.

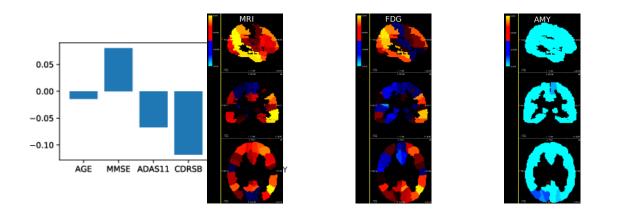


Figure 9. Joint relationships among Alzheimer's disease biomarkers discovered by our multi-channel model in the ADNI dataset. Relationships in line with the current literature discoveries. Clinical biomarkers on the left; brain imaging biomarkers on the right: gray matter density (MRI), glucose uptake (FDG), amyloid uptake (AMY).

#### 6.2.3. Joint Biological & Imaging markers for the Diagnosis of severe lung diseases

Participants: Benoît Audelan [Correspondant], Hervé Delingette, Nicholas Ayache.

Lung cancer, Early detection, Sparse Bayesian Learning

Lung cancer is among the most common cancer and is considered to be one of the most important public health problem. The aim of this work is to improve the detection of lung cancer by combining imaging and biological markers. Exploratory analysis have been conducted to discriminate cancer patients versus controls from circulating miRNAs data using sparse Bayesian learning and to automatically pre-process lung CT images (Fig. 10).

<sup>&</sup>lt;sup>0</sup>http://adni.loni.usc.edu/

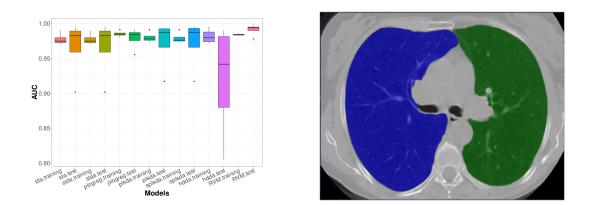


Figure 10. Comparison of statistical methods for classifying lung cancer patient from miRNAs data and lung segmentation

### 6.2.4. A data-driven model of mechanistic brain atrophy propagation in dementia

Participants: Sara Garbarino [Correspondant], Marco Lorenzi.

Sara Garbarino acknowledges financial support from the French government managed by L'Agence Nationale de la Recherche under Investissements d'Avenir UCA JEDI (ANR-15-IDEX-01) through the project "AtroPro-Dem: A data-driven model of mechanistic brain Atrophy Propagation in Dementia".

Gaussian Processes, Bayesian non-parametric modelling, neuroimaging data, protein dynamics, brain network

Models of misfolded proteins aim at discovering the bio-mechanical properties of neurological diseases by identifying plausible associated dynamical systems. Solving these systems along the full disease trajectory is usually challenging, due to the lack of a well defined time axis for the pathology. This issue is solved by disease progression models where long-term progression trajectories are estimated via time reparametrization of individual observations. However, due to their loose assumptions on the dynamics, they do not provide insights on the bio-mechanical properties of protein propagation.

In this project we propose a unified model of spatio-temporal protein dynamics based on the joint estimation of long-term protein dynamics and time reparameterization of individuals observations (Figure 11). The model is expressed within a Gaussian Process regression setting, where constraints on the dynamics are imposed through non–linear dynamical systems.

## 6.2.5. Federated Learning in Distributed Medical Databases: Meta-Analysis of Large-Scale Subcortical Brain Data

**Participants:** Santiago Silva [Correspondant], Marco Lorenzi, Boris Gutman, Andre Altman, Eduardo Romero, Paul M. Thompson.

This work was supported by the French government, through the UCAJEDI Investments in the Future project managed by the National Research Agency (ANR) with the reference number ANR-15-IDEX-01 (project Meta-ImaGen).

Federated learning, distributed databases, PCA, SVD, meta-analysis, brain disease.

We proposed a federated learning framework for securely accessing and meta-analyzing any biomedical data without sharing individual information.

• A frontend pipeline for preprocessing and analyzing data was proposed, including: standardization, confounders correction, and variability analysis via federated PCA.

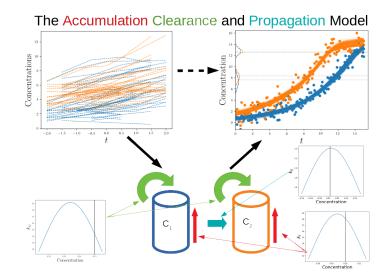


Figure 11. Schematic representation of our framework. Here we have two brain regions whose concentrations are collected for many subjects over a short term time span. The dynamics of such concentrations is described in terms of accumulation, clearance and propagation parameters. The proposed Bayesian framework estimates the distribution of such parameters and the long term trajectories with respect to the estimated disease time axis.

- Tested on multi-centric and multi-diagnosis databases (ADNI, PPMI and UK-Biobank) showed a clear differentiation between control and Alzheimer's subjects (Figure 12).
- Further developments of this study will extend the proposed analysis to large-scale imaging genetics data, such as in the context of the ENIGMA meta-study.

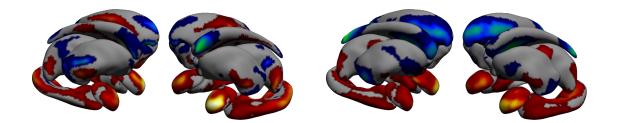


Figure 12. First principal component estimated with the proposed federated framework. The component maps prevalently hippocampi and amigdalae. Left: Thickness. Right: Log-Jacobians.

## 6.3. Computational Anatomy

6.3.1. Statistical Learning of Heterogeneous Data in Large-Scale Clinical Databases Participants: Clement Abi Nader [Correspondant], Nicholas Ayache, Philippe Robert, Marco Lorenzi. Gaussian Process, Alzheimer's Disease, Disease Progression Modelling

The aim of this project is to develop a spatio-temporal model of Alzheimer's Disease (AD) progession [47]. We assume that the brain progression is characterized by independent spatio-temporal sources that we want to separate. We estimate brain structures involved in the disease progression at different resolutions thus dealing with the non-stationarity of medical images, while assigning to each of them a monotonic temporal progression using monotonic Gaussian processes (Figure 13, left-middle panel). We also compute an individual time-shift parameter to assess the disease stage of each subject (Figure 13, right panel).

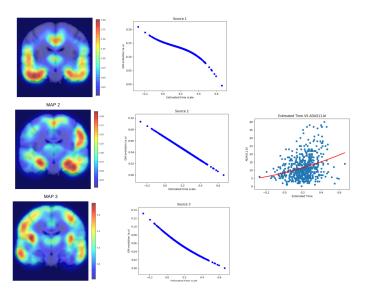


Figure 13. Left-Middle: Brain structures involved in AD along with their temporal evolution. Right: Correlation between ADAS11 cognitive score and the individual time-shift.

#### 6.3.2. A model of brain morphological evolution

**Participants:** Raphaël Sivera [Correspondant], Hervé Delingette, Marco Lorenzi, Xavier Pennec, Nicholas Ayache.

Longitudinal modeling, Deformation framework, Brain morphology, Alzheimer's disease, Aging.

We proposed a deformation-based generative model of the brain morphological evolution that can jointly describes the effect of aging and Alzheimer's disease. It relies on longitudinal description of the aging and disease consequences and can be use to compute image-based cross-sectional progression markers. This approach is able to propose a description of the disease evolution, population and subject-wise(see Figure 14) and open the way to a better modeling of the disease progression.

#### 6.3.3. Geometric statistics

Participant: Xavier Pennec [Correspondant].

*This work is partially funded by the ERC-Adv G-Statistics.* Statistics on manifolds, Differential geometry,

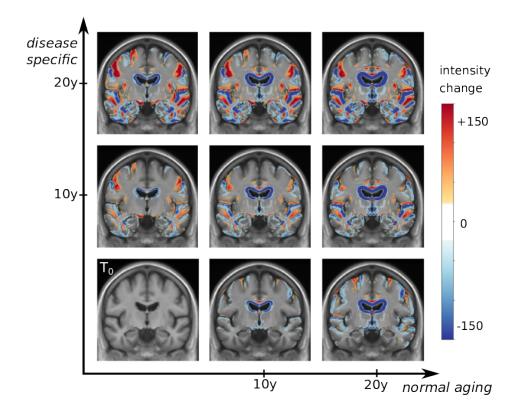


Figure 14. Representation of the 2D parametric template subspace generated by the model. In these images, the bottom row correspond to a healthy evolution, and the diagonal (from bottom left to top right) to a typical pathological evolution. The colors represent the voxel-wise intensity differences between the images and the reference  $T_0$  to highlight the boundary shifts between tissues and CSF.

Beyond the mean value, Principal Component Analysis (PCA) is often used to describe the main modes of variability and to create low dimensional models of the data. Generalizing these tools to manifolds is a difficult problem. In order to define low dimensional parametric subspaces in manifolds, we proposed in [22] to use the locus of points that are weighted means of a number of reference points. These barycentric subspaces locally define submanifolds which can naturally be nested to provide a hierarchy of properly embedded subspaces of increasing dimension (a flag) approximating the data better and better. This defines a generalization of PCA to manifolds called Barycentric Subspace Analysis (BSA) which provides a new perspective for dimension reduction. It appears to be well suited for implicit manifolds such as the ones defined by multiple registrations in longitudinal or cross-section image analysis. An example of such an application was provided in [23] for 4D cardiac image sequences.

In classical estimation problems, the number of samples is always finite. The variability that this induces on the estimated empirical mean is a classical result of the law of large numbers in the asymptotic regime. In manifolds, it is not clear how the curvature influences the estimation of the empirical Fréchet mean with a finite number of samples. Preliminary results showed that there is an unexpected bias inversely proportional to the number of samples induced by the gradient of the curvature and a correction term of the same order on the covariance matrix slowering or accelerating the effective convergence rate towards the Fréchet mean of the underlying distribution. These preliminary results were derived using a new simple methodology that is also extending the validity from Riemannian manifolds to affine connection spaces [45].

#### 6.3.4. Brain template as a Fréchet mean in quotient spaces

Participants: Nina Miolane [Correspondant], Xavier Pennec.

Computational anatomy, Morphological brain template, Hierarchical modeling.

Geometrically, the procedure used to construct the reference anatomy for normalizing the measurements of individual subject in neuroimaging studies can be summarized as the Fréchet mean of the images projected in a quotient space. We have previously shown that this procedure is asymptotically biased, therefore inconsistent. In [15], we presented a methodology that quantifies spatially the brain template's asymptotic bias. We identify the main variables controlling the inconsistency. This leads us to investigate the topology of the template's intensity levels sets, represented by its Morse-Smale complex. We have proposed a topologically constrained adaptation of the template computation that constructs a hierarchical template with bounded bias. We apply our method to the analysis of a brain template of 136 T1 weighted MR images from the Open Access Series of Imaging Studies (OASIS) database.

## 6.3.5. Cardiac Motion Evolution Modeling from Cross-Sectional Data using Tensor Decomposition

Participants: Kristin Mcleod [Simula Research Laboratory], Maxime Sermesant, Xavier Pennec.

Cardiac motion tracking, modeling cardiac motion evolution over time

Cardiac disease can reduce the ability of the ventricles to function well enough to sustain long-term pumping efficiency. We proposed in [14] a cardiac motion tracking method to study and model cohort effects related to age with respect to cardiac function. The proposed approach makes use of a Polyaffine model for describing cardiac motion of a given subject, which gives a compact parameterisation that reliably and accurately describes the cardiac motion across populations. Using this method, a data tensor of motion parameters is extracted for a given population. The partial least squares method for higher-order arrays is used to build a model to describe the motion parameters with respect to age, from which a model of motion given age is derived. Based on cross-sectional statistical analysis with the data tensor of each subject treated as an observation along time, the left ventricular motion over time of Tetralogy of Fallot patients is analysed to understand the temporal evolution of functional abnormalities in this population compared to healthy motion dynamics (see Figure 15).

#### 6.3.6. Challenging cardiac shape and motion statistics

Participants: Marc-Michel Rohé [correspondant], Maxime Sermesant, Xavier Pennec.

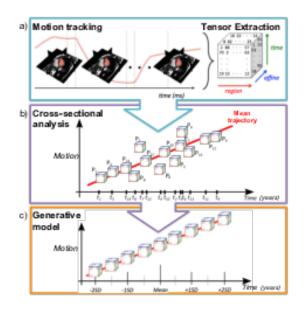


Figure 15. Building a generative model of the long-term motion changes in a population (c) by a) building a data tensor of polyaffine motion parameters that represent the motion over the cardiac cycle for each subject in the population using cross-sectional statistical analysis of polyaffine tensors and b) performing cross-sectional statistical analysis of the data tensors.

Shape statistics, Non-rigid registration, Deep learning, Cardiac shape and motion

Two of the methods previously developed by Marc-Michel Rohé in his PhD were benchmarked against other state of the art methods in two successive MICCAI challenges. First, the SVF-net developed to perform a very-fast inter-subject heart registration based on convolutional neural networks was embedded into a multiatlas segmentation pipeline and tested against other deep learning techniques for the automatic MRI cardiac multi-structures segmentation [2]. Second, a combination of polyaffine cardiac motion tracking and supervised learning was used to predict myocardial infarction [25]. Both challenges demonstrate the good performances of the tested methods.

## 6.4. Computational Physiology

### 6.4.1. CIMPLE : Cochlear Implantation Modeling, PLanning & Evaluation

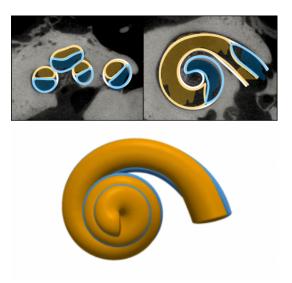
**Participants:** Zihao Wang [Correspondant], Hervé Delingette, Thomas Demarcy [Oticon Medical], Clair Vandersteen [IUFC], Nicolas Guevara [IUFC], Charles Raffaelli [CHU], Dan Gnansia [Oticon Medical], Nicholas Ayache.

This work is funded by the Provence-Alpes-Côte-d'Azur region, the Université Côte d'Azur and Oticon Medical.

Statistic Learning, Image segmentation, Cochlea Implantation

The work aims to establish an effective, quantitative and rapid assessment method for human cochlear implantation planning and adjustment.

During last one year, our team explored a cost-effectively and practically algorithm to achieve the goal.



*Figure 16. The figure shown a example segmentation on micro-CT image. Lower is the parametric model that quantitative mesure the cochea shape.* 

## 6.5. Computational Cardiology & Image-Based Cardiac Interventions

#### 6.5.1. Population-based priors for group-wise Personalisation

**Participants:** Roch Molléro [Correspondant], Hervé Delingette, Xavier Pennec, Nicholas Ayache, Maxime Sermesant.

#### The authors acknowledge the partial funding by the MD-Paedigree EU Project.

Personalised cardiac model, Parameter observability, Statistical modeling, Dimensionality reduction, Heterogeneous clinical data, Imputation

Personalised cardiac models have a large number of parameters while the available data for a given patient is typically limited to a small set of measurements, thus the parameters cannot be estimated uniquely. This is a practical obstacle for clinical applications, where accurate parameter values can be important. Here we explore an original approach based on an algorithm called Iteratively Updated Priors (IUP), in which we perform successive personalisations of a full database through Maximum A Posteriori (MAP) estimation, where the prior probability at an iteration is set from the distribution of personalised parameters in the database at the previous iteration (Figure 17). At the convergence of the algorithm, estimated parameters of the population lie on a linear subspace of reduced (and possibly sufficient) dimension in which for each case of the database, there is a (possibly unique) parameter value for which the simulation fits the measurements. We first show how this property can help the modeler select a relevant parameter subspace for personalisation. In addition, since the resulting priors in this subspace represent the population statistics in this subspace, they can be used to perform consistent parameter estimation for cases where measurements are possibly different or missing in the database, which we illustrate with the personalisation of a heterogeneous database of 811 cases [18].

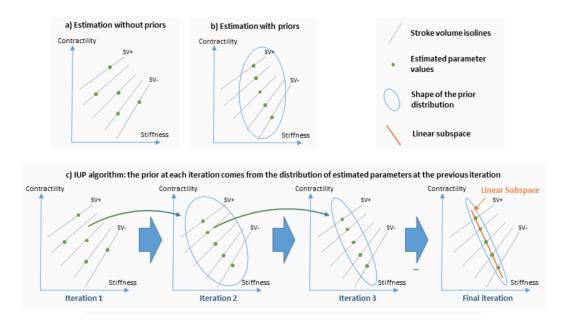


Figure 17. Schematic representation of parameter estimation problem: both contractility and stiffness are estimated from the stroke volume (SV). Both have an influence on the stroke volume (SV) so there are isolines of stroke volume (in grey) for varying parameters. (a) estimation without priors, the estimated values (green) for each case can be anywhere on an isoline (grey). (b) estimation performed with a prior (Gaussian covariance in blue), estimated values are grouped closer to prior mean. (c) Iteratively Updated Priors (IUP) algorithm performs successive estimations where the prior is set from the distribution of estimated parameters at the previous iteration. This leads the parameters to lie on a reduced linear subspace (orange).

### 6.5.2. Fast Personalized Computer Simulation of Electrical Activation from CT Imaging in Post-infarction Ventricular Tachycardia

Participants: Nicolas Cedilnik [Correspondant], Hubert Cochet [IHU Liryc, Bordeaux], Maxime Sermesant.

#### This work is funded by the IHU Liryc, in Bordeaux.

Cardiac modeling, Personalised simulation, ablation, intervention guidance.

In the vast majority of post-MI VT ablation procedures, VT is either non inducible or non mappable. We introduce a fast and robust model of cardiac electrophysiology that can be directly parameterized from CT images to predict activation maps (Figure 18). The model is based on the Eikonal equation for wave propagation, where local conduction velocities are estimated from CT. A fully automated method is used to segment the LV wall and assign local conduction velocity according to local LV thickness. Then, a "channelness" filter automatically detects potential VT isthmuses as channels of preserved thickness within severely thinned scar. The model can then be paced within each channel to produce simulated activation maps within seconds. A neural network for automated LV wall segmentation was trained on 450 CTs segmented by experts. Validation, performed on another 50 cases, showed excellent accuracy (Dice score vs. expert 0.95). In 11 patients undergoing post-MI VT ablation (age 58±13, 9 men), simulated activation maps were validated vs. 25 high density maps acquired in Rhythmia (16 paced, 9 VT). Quantitative differences between predicted and measured local activation times remained substantial, particularly in dense scar (> 50ms). Nonetheless, activation patterns were well predicted in most cases (22/25), the 3 poor correlations being observed in patients with fewer scar. Personalized simulation of activation maps from CT scan is feasible and reliably reproduces activation patterns in post-MI VT. The method is fast enough to be used clinically in an interactive fashion for procedural planning [4].

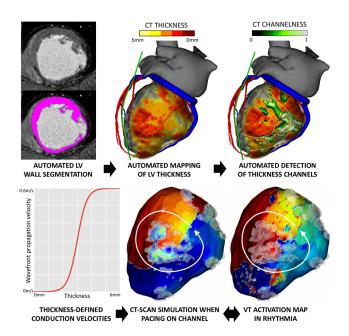


Figure 18. Our image-based model personalization pipeline

## 6.5.3. Cardiac Modeling, Medical Imaging and Machine Learning for Electrostructural Tomography

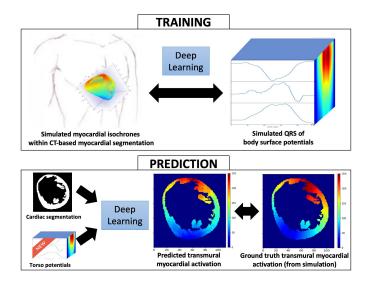
**Participants:** Tania Marina Bacoyannis [Correspondant], Hubert Cochet [IHU Liryc, Bordeaux], Maxime Sermesant.

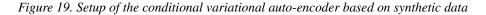
This work is funded within the ERC Project ECSTATIC with the IHU Liryc, in Bordeaux.

Machine Learning, Cardiac modeling, Personalised simulation, Inverse problem of ECG, Electrical simulation. Electrocardiographic imaging (ECGI) aims at reconstructing cardiac activity from torso measurements. To achieve this one has to solve the ill-posed inverse problem of the torso propagation. We propose a novel application for Deep Learning Networks to learn spatio-temporal correlations on ECGI (Figure 19). We developped a conditional variational auto-encoder (CVAE). The input are activation maps and the model takes two conditions: on one hand the cardiac shape(cardiac segmentation) and the other one the ECG signals.

The model currently involves simulated data: 120 activations maps were simulated from one cardiac geometry along with simulated body surface potential maps.80% of the data was used for training and the remaining 20% for testing. As a result we were able to observe a good prediction of the activation pattern.

Next, we will test the model with real data provided by the IHU Liryc.





## 6.5.4. Discovering the link between cardiovascular pathologies and neurodegeneration through biophysical and statistical models of cardiac and brain images Participants: Jaume Banus Cobo [Correspondant], Maxime Sermesant, Marco Lorenzi.

Université Côte d'Azur (UCA)

Lumped models - Biophysical simulation - Statistical learning

The project aims at developing a computational model of the relationship between cardiac function and brain damage from large-scale clinical databases of multi-modal and multi-organ medical images. The model is based on advanced statistical learning tools for discovering relevant imaging features related to cardiac dysfunction and brain damage; these features are combined within a unified mechanistic framework to providing a novel understanding of the relationship between cardiac function, vascular pathology and brain damage (Fig. 20). We are also testing data-driven statistical learning models for the discovery of associations between cardiac function and brain damage. For example, by applying CCA we identified a first component that shows a positive correlation between the volume of white matter hyper intensities (WMHs), the number of WMHs lesions, the brain ventricles volume and high blood pressure values. On the other side we observed a second component, inversely associated to the first one, in which we observe a strong correlation between ejection fraction (EF) and total brain volume (white matter plus grey matter).

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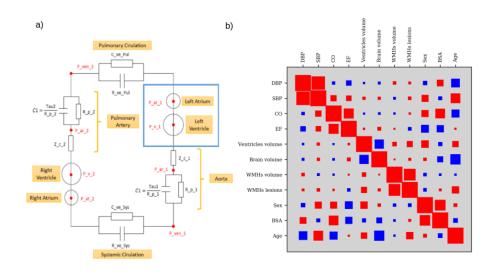


Figure 20. a) Schematic representation of the 0D model used to simulate the whole body circulation, its parameters are optimized to fit the available clinical measurements b) Partial correlations between cardiovascular, brain and demographic variables. Red represents positive correlation and blue negative correlation.

#### 6.5.5. Automatic Image Segmentation of cardiac structures with Adapted U-Net

**Participants:** Shuman Jia [Correspondant], Antoine Despinasse, Zihao Wang, Hervé Delingette, Xavier Pennec, Hubert Cochet, Maxime Sermesant.

The authors acknowledge the partial funding by the Agence Nationale de la Recherche (ANR)/ERA CoSysMedSysAFib and ANR MIGAT projects.

We proposed automated, two-stage, three-dimensional U-Nets with a contour loss, to segment the left atrium, as explained in [28], which obtained state-of-the-art results in the STACOM international challenge (Figure 21). Using similar method, we participated in Data Challenge organised at Journées Francophones de Radiologie and obtained a second place for renal cortex segmentation.

#### 6.5.6. Parallel Transport of Surface Deformation

**Participants:** Shuman Jia [Correspondant], Nicolas Duchateau, Pamela Moceri, Xavier Pennec, Maxime Sermesant.

The authors acknowledge the partial funding by the Agence Nationale de la Recherche (ANR)/ERA CoSysMedSysAFib and ANR MIGAT projects.

We looked into normalization of temporal deformation and proposed a more symmetric mapping scheme for pole ladder, which relies on geodesic symmetries around mid-points, as illustrated in [29] (Figure 22 )). This modified parallel transport method method was shown to be of order 4 on general manifolds and exact in symmetric spaces [58].

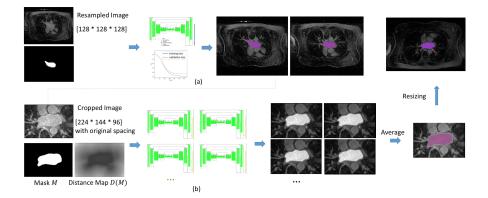


Figure 21. The framework of successive U-Nets training. (a) The fist U-Net - cropping; (b) the second U-Net - segmenting, with ensemble prediction models. We show here axial slices of MR images, overlapped with manual segmentation of the left atrium in blue, our segmentation in red, intersection of the two in purple.

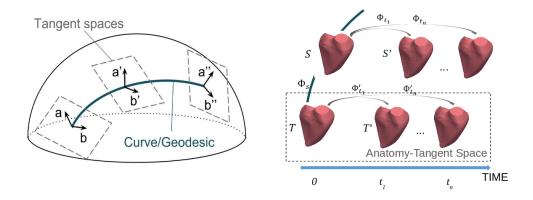


Figure 22. Illustration of parallel transport of vectors a and b along a curve (left) and its application to cardiac imaging (right) with a focus on surfaces.

## **LEMON Team**

## 7. New Results

## 7.1. Inland flow processes

#### 7.1.1. Shallow water models with porosity

#### 7.1.1.1. DDP model.

A new porosity model was published in 2018. The Depth-Dependent Porosity (DDP) model [4] was developed to account for subgrid-scale topographical features in shallow water models. The purpose is to allow flows to be modelled using coarse grids in the presence of strongly contrasted topography (e.g. ditches, narrow channels, submerged obstacles). Applications range from the modelling of lagoon/wetland dynamics to the submersion of urban areas by dambreak or tsunami waves. The development is the result of a team work in cooperation with the Tour du Valat research institute (O. Boutron). The developments are incorporated in the SW2D code.

#### 7.1.1.2. Porosity model validation.

The first experimental results validating the Dual Integral Porosity (DIP) model were presented at the RiverFlow 2018 International conference [9]. This work was carried out in collaboration with S. Soares-Frazão at Université Catholique de Louvain (UCL). Two stays of Carole Delenne and Vincent Guinot at UCL to participate in the experimental campaign in 2017 had been supported financially by the LEMON budget. A journal article presenting these experiments in detail has been submitted to the Journal of Hydraulic Research and is currently awaiting the final decision.

#### 7.1.2. Forcing

Stochastic approaches can be used to generate forcing scenarios randomly. To this end, an accurate characterization of the spatio-temporal variability and rainfall intensity distribution must be obtained from available data. So we have deeply studied a gridded hourly rainfall dataset in a region in Mediterranean France and proposed a semiparametric method to simulate spatio-temporal scenarios for extreme events. Our work was presented in the following international conferences: METMA 2018 - 9th Workshop on Spatio-temporal modelling (June 2018, Montpellier) [11] and SWGEN 2018 - Stochastic Weather Generators Conference (October 2018, Boulder, United States)[10]. Moreover we have invited P. Naveau (CNRS, LSCE) during two weeks and we have begun a collaboration concerning the construction of a unique temporal model permitting to deal with both ordinary and extreme events.

#### 7.1.3. Inland hydrological systems

The PhD of Joseph Luis Kahn Casapia (co-advised by Antoine Rousseau and Céline Casenave from INRA) has just started (Oct. 2018). The objective of the thesis is the modelling of cyanobacteria blooms in shallow water lakes such as TaiHu, in China. This work is done in the framework of the ANSWER research project funded by ANR, with a co-funding by labex NUMEV in Montpellier.

A publication presenting the KarstMod modelling platform was accepted in Environmental Modelling & Software [6]. KarstMod incorporates a number of developments by Vincent Guinot, including the Hysteretic [90] and the infinite characteristic time [60] transfer functions.

A family of multi-region transport models in heterogeneous porous media have been derived and validated experimentally [5]. The publication with Carole Delenne and Vincent Guinot as co-authors presents not only experimental results, but also a theoretical analysis of the transport and dispersion properties of a variety of models, depending on the structure of the flow field.

#### 7.1.4. Parametrization

With an objective of assessing flood hazard at large scale, the CASACADE project has been funded by the Luxembourg National Research Fund and provides for a phD (started in November 2018 by Vita Ayoub) concerning assimilation of satellite derived flood information for better parameterizing and controlling large scale hydraulic models over data scarce areas. One of the model used will be the DDP model [4]. The effective integration of remote sensing-derived flood information into this model will be investigated in this project for retrieving uncertain model parameters and boundary conditions. The PhD is co-directed by Carole Delenneand Renaud HOSTACHE from the Luxembourg Institute of Sciences and Technologies (LIST).

## 7.2. Marine and coastal systems

#### 7.2.1. Multi-scale ocean modelling

We proposed in [2] a Schwarz-based domain decomposition method for solving a dispersion equation consisting on the linearized KdV equation without the advective term, using simple interface operators based on the exact transparent boundary conditions for this equation. An optimization process is performed for obtaining the approximation that provides the method with the fastest convergence to the solution of the monodomain problem.

We also moved towards more complex equations and derived in [13], [12] discrete transparent boundary conditions for a class of linearized Boussinesq equations. These conditions happen to be non-local in time and we test numerically their accuracy with a Crank-Nicolson time-discretization on a staggered grid. We used the derived transparent boundary conditions as interface conditions in a domain decomposition method, where they become local in time. We analyzed numerically their efficiency thanks to comparisons made with other interface conditions. A paper [19] is submitted for publication in addition to the aforementioned talks.

#### 7.2.2. Data-model interactions

To go further with what have been explained in subsection Forcings, there are clear advantages of thresholding techniques in stochastic approaches aiming to simulate extreme events. They permit to exploit information from more data (compared to the block-maxima approach) and to explicitely model the original event. Pareto processes have been mostly used in a parametric framework, thereby using assumptions on the choce of the underlying dependence structure that may be strong. We have proposed a semi-parametric approach ([10], [11]) and we have shown the links between this semi-parametric method and the Pareto processes. A key benefit of the proposed method is to allow the generation of an unlimited number of realizations of these extreme fields. This work will be submitted for publication during the first trimester of 2019.

## 7.3. Methodological developments

#### 7.3.1. Stochastic models for extreme events

In extreme value theory, there is two main approaches. The first one is based on block maxima and involve max-stable models. Indeed the use of extreme value copula for extreme events is justified by the theory of multivariate extreme. The most accessible models are too simplistic when they are used in a high-dimensional framework. That is why we have proposed in a spatial context to combine two Gumbel copulas. By doing that, we reduce the complexity considering the weight parameter as a function depending on covariates. Moreover interpolation becomes straightforward and enable the interpretation of the parameters with distances between sites. Properties of the proposed model such as the possible extremal dependencies varying in space are studied and inference relies on ABC techniques. This work will be submitted for publication during the first quarter of 2019 (see also [14]).

The second approach is based on high threshold exceedances. We have proposed a novel hierarchical model for this kind of data leading to asymptotic independence in space and time. Our approach is based on representing a generalized Pareto distribution as a Gamma mixture of an exponential distribution, enabling us to keep marginal distributions which are coherent with univariate extreme value theory. The key idea is to use a kernel convolution of a space-time Gamma random process based on influence zones defined as cylinders with an ellipsoidal basis to generate anisotropic spatio-temporal dependence in exceedances. Statistical inference is based on a composite likelihood for the observed censored excesses. The practical usefulness of our model is illustrated on the previously mentionned hourly precipitation data set from a region in Southern France. This work has been presented in two invited talks in 2018 ([16], [17]) and is under revision in JASA [27].

#### 7.3.2. Integrating heterogeneous data

In the framework of the Cart'Eaux project, a stochastic algorithm has been set up to provide a set of probable wastewater networks geometries, obtained from manhole covers positions and cost functions based on general guidelines for such networks construction. The methodology and results are presented in a publication submitted to Computers, Environment and Urban Systems Journal.

Meanwhile, the MeDo project led by N. CHAHINIAN in collaboration with linguists, aims at identifying thematic entities related to wastewater networks in automatically collected documents on the web. This project has been presented in [8].

A PhD thesis has just been funded by ANRT and Berger-Levrault company concerning the fusion of the heterogeneous and uncertain data collected. This PhD (Yassine BEL-GHADDAR) will starts at the beginning of 2019 and will be co-directed by Carole Delenne and Ahlame BEGDOURI from the LSIA laboratory of FST Fes (Maroc).

## **MATHNEURO Team**

## 4. New Results

### 4.1. Neural Networks as dynamical systems

#### 4.1.1. Latching dynamics in neural networks with synaptic depression

**Participants:** Elif Köksal Ersöz, Carlos Aguilar [Université de Nice - BCL], Pascal Chossat [Université de Nice - LJAD, Inria MathNeuro], Martin Krupa [Université de Nice - LJAD, UCA, Inria MathNeuro], Frédéric Lavigne [Université de Nice - BCL].

Prediction is the ability of the brain to quickly activate a target concept in response to a related stimulus (prime). Experiments point to the existence of an overlap between the populations of the neurons coding for different stimuli, and other experiments show that prime-target relations arise in the process of long term memory formation. The classical modelling paradigm is that long term memories correspond to stable steady states of a Hopfield network with Hebbian connectivity. Experiments show that short term synaptic depression plays an important role in the processing of memories. This leads naturally to a computational model of priming, called latching dynamics; a stable state (prime) can become unstable and the system may converge to another transiently stable steady state (target). Hopfield network models of latching dynamics have been studied by means of numerical simulation, however the conditions for the existence of this dynamics have not been elucidated. In this work we use a combination of analytic and numerical approaches to confirm that latching dynamics can exist in the context of a symmetric Hebbian learning rule, however lacks robustness and imposes a number of biologically unrealistic restrictions on the model. In particular our work shows that the symmetry of the Hebbian rule is not an obstruction to the existence of latching dynamics, however fine tuning of the parameters of the model is needed.

A natural follow-up of the work which has lead to the article [1] has been initiated through the postdoc project of Elif Köksal Ersöz. The objective is to extend the previous results in several ways. First, to gain more robustness in the heteroclinic chains sustained by the network model. Second, to be able to simulate much larger networks and exhibit heteroclinic dynamics in them. Third, to link with experimental data. The postdoc of Elif Köksal Ersöz, which finished at the end of December 2018, has been funded by the "tail" of the ERC Advanced Grant NerVi held by Olivier Faugeras.

#### 4.1.2. Pseudo-simple heteroclinic cycles in $\mathbb{R}^4$

**Participants:** Pascal Chossat [Université de Nice - LJAD, Inria MathNeuro], Alexander Lohse [Universität Hamburg, Germany], Olga Podvigina [Institute of Earthquake Prediction Theory and Mathematical Geophysics, Russia].

We study pseudo-simple heteroclinic cycles for a  $\Gamma$ -equivariant system in  $\mathbb{R}^4$  with finite  $\Gamma \subset O(4)$ , and their nearby dynamics. In particular, in a first step towards a full classification – analogous to that which exists already for the class of simple cycles – we identify all finite subgroups of O(4) admitting pseudo-simple cycles. To this end we introduce a constructive method to build equivariant dynamical systems possessing a robust heteroclinic cycle. Extending a previous study we also investigate the existence of periodic orbits close to a pseudo-simple cycle, which depends on the symmetry groups of equilibria in the cycle. Moreover, we identify subgroups  $\Gamma \subset O(4)$ ,  $\Gamma \neg \subset SO(4)$ , admitting fragmentarily asymptotically stable pseudo-simple heteroclinic cycles (It has been previously shown that for  $\Gamma \subset SO(4)$  pseudo-simple cycles generically are completely unstable). Finally, we study a generalized heteroclinic cycle, which involves a pseudo-simple cycle as a subset.

This work has been published in Physica D and is available as [13].

# 4.1.3. Qualitative stability and synchronicity analysis of power network models in port-Hamiltonian form

**Participants:** Volker Mehrmann [Technical University of Berlin, Germany], Riccardo Morandin [Technical University of Berlin, Germany], Simona Olmi, Eckehard Schöll [Technical University of Berlin, Germany].

In view of highly decentralized and diversified power generation concepts, in particular with renewable energies, the analysis and control of the stability and the synchronization of power networks is an important topic that requires different levels of modeling detail for different tasks. A frequently used qualitative approach relies on simplified nonlinear network models like the Kuramoto model with inertia. The usual formulation in the form of a system of coupled ordinary differential equations is not always adequate. We present a new energy-based formulation of the Kuramoto model with inertia as a polynomial port-Hamiltonian system of differential-algebraic equations, with a quadratic Hamiltonian function including a generalized order parameter. This leads to a robust representation of the system with respect to disturbances: it encodes the underlying physics, such as the dissipation inequality or the deviation from synchronicity, directly in the structure of the equations, and it explicitly displays all possible constraints and allows for robust simulation methods. The model is immersed into a system of model hierarchies that will be helpful for applying adaptive simulations in future works. We illustrate the advantages of the modified modeling approach with analytics and numerical results.

This work has been published in Chaos and is available as [18].

#### 4.1.4. Collective behavior of oscillating electric dipoles

**Participants:** Simona Olmi, Matteo Gori [Centre de Physique Théorique, Marseille], Irene Donato [Centre de Physique Théorique, Marseille], Marco Pettini [Centre de Physique Théorique, Marseille].

We investigate the dynamics of a population of identical biomolecules mimicked as electric dipoles with random orientations and positions in space and oscillating with their intrinsic frequencies. The biomolecules, beyond being coupled among themselves via the dipolar interaction, are also driven by a common external energy supply. A collective mode emerges by decreasing the average distance among the molecules as testified by the emergence of a clear peak in the power spectrum of the total dipole moment. This is due to a coherent vibration of the most part of the molecules at a frequency definitely larger than their own frequencies corresponding to a partial cluster synchronization of the biomolecules. These results can be verified experimentally via spectroscopic investigations of the strength of the intermolecular electrodynamic interactions, thus being able to test the possible biological relevance of the observed macroscopic mode.

This work has been published in Scientific Reports and is available as [19].

#### 4.1.5. Controlling seizure propagation in large-scale brain networks

**Participants:** Simona Olmi, Spase Petkoski [Institut de Neurosciences des Systèmes, Marseille], Maxime Guye [Centre d'Exploration Métabolique par Résonance Magnétique, Marseille], Fabrice Bartolomei [Epilepsies, Lésions Cérébrales et Systèmes Neuraux de la Cognition, Marseille], Viktor Jirsa [Institut de Neurosciences des Systèmes, Marseille].

Information transmission in the human brain is a fundamentally dynamic network process. In partial epilepsy, this process is perturbed and highly synchronous seizures originate in a local network, the so-called epileptogenic zone (EZ), before recruiting other close or distant brain regions. We studied patient-specific brain network models of 15 drug-resistant epilepsy patients with implanted stereotactic electroencephalography (SEEG) electrodes. Each personalized brain model was derived from structural data of magnetic resonance imaging (MRI) and diffusion tensor weighted imaging (DTI), comprising 88 nodes equipped with region specific neural mass models capable of demonstrating a range of epileptiform discharges. Each patients virtual brain was further personalized through the integration of the clinically hypothesized EZ. Subsequent simulations and connectivity modulations were performed and uncovered a finite repertoire of seizure propagation patterns. Across patients, we found that (i) patient-specific network connectivity is predictive for the subsequent seizure propagation pattern; (ii) seizure propagation is characterized by a systematic sequence of brain

states; (iii) propagation can be controlled by an optimal intervention on the connectivity matrix; (iv) the degree of invasiveness can be significantly reduced via the here proposed seizure control as compared to traditional resective surgery. To stop seizures, neurosurgeons typically resect the EZ completely. We showed that stability analysis of the network dynamics using graph theoretical metrics estimates reliably the spatiotemporal properties of seizure propagation. This suggests novel less invasive paradigms of surgical interventions to treat and manage partial epilepsy.

This work has been submitted for publication and is available as [28].

#### 4.1.6. Effect of disorder and noise in shaping the dynamics of power grids

**Participants:** Liudmila Tumash [Technical University of Berlin, Germany], Simona Olmi, Eckehard Schöll [Technical University of Berlin, Germany].

The aim of this paper is to investigate complex dynamic networks which can model high-voltage power grids with renewable, fluctuating energy sources. For this purpose we use the Kuramoto model with inertia to model the network of power plants and consumers. In particular, we analyse the synchronization transition of networks of N phase oscillators with inertia (rotators) whose natural frequencies are bimodally distributed, corresponding to the distribution of generator and consumer power. First, we start from globally coupled networks whose links are successively diluted, resulting in a random Erdös-Renyi network. We focus on the changes in the hysteretic loop while varying inertial mass and dilution. Second, we implement Gaussian white noise describing the randomly fluctuating input power, and investigate its role in shaping the dynamics. Finally, we briefly discuss power grid networks under the impact of both topological disorder and external noise sources.

This work has been published in Europhysics Letters and is available as [20].

## 4.2. Mean field theory and stochastic processes

#### 4.2.1. Emergence of collective phenomena in a population of neurons

Participants: Benjamin Aymard, Fabien Campillo, Romain Veltz.

In this work, we propose a new model of biological neural network, combining a two-dimensional integrateand-fire neuron model with a deterministic model of electrical synapse, and a stochastic model of chemical synapse. We describe the dynamics of a population of neurons in interaction as a piecewise deterministic Markov process. We prove the weak convergence of the associated empirical process, as the population size tends to infinity, towards a McKean-Vlasov type process and we describe the associated PDE. We are also interested in the simulation of these dynamics, in particular by comparing "detailed" simulations of a finite population of neurons with a simulation of the system with infinite population. Benjamin Aymard has the adapted toolkit to attack these questions numerically. The mean field equations studied by Benjamin are of transport type for which numerical methods are technical. However, they are the domain of expertise of Benjamin. His postdoc is funded by the Flagship Human Brain Project.

Latest results are as follows. A first manuscript concerning the numerical simulation of the mean field model is in preparation. We managed to find a new numerical scheme which is positive, semi-implicit and adaptive in time (of order 2). A second manuscript concerning the existence of stationary distribution for the mean field limit is also in preparation.

### 4.2.2. Long time behavior of a mean-field model of interacting neurons

Participants: Quentin Cormier [Inria TOSCA], Étienne Tanré [Inria TOSCA], Romain Veltz.

We study the long time behavior of the solution to some McKean-Vlasov stochastic differential equation (SDE) driven by a Poisson process. In neuroscience, this SDE models the asymptotic dynamic of the membrane potential of a spiking neuron in a large network. We prove that for a small enough interaction parameter, any solution converges to the unique (in this case) invariant measure. To this aim, we first obtain global bounds on the jump rate and derive a Volterra type integral equation satisfied by this rate. We then replace temporary the interaction part of the equation by a deterministic external quantity (we call it the external current). For constant current, we obtain the convergence to the invariant measure. Using a perturbation method, we extend this result to more general external currents. Finally, we prove the result for the non-linear McKean-Vlasov equation.

This work has been submitted for publication and is available as [24].

# 4.2.3. Exponential stability of the stationary distribution of a mean field of spiking neural network

Participants: Audric Drogoul [Thales, France], Romain Veltz.

In this work, we study the exponential stability of the stationary distribution of a McKean-Vlasov equation, of nonlinear hyperbolic type which was recently derived in [33], [40]. We complement the convergence result proved in [40] using tools from dynamical systems theory. Our proof relies on two principal arguments in addition to a Picard-like iteration method. First, the linearized semigroup is positive which allows to precisely pinpoint the spectrum of the infinitesimal generator. Second, we use a time rescaling argument to transform the original quasilinear equation into another one for which the nonlinear flow is differentiable. Interestingly, this convergence result can be interpreted as the existence of a locally exponentially attracting center manifold for a hyperbolic equation.

This work has been submitted for publication and is available as [23].

#### 4.2.4. On a toy network of neurons interacting through their dendrites

**Participants:** Nicolas Fournier Cormier [LPSM, Sorbonne Université, Paris], Étienne Tanré [Inria TOSCA], Romain Veltz.

Consider a large number n of neurons, each being connected to approximately N other ones, chosen at random. When a neuron spikes, which occurs randomly at some rate depending on its electric potential, its potential is set to a minimum value vmin, and this initiates, after a small delay, two fronts on the (linear) dendrites of all the neurons to which it is connected. Fronts move at constant speed. When two fronts (on the dendrite of the same neuron) collide, they annihilate. When a front hits the soma of a neuron, its potential is increased by a small value  $w_n$ . Between jumps, the potentials of the neurons are assumed to drift in  $[v_{min}, \infty)$ , according to some well-posed ODE. We prove the existence and uniqueness of a heuristically derived mean-field limit of the system when  $n, N \to \infty$  with  $w_n \simeq N1/2$ . We make use of some recent versions of the results of Deuschel and Zeitouni [37] concerning the size of the longest increasing subsequence of an i.i.d. collection of points in the plan. We also study, in a very particular case, a slightly different model where the neurons spike when their potential reach some maximum value  $v_{max}$ , and find an explicit formula for the (heuristic) mean-field limit.

This work has been submitted for publication and is available as [26].

#### 4.2.5. Mathematical statistical physics applied to neural populations

Participants: Émilie Soret, Olivier Faugeras, Étienne Tanré [Inria, project-team TOSCA, Sophia-Antipolis].

This project focuses on Mean-Field descriptions or thermodynamics limits of large populations of neurons. They study a system of Stochastic Differential Equations (SDEs) which describes the evolution of membrane potential of each neuron over the time when the synaptic weights are random variables (not assumed to be independent). This setup is well suited to Émilie, who has worked during her PhD and first postdoc on mathematical statistical physics and stochastic processes. Her postdoc is funded by the Flagship Human Brain Project. A manuscript is in preparation.

## 4.3. Neural fields theory

#### 4.3.1. A neural field model for color perception unifying assimilation and contrast

Participants: Anna Song [ENS Paris, France], Olivier Faugeras, Romain Veltz.

We propose a neural field model of color perception in context, for the visual area V1 in the cortex. This model reconciles into a common framework two opposing perceptual phenomena, simultaneous contrast and chromatic assimilation. Previous works showed that they act simultaneously, and can produce larger shifts in color matching when acting in synergy with a spatial pattern. At some point in an image, the color perceptually seems more similar to that of the adjacent locations, while being more dissimilar from that of remote neighbors. The influence of neighbors hence reverses its nature above some characteristic scale. Our model fully exploits the balance between attraction and repulsion in color space, combined at small or large scales in physical space. For that purpose we rely on the opponent color theory introduced by Hering, and suppose a hypercolumnar structure coding for colors. At some neural mass, the pointwise influence of neighbors is spatially integrated to obtain the final effect that we call a color sensation. Alongside this neural field model, we describe the search for a color match in asymmetric matching experiments as a mathematical projector. We validate it by fitting the parameters of the model to data from [45] and [46] and our own data. All the results show that we are able to explain the nonlinear behavior of the observed shifts along one or two dimensions in color space, which cannot be done using a simple linear model.

This work has been submitted for publication and is available as [29].

## 4.4. Slow-fast dynamics in Neuroscience

# 4.4.1. Spike-adding in a canonical three time scale model: superslow explosion & folded-saddle canards

Participants: Mathieu Desroches, Vivien Kirk [University of Auckland, New-Zealand].

We examine the origin of complex bursting oscillations in a phenomenological ordinary differential equation model with three time scales. We show that bursting solutions in this model arise from a Hopf bifurcation followed by a sequence of spike-adding transitions, in a manner reminiscent of spike-adding transitions previously observed in systems with two time scales. However, the details of the process can be much more complex in this three-time-scale context than in two-time-scale systems. In particular, we find that spikeadding can involve canard explosions occurring on two different time scales and is associated with passage near a folded-saddle singularity. We show that the character of the bursting and the form of spike-adding transitions that occur depend on the geometry of certain singular limit systems, specifically the relative positions of the critical and superslow manifolds. We also show that, unlike the case of spike-adding in two-time-scale systems, the onset of a new spike in our model is not typically associated with a local maximum in the period of the bursting oscillation.

This work has been published in SIAM Journal on Applied Dynamical Systems and is available as [14].

#### 4.4.2. Parabolic bursting, spike-adding, dips and slices in a minimal model

**Participants:** Mathieu Desroches, Jean-Pierre Françoise [LJLL, Sorbonne Université, Paris], Martin Krupa [Université de Nice - LJAD, UCA, Inria MathNeuro].

A minimal system for parabolic bursting, whose associated slow flow is integrable, is presented and studied both from the viewpoint of bifurcation theory of slow-fast systems, of the qualitative analysis of its phase portrait and of numerical simulations. We focus the analysis on the spike-adding phenomenon. After a reduction to a periodically forced 1-dimensional system, we uncover the link with the dips and slices first discussed by J. E. Littlewood in his famous articles on the periodically forced van der Pol system.

This work has been submitted for publication and is available as [25].

# 4.4.3. Piecewise-linear (PWL) canard dynamics : Simplifying singular perturbation theory in the canard regime using piecewise-linear systems

**Participants:** Mathieu Desroches, Soledad Fernández-García [University of Sevilla, Spain], Martin Krupa [Université de Nice - LJAD, UCA, Inria MathNeuro], Rafel Prohens [University of the Balearic Islands, Spain], Antonio E. Teruel [University of the Balearic Islands, Spain].

In this work we have gathered recent results on piecewise-linear (PWL) slow-fast dynamical systems in the canard regime. By focusing on minimal systems in  $\mathbb{R}^2$  (one slow and one fast variables) and  $\mathbb{R}^3$  (two slow and one fast variables), we prove the existence of (maximal) canard solutions and show that the main salient features from smooth systems is preserved. We also highlight how the PWL setup carries a level of simplification of singular perturbation theory in the canard regime, which makes it more amenable to present it to various audiences at an introductory level. Finally, we present a PWL version of Fenichel theorems about slow manifolds, which are valid in the normally hyperbolic regime and in any dimension, which also offers a simplified framework for such persistence results.

This work has been published as a chapter in the book "Nonlinear Systems, Vol. 1: Mathematical Theory and Computational Methods" published by Springer as part of the Understanding Complex Systems book series, and it is available as [22].

#### 4.4.4. Anticipation via canards in excitable systems

**Participants:** Elif Köksal Ersöz, Mathieu Desroches, Claudio Mirasso [University of the Balearic Islands, Spain], Serafim Rodrigues [Ikerbasque & Basque Center for Applied Mathematics, Spain].

Neurons can anticipate incoming signals by exploiting a physiological mechanism not well understood. This article offers a novel explanation on how a receiver neuron can predict the sender's dynamics in a unidirectionally-coupled configuration, in which both sender-receiver follow the evolution of a multi-scale excitable system. We present a novel theoretical view point based on a mathematical object, called canard, to explain anticipation in excitable systems. We provide a numerical approach, which allows to determine the transient effects of canards. To demonstrate the general validity of canard-mediated anticipation in the context of excitable systems, we illustrate our framework in two examples, a multi-scale radio-wave circuit (the van der Pol model) that inspired a caricature neuronal model (the FitzHugh-Nagumo model) and a biophysical neuronal model (a 2-dimentional reduction of the Hodgkin-Huxley model), where canards act as messengers to the senders' prediction. We also propose an experimental paradigm that would enable experimental neuroscientists to validate our predictions. We conclude with an outlook to possible fascinating research avenues to further unfold the mechanisms underpinning anticipation. We envisage that our approach can be employed to a wider class of excitable systems with appropriate theoretical extensions. Anticipation appears as a counter-intuitive observation in a wide range of dynamical systems ranging from biology to engineering applications. It can occur in unidirectionally coupled systems when the receiver is subject to a self-delayed feedback in addition to a signal coming from the sender. This particular interaction permits the receiver to predict the future trajectory of the sender. Anticipation can occur transiently, thus straightforwardly denoted anticipation, or in long-term dynamics, in which case it is referred to as anticipated synchronization. In this study, we focus on both aspects of anticipatory dynamics in the context of excitable systems and explain it via a counter-intuitive phenomenon, namely canards. Canard trajectories structure the excitability and synchronization properties of multiple timescale systems exhibiting excitable dynamics. By developing a theoretical framework enhanced by numerical continuation, we show that the underlying canard structure in excitable systems is responsible for delaying sub-threshold solutions, but anticipating the spiking ones. We also propose an experimental set up that would enable experimentalists to observe anticipated behavior in neural systems, in particular in type-II neurons.

This work has been accepted for publication in Chaos and is available as [17].

#### 4.4.5. Canard-induced complex oscillations in an excitatory network

**Participants:** Elif Köksal Ersöz, Mathieu Desroches, Antoni Guillamon [Polytechnic University of Catalunya, Spain], Joel Tabak [University of Exeter, UK].

In this work we have revisited a rate model that accounts for the spontaneous activity in the developing spinal cord of the chicken embryo [50]. The dynamics is that of a classical square-wave burster, with alternation of silent and active phases. Tabak et al. [50] have proposed two different three-dimensional (3D) models with variables representing average population activity, fast activity-dependent synaptic depression and slow activity-dependent depression of two forms. In [47], [48], [49] various 3D combinations of these four variables have been studied further to reproduce rough experimental observations of spontaneous rhythmic activity. In this work, we have first shown the spike-adding mechanism via canards in one of these 3D models from [50] where the fourth variable was treated as a control parameter. Then we discussed how a canard-mediated slow passage in the 4D model explains the sub-threshold oscillatory behavior which cannot be reproduced by any of the 3D models, giving rise to mixed-mode bursting oscillations (MMBOs); see [6]. Finally, we relateed the canard-mediated slow passage to the intervals of burst and silent phase which have been linked to the blockade of glutamatergic or GABAergic/glycinergic synapses over a wide range of developmental stages [49].

This work is in progress and is available as [27].

#### 4.4.6. High-frequency forced oscillations in neuronlike elements

**Participants:** Denis Zakharov [Institute of Applied Physics RAS, Russia], Martin Krupa [Université de Nice - LJAD, UCA, Inria MathNeuro], Boris Gutkin [Group for Neural Theory, ENS Paris, France], Alexey Kuznetsov [Indiana University - Purdue University Indianapolis, USA].

We analyzed a generic relaxation oscillator under moderately strong forcing at a frequency much greater that the natural intrinsic frequency of the oscillator. Additionally, the forcing is of the same sign and, thus, has a nonzero average, matching neuroscience applications. We found that, first, the transition to highfrequency synchronous oscillations occurs mostly through periodic solutions with virtually no chaotic regimes present. Second, the amplitude of the high-frequency oscillations is large, suggesting an important role for these oscillations in applications. Third, the 1:1 synchronized solution may lose stability, and, contrary to other cases, this occurs at smaller, but not at higher frequency differences between intrinsic and forcing oscillations. We analytically built a map that gives an explanation of these properties. Thus, we found a way to substantially "overclock" the oscillator with only a moderately strong external force. Interestingly, in application to neuroscience, both excitatory and inhibitory inputs can force the high-frequency oscillations.

This work has been published in Physical Review E and is available as [21].

## **MORPHEME Project-Team**

## 6. New Results

## **6.1.** Exact biconvex reformulation of the $\ell_2 - \ell_0$ minimization problem

Participants: Gilles Aubert, Arne Henrik Bechensteen, Laure Blanc-Féraud.

We focus on the problem of minimizing the least-squares loss function under the constraint that the reconstructed signal is at maximum k-sparse. This is called the  $\ell_2$ - $\ell_0$  constrained problem. The  $\ell_0$  pseudo-norm counts the number of non-zero elements in a vector. The minimization problem is of interest in signal processing, with a wide range of applications such as compressed sensing, source separation, and super-resolution imaging.

Based on the results of [20], we reformulate the  $\ell_0$  pseudo-norm exactly as a convex minimization problem by introducing an auxiliary variable. We then propose an exact biconvex reformulation of the  $\ell_2 - \ell_0$  constrained and penalized problems. We give correspondence results between minimizer of the initial function and the reformulated ones. The reformulation is biconvex. This property is used to derive a minimization algorithm.

We apply the algorithm to the problem of Single-Molecule Localization Microscopy and compare the results with the well-known IHT algorithm [13]. Both visually and numerically the biconvex reformulations perform better. This work has been presented at the iTWIST 2018 workshop [5].

Furthermore, the algorithm has been compared to the IRL1-CEL0 [14] and Deep-STORM [15] (see figure 1). The IRL1-CEL0 minimizes an exact relaxation [19] of the  $\ell_2 - \ell_0$  penalized form and Deep-STORM is an algorithm that uses deep-learning and convolutional network to localize the molecules. This work has been accepted to the ISBI 2019 conference.

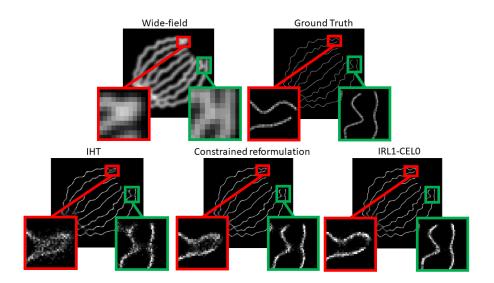


Figure 1. Reconstruction by the different algorithms. Data set from ISBI 2013 challenge [18].

### 6.2. Reconstruction of mosaic of microscopic images

Participants: Kevin Giulietti, Eric Debreuve, Grégoire Malandain.

#### This work takes place within the ANR PhaseQuant.

In microscopy imaging, a trade-off has to be made between a high resolution, that enables to see details, and the width of the field of view, that enables to see many objects. Such a trade-off is avoided by mosaicing, which consists in the acquisition of several images, say  $N \times N$ , with a small overlap between images. This way, an image with a N larger field of view can be reconstructed with the same resolution than a single microscopic image.

Such an imaging protocol is available on many microscopy software. Basically, displacements of the table on which lies the material to be imaged are programmed, and used to reconstruct the mosaic. However, it appears (at the overlapping areas) that a residual offset is still present. Analysis of acquisitions of both real and controlled experiments demonstrate that the table motions are not exactly reproducible (see figure 2), and that the cause of the offset is twofold: first a mis-alignement of the micrometer table axis with respect to the microscope axis, and second errors in the displacement computed by the micrometer table. Thanks to an image-based calculation of the axis mis-alignement, it has been shown that the first type error can easily be corrected.

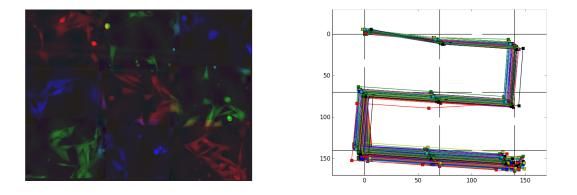


Figure 2. Example of a mosaic reconstructed for one acquisition timepoint. Estimation of the relative image position through time for the whole sequence (displacements with respect to the expected position have been magnified for visualization purpose).

## 6.3. Cytoplasm segmentation from cells confocal microscopy images

Participants: Somia Rahmoun, Fabienne de Graeve, Eric Debreuve, Xavier Descombes.

#### This work takes place within the ANR RNAGRIMP.

As part of the ANR project RNAGRIMP, two series of images have been acquired using fluorescence microscopy: one where the cell cytoplasm has been stained with GFP (Green Fluorescent Protein), the second where the nuclei have been stained with DAPI (4',6-diamidino-2-phenylindole). The first steps are detecting the nuclei on the DAPI images and learning a classification procedure into living cell or dead cell based on morphological and radiometric nuclei properties (average intensity, area, granularity, circularity ...).

A specific CellProfiler pipeline has been developed for this, and CellProfiler Analyst has been used to learn a decision tree for automatic nuclei (hence, cell) classification.

The next step is to segment the cell cytoplasms on the GFP images. Indeed, the target RNP-IMP granules appear in that compartment of the cell and are visible through their GFP response. This segmentation problem is particularly difficult due the heterogeneity of the cells intensity. This heterogeneity even appears within a given cell. Besides, cells sometimes form clusters in which there is no clear separation between adjacent cells.

In this context, we have considered a two steps algorithm to segment the cytoplasm. The first step consists of the image segmentation in small areas called superpixels that represent adjacent pixels with similar intensity. We have evaluated and compared different strategies (based on iterative clustering, minimum spanning tree, persistent edge selection ...) to achieve such a segmentation. Finally, we have selected an automatic algorithm based on the watershed transform. We are currently developing an algorithm to merge superpixels into the final segmentation.

Meanwhile, we have developed a supervised software to manually merge the superpixels (see Fig. 3). This tool can also be used by biologist to correct any segmentation error.



Figure 3. Superpixels merging: each color corresponds to a cell that is obtained by merging several superpixels.

## 6.4. Cytoneme detection and characterization

Participants: Eric Debreuve, Xavier Descombes.

#### This work is made in collaboration with Caterina Novelli, Tamas Matusek, Pascal Thérond (iBV).

This work is supported by the ANR project HMOVE. Cellular communication is one of the most important processes for controlling the morphogenesis of organs (i.e. the set of laws that determine the structure of tissues and organs during embryonic development). Understanding the communication both ways is an important issue in the field of developmental biology and it has recently been shown that the exchange of information between cells is controlled by long cellular extensions called "cytonemes". Last year, we had developed a pipeline for automatic cell membrane detection and cytoneme extraction from in vivo images obtained by confocal microscopy. When testing the proposed method on new images with varying acquisition conditions, we found it to be less reliable than expected. While retaining the same general philosophy (use of Frangi enhancement filter, skeletonization, and Dijkstra shortest path algorithm), we largely rethought the approach to make it more robust to acquisition conditions, more reliable in general, and faster (see Fig. 4). Some topological and geometrical features are then computed on the graph-based representation of the cytonemes in order to characterize in which respect wild-type and mutant conditions are different or similar. A journal paper is in preparation based on the analysis and interpretation of these results by our biologist colleagues.

## 6.5. Classification and Modeling of the Fibronectin Network in Extracellular Matrices

Participants: Anca-Ioana Grapa, Laure Blanc-Féraud, Xavier Descombes, Sébastien Schaub.

This work is done in collaboration with Ellen Van Obberghen-Schilling and Georgios Efthymiou (iBV).

We are interested in the numerical analysis and modeling of the Fibronectin (FN) network, a major extracellular matrix (ECM) molecule expressed in pathological states (fibrosis, cancer, etc). Our goal is to develop numerical quantitative biomarkers that describe the organization of the different FN networks from 2D confocal miscroscopy images (Figure 5).

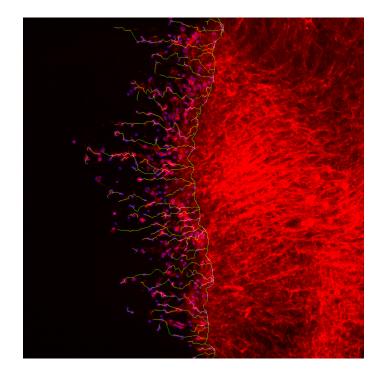
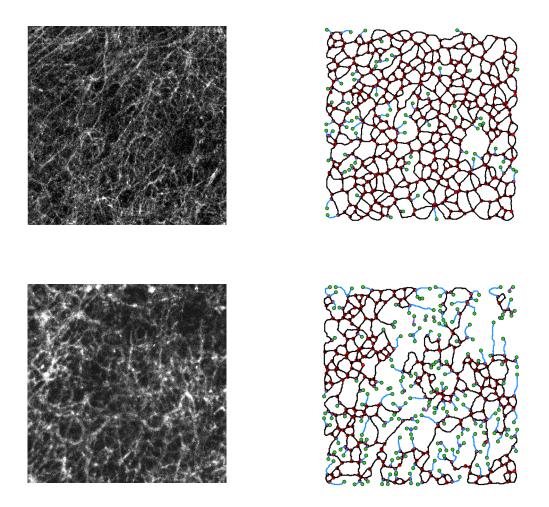


Figure 4. A result of membrane detection and cytoneme extraction.



*Figure 5. Different variants of FN and their associated graph networks. Top row:* A+ *fibronectin; bottom row:* A-*B*-*fibronectin. Left: confocal images; right: associated graphs.* 

In a previous work, we have derived a pipeline to classify a given tissue among the four FN variants (cellderived matrices), based on a decomposition into discrete fast curvelet transform coefficients. We ensured the invariance to rotation of the coefficients and then fed them to a DAG-SVM multiclassifier, in order to prove their discriminative ability in the context of classification of the four FN variants. The results were published in [7].

The second step of our work consists in setting up the modeling of the FN networks starting from a graph-based representation, built on top of Gabor features (fiber scale, orientation, etc). More specifically, Gabor filters are used to enhance the fibrillar structures, followed by a morphological skeletonization of the maximum response of the Gabor filter set. We then derive the corresponding graph networks that generate relevant fiber geometry statistics (e.g fiber length, node degree, node density, etc).

Starting from the graph networks, we manage to reconnect the missing fibers in the skeleton, that are due to previous morphological operations. To do so, we use the Gabor maximum response as a guideline for reconnection, and connect the fibers within a predefined cone sector around the local fiber orientation. The graph parameters corresponding to the improved skeletonizations of the four FN variants, are then classified by a DAG-SVM. It is thus shown that graph features can discriminate among the FN variants.

The next step concerns the development of a metric between graph networks that takes into account their topology, to provide a meaningful distance between them. We currently investigate methods based on optimal transport, that are able to compare discrete probability distributions and respect the local geometry. The techniques that rely on graph structures to compute a geodesic distance (e.g. Gromov-Wasserstein) and/or barycenter of structured data (e.g. mesh structures) [16], serve as inspiration for our work. The distance is obtained following a minimization of the cost of transport of the mass from one distribution to the other. Despite the fact that they consider the intrinsic distance within each space (i.e graphs) in the cost formulation, these methods don't explicitly take into account the graph structure defined by the adjacency matrices. To counteract some of the shortcomings, we consider parallel graph-matching methods and redefine our problem in a many-to-many graph matching context, where the distance between the graphs is given by the optimal alignment of their structure determined by the mapping between the vertices [21].

Finally, we analyze the advantages and drawbacks of the two techniques both for small-size graphs as well as for FN graphs to derive an appropriate formulation of the distance among them, which will be useful to compare the FN fiber networks.

# 6.6. Detection of Brain Strokes Using Microwave Tomography

Participant: Laure Blanc-Féraud.

This work is done in collaboration with Vanna Lisa Coli and Juliette Leblond (EPI Factas, Inria Sophia), Pierre-Henri Tournier (Université Sorbonne, CNRS, LJLL, Inria, Paris), Victorita Dolean (Université Côte d'Azur, CNRS, LJAD, Nice), Ibtissam El Kanfoud, Christian Pichot, Claire Migliaccio (Université Côte d'Azur, CNRS, LEAT, Sophia Antipolis).

Brain strokes are one of the leading causes of disability and mortality in adults in developed countries. The ischemic stroke (85% of total cases) and hemorrhagic stroke (15%) must be treated with opposite therapies, so that the determination of the stroke nature must be made quickly to apply the appropriate treatment. Recent works in biomedical imaging showed that strokes produce variations on brain tissues complex electric permittivity that can be detected by means of microwave tomography.

We present here some synthetic results obtained with an experimental microwave tomography-based portable system for the early detection and monitoring of brain strokes (Figure 6). The determination of electric permittivity requires the solution of a coupled direct-inverse problem, where massive parallel computation from domain decomposition method and regularization techniques for optimization methods are employed. Synthetic data are obtained with electromagnetic simulations and a noise model developed for the specific problem, which has been derived from measurements errors with the experimental imaging system.

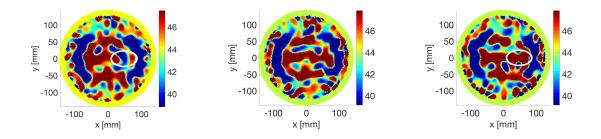


Figure 6. From left to right: brain with ischemic stroke, healthy brain and brain with hemorrhagic stroke (real part of permittivity  $\epsilon_r$ ).

# 6.7. Organoid growth tracking

Participants: Cédric Girard Riboulleau, Xavier Descombes.

This work is a collaboration with F.-R. Roustan, S. Torrino, S. Clavel and F. Bost from C3M. It was partially supported by the UCA Jedi Idex.

Organoid culture is a major challenge toward personalized medicine. It is now possible to partially reconstruct the structure of organs from a single biopsy. This new technology named organoid for sane cells or tumoroid for cancer cells allows the test of different molecules on cells withdrawn on a patient to retrieve the most efficient one for this patient. In this context, the main goal of this work is to develop a numerical scheme to automatically assess the effect of a given treatment on the organoid growth. We consider a time sequence of 2D confocal microscopy images of a population of organoids. We have considered different approaches to detect the organoids in the images. These approaches include edge detection using Canny filter, thresholding combined with mathematical morphology tools, texture analysis through Markov Random Fields, marked point processes. We have also modified several times the imaging protocol in order to simplify the object detection. To evaluate the growth of each organoid we have to match the objects detected in two consecutive frames. We have developed a matching algorithm based on a majority voting. We compute the vector between every pair of detected objects on both frames. Assuming that there is only a translation between the two frames we estimate it as the most represented vector. With this framework we have shown that the studied treatment has stopped the organoid growth (see figure 7).

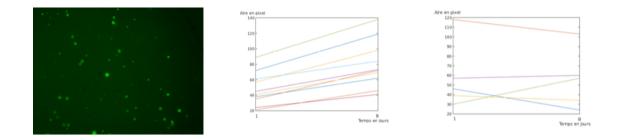


Figure 7. Image of organoids (left), Temporal evolution of some organoid size without treatment (middle) and with treatment (right).

# 6.8. Vesicles tracking

Participants: Raphael Pages, Xavier Descombes.

# This work is a collaboration with P. Juan, M. Furthauer from iBV. It was partially supported by the UCA Jedi Idex.

We take advantage of the optical transparency of the zebrafish to study the formation, transport and function of extracellular vesicles in vivo. In the zebrafish Left/Right Organizer (LRO) a cilia-driven fluid flow promotes the directional transport of extracellular vesicles in the organ lumen. We have developed a software to analyze the vesicles trajectory. Assuming that the speed is slow enough, the detection is performed by considering the 2D+t time sequence of data as a 3D volume in which the vesicle trajectories are represented by tubular shapes. We first remove the background in each slice by subtracting a temporal mean computed on a sliding window. The trajectories are than enhanced by a Frangi filter followed by a top hat operator. Finally, the trajectories are obtained by a threshold and filtered to remove those corresponding to cilia movement. To compare different populations we then compute a mean shape of the LRO using an elastic shape metric. The trajectories detected on the different samples of a given population are then projected onto this common space. To have a dense representation of the vesicles speed inside the LRO we then extrapolate the detected trajectories on the whole population using a Markov random field regularization (see figure 8).

# 6.9. Comparison of tracking strategies

Participants: Sarah Laroui, Grégoire Malandain, Gaël Michelin.

#### This work takes place within the ANR PhaseQuant.

In video-microscopy, subject-based studies require the tracking of every individual to both quantify its dynamics (speed, etc) and detect special events (mitosis). In high throughput experiments, manual annotation or correction of sequences is not feasible, and computed-based strategies are definitevely prefered. In such a context, where cells have already been segmented in video-microscopy images (by a third party method), this work aims to assess different tracking strategies in presence of unavoidable segmentation errors (missing cells, over- or under-segmentations).

Two main strategies have been under examination. In the first one, all pairing hypothesis (based on a proximity criteria) have been generated. Further stages of both selection of plausible pairings or rejection of non-plausible ones have been tested to end up with tracking results. In the second one, pairings are built progressively based on their plausibility (one cell can be paired forward to 0, 1 or 2 cells; one cell can be paired backward to 0 or 1 cell). In both strategies, jumps are allowed to take into account possible segmentation errors.

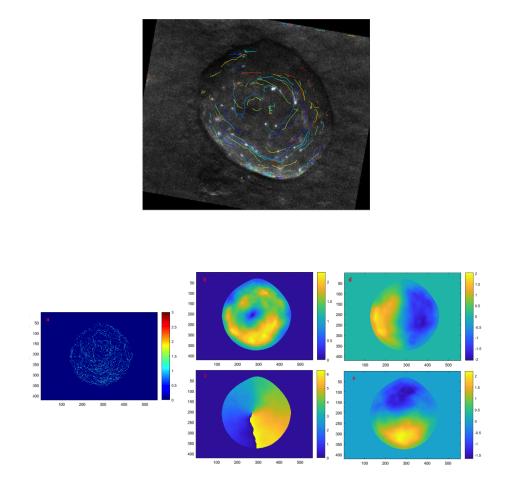
It appears that the first strategie is more likely to end up with undecidable unplausible situations, that can not occur, by construction, with the second one.

# 6.10. 3D Coronary vessel tracking in x-ray projections

Participants: Emmanuelle Poulain, Grégoire Malandain.

# This work is made in collaboration with Régis Vaillant (GE-Healthcare, Buc, France) and Nicholas Ayache (Inria Epione team).

Percutaneous Coronary Intervention (PCI) is a minimally procedure which is used to treat coronary artery narrowing. The physician intervenes on the patient under the guidance of an x-ray imaging system. This system is not able to display a visual assessment of the coronary wall, contrary to the pre-operative Computed Tomography Angiography (CTA). To help physician to exploit this information during the course of the procedure, registering these two modalities would be useful. To this aim, we first proposed in a previous work a method of 3D coronary tracking of the main vessel in x-ray projections [17]. Although, we faced a segmentation problem when we wanted to move from the tracking of one vessel to the entire set. For this reason, we have worked this year on the vessel centerline extraction in x-ray projection images.



*Figure 8. Trajectories detected on one LRO (top). Bottom: trajectories detected the whole population (right a), horizonal (b), vertical (c) radial (d) and angular (e) speeds.* 

2D Angiographic images are often first enhanced, before centerline extraction, by dedicated filters, e.g. Hessian based filters. Such filters exhibit critical defects, one of them being the non-uniform response for vessels of different sizes. This fact largely compromised the next step of centerline extraction. This last step requires a threshold step which is usually not clearly explained in other established methods. We worked on a model-based study of two widely used Hessian-based filter. It demonstrates that the non-uniform response for vessels of different sizes is due to the projective effect, and further enables to propose an X-ray projection dedicated method for centerline extraction which overpass this behavior. It is complemented by a component-based hysteresis thresholding. Last, the huge variability of coronary image aspect, due to imaging parameters, makes the threshold choice quite complex. We have shown that the thresholds can be determined automatically taking into account the kilovoltage peak (kVp), one key technical parameter of the X-ray acquisition. These thresholds are determined without any a priori on the image content. This technique not only allows to obtain an almost optimal segmentation, but also performs well for non-injected frames. Results of our proposed method and methods from state of the art are presented in Fig. 9.

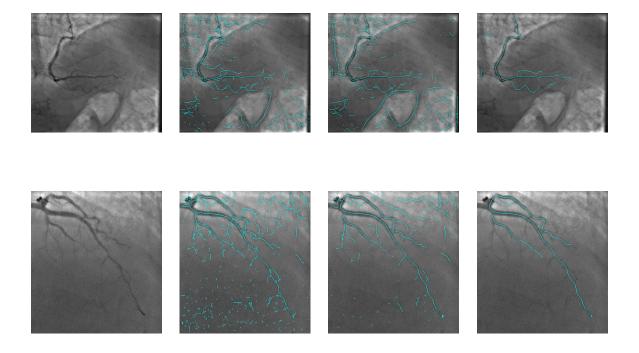


Figure 9. The obtained results of the different methods on a right coronary sample (first line), and left coronary sample (second line). From left to right: the original image, the result of Frangi (OPHT), the result of Krissian (OPHT), and the result of the proposed method (CCHT). The two first methods were tuned to obtain the same sensitivity than the third one.

# 6.11. Mitochondrial network detection and classification

Participants: Guillaume Lavisse, Xavier Descombes.

This work is a collaboration with C. Badot and M. Chami from IPMC and A. Charezac, S. Clavel and F. Bost from C3M. It was partially supported by the UCA Jedi Idex.

Last year we had developed a framework to classify mitochondrial networks. In this framework, mitchondrial networks are first binarized using our algorithm ATOLS. Some geometrical features are then computed for each connected component providing a clustering at the object level in the feature space. A signature of a

given image is then defined by the ratio of objects in the different classes. A second classification, performed by an SVM on this signature, provides a global class for the image. The different classes are defined as fragmented, tubular and filamentous. This year, we have validated this framework on two other databases, one consisting of cultured cells, the other being constituted of Alzheimer neuronal cells. The results were not satisfactory compared to those obtained on the first database last year. This is mainly due to the signal heterogeneity within an image. To compensate this heterogeneity we have applied a local normalization (see figure 10). We then have recovered classification performances comparable to those obtained by an expert. The next step consists in following in time the mitochondria of Alzheimer neuron. To this aim, we have developed a matching algorithm between two sets of mitochondria based on geometrical features and location of detected objects at two different instants.

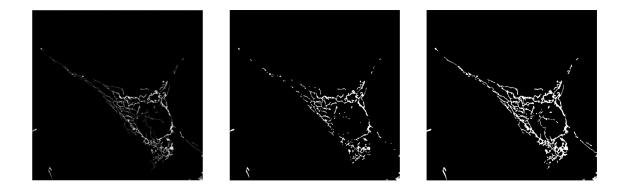


Figure 10. Image of Mitochondria (left), Binarization obtained without local normalization (middle) and with local normalization (right).

# 6.12. Botrytis cinerea phenotype recognition and classification: toward the establishment of links between phenotypes and antifungal molecules

Participants: Sarah Laroui, Eric Debreuve, Xavier Descombes.

This work is a collaboration with Aurelia Vernay (Bayer, Lyon, France).

Botrytis cinerea is a reference model of filamentous phytopathogen fungi. Some chemical treatments can lead to characteristic morphological changes, or phenotypic signatures, observable with transmitted light microscopy. These phenotypes could be associated with the treatment Mode of Action (figure 11). The goal of this work is the recognition of already known phenotypes but also the detection of new phenotypes. Because of the different dose-response effects, each given molecule is tested at ten concentrations.

In this context, we are developing a robust image analysis and classification framework relying on morphometric and topological characteristics to automatically recognize such phenotypes. Specifically, these characteristics are used in a supervised machine-learning framework to learn a Random Forest classifier.

After object detection, we calculate the skeleton of each object and we converted them into graphs, a more convenient data structure. Two types of parameters were extracted: those calculated globally on all the objects of an image like for example the number of objects and the skeleton length variance, and those computed on each object of an image like the number of nodes, the mean branch length and the object area.

#### 6.13. Automatic zooplankton classification using hierarchical approaches

Participants: Eric Debreuve, Baptiste Pouthier.

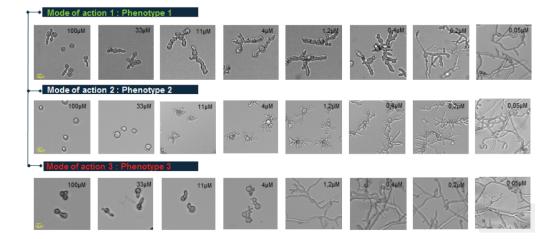


Figure 11. Each row depicts the observed phenotypic signatures associated with a given molecules. Columns correspond to different molecule concentrations.

This work is made in collaboration with Frédéric Precioso (I3S) and Jean-Olivier Irisson (Laboratoire d'Océanographie de Villefranche-sur-mer).

In marine ecology routine, zooplankton organisms are imaged using a single camera system. With the purpose of building an automatic classifier of plankton images, databases of annotated images are built. For each species, such databases contain a set of images of similar organisms, but seen under different point of views, i.e., having potentially very different appearances. Hence, learning an automatic classifier for zooplankton from such databases is difficult. In consequence, feeding the learning process with as much information as possible is essential. One piece of information we have access to is a taxonomic structure (hence hierarchical structure) of zooplankton species established by environmental biologists (see Fig. 12). Therefore, we have explored (and we continue to explore) different strategies to use such a hierarchy in the learning process, from the straightforward one consisting of learning a coarse-to-fine tree of independent convolutional neural networks (CNNs) to using neural network architectures explicitly accounting for hierarchical constraints.

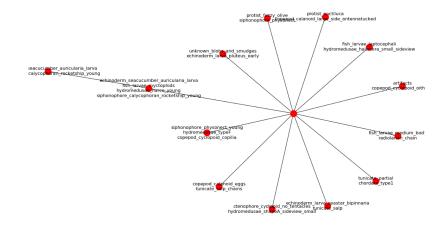


Figure 12. An Illustration of the zooplankton taxonomy.

# **COATI Project-Team**

# 7. New Results

## 7.1. Network Design and Management

**Participants:** Jean-Claude Bermond, Christelle Caillouet, David Coudert, Frédéric Giroire, Frédéric Havet, Nicolas Huin, Joanna Moulierac, Nicolas Nisse, Stéphane Pérennes, Andrea Tomassilli.

Network design is a very wide subject which concerns all kinds of networks. In telecommunications, networks can be either physical (backbone, access, wireless, ...) or virtual (logical). The objective is to design a network able to route a (given, estimated, dynamic, ...) traffic under some constraints (e.g. capacity) and with some quality-of-service (QoS) requirements. Usually the traffic is expressed as a family of requests with parameters attached to them. In order to satisfy these requests, we need to find one (or many) paths between their end nodes. The set of paths is chosen according to the technology, the protocol or the QoS constraints.

We mainly focus on the following topics: Firstly, we study the new network paradigms, Software-Defined Networks (SDN) and Network Function Virtualization (NFV). On the contrary to legacy networks, in SDN, a centralized controller is in charge of the control plane and takes the routing decisions for the switches and routers based on the network conditions. This new technology brings new constraints and therefore new algorithmic problems such as the problem of limited space in the switches to store the forwarding rules. We then tackle the problem of placement of virtualized resources. We validated our algorithms on a real SDN platform <sup>0</sup>. Secondly, we consider different scenarios regarding wireless networks and connected Unmanned Aerial Vehicules (UAVs). Third, we tackle routing in the Internet. Last, we study live streaming in distributed systems.

#### 7.1.1. Software Defined Networks (SDN)

Software-defined Networks (SDN) is a new networking paradigm enabling innovation through network programmability. SDN is gaining momentum with the support of major manufacturers. Over past few years, many applications have been built using SDN such as server load balancing, virtual-machine migration, traffic engineering and access control.

#### 7.1.1.1. Bringing Energy Aware Routing Closer to Reality With SDN Hybrid Networks

Energy-aware routing aims at reducing the energy consumption of Internet service provider (ISP) networks. The idea is to adapt routing to the traffic load to turn off some hardware. However, it implies to make dynamic changes to routing configurations which is almost impossible with legacy protocols. The software defined network (SDN) paradigm bears the promise of allowing a dynamic optimization with its centralized controller. In [34], we propose smooth energy aware routing (SENAtoR), an algorithm to enable energy-aware routing in a scenario of progressive migration from legacy to SDN hardware. Since in real life, turning off network devices is a delicate task as it can lead to packet losses, SENAtoR also provides several features to safely enable energy saving services: tunneling for fast rerouting, smooth node disabling, and detection of both traffic spikes and link failures. We validate our solution by extensive simulations and by experimentation. We show that SENAtoR can be progressively deployed in a network using the SDN paradigm. It allows us to reduce the energy consumption of ISP networks by 5%–35% depending on the penetration of SDN hardware while diminishing the packet loss rate compared to legacy protocols.

<sup>&</sup>lt;sup>0</sup>Testbed with SDN hardware, in particular a switch HP 5412 with 96 ports, hosted at I3S laboratory. A complete fat-tree architecture with 16 servers can be built on the testbed.

#### 7.1.1.2. Energy-Aware Routing in Software-Defined Network using Compression

Over past few years, many applications have been built using SDN such as server load balancing, virtualmachine migration, traffic engineering and access control. In [31], we focus on using SDN for energy-aware routing (EAR). Since traffic load has a small influence on the power consumption of routers, EAR allows putting unused links into sleep mode to save energy. SDN can collect traffic matrix and then computes routing solutions satisfying QoS while being minimal in energy consumption. However, prior works on EAR have assumed that the SDN forwarding table switch can hold an infinite number of rules. In practice, this assumption does not hold since such flow tables are implemented in Ternary Content Addressable Memory (TCAM) which is expensive and power-hungry. We consider the use of wildcard rules to compress the forwarding tables. In [31], we propose optimization methods to minimize energy consumption for a backbone network while respecting capacity constraints on links and rule space constraints on routers. In details, we present two exact formulations using Integer Linear Program (ILP) and introduce efficient heuristic algorithms. Based on simulations on realistic network topologies, we show that using this smart rule space allocation, it is possible to save almost as much power consumption as the classical EAR approach.

#### 7.1.1.3. Complexity of Compressing Two Dimensional Routing Tables with Order

Motivated by routing in telecommunication network using Software Defined Network (SDN) technologies, we consider the following problem of finding short routing lists using aggregation rules. We are given a set of communications  $\mathcal{X}$ , which are distinct pairs  $(s,t) \subseteq S \times T$ , (typically S is the set of sources and T the set of destinations), and a port function  $\pi : \mathcal{X} \to P$  where P is the set of ports. A *routing list* $\mathcal{R}$  is an ordered list of triples which are of the form (s,t,p), (\*,t,p), (s,\*,p) or (\*,\*,p) with  $s \in S$ ,  $t \in T$  and  $p \in P$ . It *routes* the communication (s,t) to the port r(s,t) = p which appears on the first triple in the list  $\mathcal{R}$  that is of the form (s,t,p), (\*,t,p), (s,\*,p) or (\*,\*,p), then we say that (s,t) is *properly routed* by  $\mathcal{R}$  and if all communications of  $\mathcal{X}$  are properly routed, we say that  $\mathcal{R}emulates(\mathcal{X},\pi)$ . The aim is to find a shortest routing list emulating  $(\mathcal{X},\pi)$ . In [30], we carry out a study of the complexity of the two dual decision problems associated to it. Given a set of communication  $\mathcal{X}$ , a port function  $\pi$  and an integer k, the first one called ROUTING LIST (resp. the second one, called LIST REDUCTION) consists in deciding whether there is a routing list emulating  $(\mathcal{X},\pi)$  of size at most k (resp.  $|\mathcal{X}| - k$ ). We prove that both problems are NP-complete. We then give a 3-approximation for LIST REDUCTION, which can be generalized to higher dimensions. We also give a 4-approximation for ROUTING LIST in the fundamental case when there are only two ports (i.e. |P| = 2),  $\mathcal{X} = S \times T$  and |S| = |T|.

#### 7.1.2. Provisioning Service Function Chains

#### 7.1.2.1. Optimal Network Service Chain Provisioning

Service chains consist of a set of network services, such as firewalls or application delivery controllers, which are interconnected through a network to support various applications. While it is not a new concept, there has been an extremely important new trend with the rise of Software-Defined Network (SDN) and Network Function Virtualization (NFV). The combination of SDN and NFV can make the service chain and application provisioning process much shorter and simpler. In [33], [48], we study the provisioning of service chains jointly with the number/location of Virtual Network Functions (VNFs). While chains are often built to support multiple applications, the question arises as how to plan the provisioning of service chains in order to avoid data passing through unnecessary network devices or servers and consuming extra bandwidth and CPU cycles. It requires choosing carefully the number and the location of the VNFs. We propose an exact mathematical model using decomposition methods whose solution is scalable in order to conduct such an investigation. We conduct extensive numerical experiments, and show we can solve exactly the routing of service chain requests in a few minutes for networks with up to 50 nodes, and traffic requests between all pairs of nodes. Detailed analysis is then made on the best compromise between minimizing the bandwidth requirement and minimizing the number of VNFs and optimizing their locations using different data sets.

#### 7.1.2.2. Energy-Efficient Service Function Chain Provisioning

Network Function Virtualization (NFV) is a promising network architecture concept to reduce operational costs. In legacy networks, network functions, such as firewall or TCP optimization, are performed by specific

hardware. In networks enabling NFV coupled with the Software Defined Network (SDN) paradigm, Virtual Network Functions (VNFs) can be implemented dynamically on generic hardware. This is of primary interest to implement energy efficient solutions, in order to adapt the resource usage dynamically to the demand. In [35], we study how to use NFV coupled with SDN to improve the energy efficiency of networks. We consider a setting in which a flow has to go through a Service Function Chain, that is several network functions in a specific order. We propose an ILP formulation, an ILP-based heuristic, as well as a decomposition model that relies on joint routing and placement configuration to solve the problem. We show that virtualization provides between 22% to 62% of energy savings for networks of different sizes.

#### 7.1.2.3. Placement of Service Function Chains with Ordering Constraints

A Service Function Chain (SFC) is an ordered sequence of network functions, such as load balancing, content filtering, and firewall. With the Network Function Virtualization (NFV) paradigm, network functions can be deployed as pieces of software on generic hardware, leading to a flexibility of network service composition. Along with its benefits, NFV brings several challenges to network operators, such as the placement of virtual network functions. In [49], [50], [62], we study the problem of how to optimally place the network functions within the network in order to satisfy all the SFC requirements of the flows. Our optimization task is to minimize the total deployment cost. We show that the problem can be seen as an instance of the Set Cover Problem, even in the case of ordered sequences of network functions. It allows us to propose two logarithmic factor approximation algorithms which have the best possible asymptotic factor. Further, we devise an optimal algorithm for tree topologies. Finally, we evaluate the performances of our proposed algorithms through extensive simulations. We demonstrate that near-optimal solutions can be found with our approach.

#### 7.1.2.4. Resource Requirements for Reliable Service Function Chaining

We study in [51], [49] the problem of deploying reliable Service Function Chains over a virtualized network function architecture. While there is a need for reliable service function chaining, there is a high cost to pay for it in terms of bandwidth and VNF processing requirements. We investigate two different protection mechanisms and discuss their resource requirements, as well as the latency of their paths. For each mechanism, we develop a scalable exact mathematical model using column generation.

#### 7.1.2.5. Path protection in optical flexible networks with distance-adaptive modulation formats

Thanks to a flexible frequency grid, Elastic Optical Networks (EONs) will support a more efficient usage of the spectrum resources. On the other hand, this efficiency may lead to even more disruptive effects of a failure on the number of involved connections with respect to traditional networks. In [52], we study the problem of providing path protection to the lightpaths against a single fiber failure event in the optical layer. Our optimization task is to minimize the spectrum requirements for the protection in the network. We develop a scalable exact mathematical model using column generation for both shared and dedicated path protection schemes. The model takes into account practical constraints such as the modulation format, regenerators, and shared risk link groups. We demonstrate the effectiveness of our model through extensive simulation on two real-world topologies of different sizes. Finally, we compare the two protection schemes under different scenario assumptions, studying the impact of factors such as number of regenerators and demands on their performances.

#### 7.1.2.6. Reconfiguring Service Functions chains with a make-before-break approach

The centralized routing model of SDN jointly with the possibility of instantiating VNFs on-demand open the way for a more efficient operation and management of networks. In [58], we consider the problem of reconfiguring network connections with the goal of bringing the network from a sub-optimal to an optimal operational state. We propose optimization models based on the *make-before-break* mechanism, in which a new path is set up before the old one is torn down. Our method takes into consideration the chaining requirements of the flows and scales well with the number of nodes in the network. We show that, with our approach, the network operational cost defined in terms of both bandwidth and installed network function costs can be reduced and a higher acceptance rate can be achieved.

#### 7.1.3. Capacity defragmentation

Optical multilayer optimization continuously reorganizes layer 0-1-2 network elements to handle both existing and dynamic traffic requirements in the most efficient manner. This delays the need to add new resources for new requests, saving CAPEX and leads to optical network defragmentation.

In [46], [47], we focus on Layer 2, i.e., on capacity defragmentation at the Optical Transport Network (OTN) layer when routes (e.g., LSPs in MPLS networks) are making unnecessarily long detours to evade congestion. Reconfiguration into optimized routes can be achieved by redefining the routes, one at a time, so that they use the vacant resources generated by the disappearance of services using part of a path that transits the congested section. For the Quality of Service, it is desirable to operate under Make-Before-Break (MBB), with the minimum number of rerouting. The challenge is to identify the rerouting order, one connection at a time, while minimizing the bandwidth requirement. We propose in [46], [47] an exact and scalable optimization model for computing a minimum bandwidth rerouting scheme subject to MBB in the OTN layer of an optical network. Numerical results show that we can successfully apply it on networks with up to 30 nodes, a very significant improvement with the state of the art. We also provide some defragmentation analysis in terms of the bandwidth requirement vs. the number of reroutings.

In [37], we focus on wavelength defragmentation in WDM networks. We propose a MBB wavelength defragmentation process which minimizes the bandwidth requirement of the resulting provisioning. Comparisons with minimum bandwidth provisioning that is not subject to MBB show that, on average, the best seamless lightpath rerouting is never more than 5% away (less than 1% on average) from an optimal lightpath provisioning.

#### 7.1.4. Spectrum assignment in elastic optical tree-networks

To face the explosion of the Internet traffic, a new generation of optical networks is being developed; the Elastic Optical Networks (EONs). EONs use the optical spectrum efficiently and flexibly, but that gives rise to more difficulty in the resource allocation problems. In [16], we study the problem of Spectrum Assignment (SA) in Elastic Optical Tree-Networks. Given a set of traffic requests with their routing paths (unique in the case of trees) and their spectrum demand, a spectrum assignment consists in allocating to each request an interval of consecutive slots (spectrum units) such that a slot on a given link can be used by at most one request. The objective of the SA problem is to find an assignment minimizing the total number of spectrum slots to be used. We prove that SA is NP-hard in undirected stars of 3 links and in directed stars of 4 links, and show that it can be approximated within a factor of 4 in general stars. Afterwards, we use the equivalence of SA with a graph coloring problem (interval coloring) to find constant-factor approximation algorithms for SA on binary trees with special demand profiles.

#### 7.1.5. Optimizing drone coverage

In the context of a collaboration with Tahiry Razafindralambo from the University of la Réunion we have studied several problems related to deployment of drones in order to collect data generated from sensors. Those problems may be seen as belonging to the category of "cover" problems and we have designed and proposed efficient formulations using linear programming models with columns generation.

Drones (Unmanned Aerial Vehicles, UAV) can be used to provide anytime and anywhere network access to targets located on the ground, using air-to-ground and air-to-air communications through directional antennas. In [43] we study how to deploy these drones to cover a set of fixed targets. It is a complex problem since each target should be covered, while minimizing (i) the deployment cost and (ii) the drones altitudes to ensure good communication quality. We also consider connectivity between the drone and a base station in order to collect and send information to the targets, which is not considered in many similar studies. We provide an efficient optimal program to solve the problem and show the trade-off analysis due to conflicting objectives. We propose a fair trade-off optimal solution and also evaluate the cost of adding connectivity to the drone deployment.

In [41], [42] we introduce a Linear Programming (LP) model for the problem of data gathering with mobile drones. The goal is to deploy a connected set of Unmanned Aerial Vehicles (UAVs) continuously monitoring mobile sensors and reporting information to a fixed base station for efficient data collection. We propose an effective optimization model reducing the number of variables of the problem and solved using column generation. Results show that our model is tractable for large topologies with several hundreds of possible 3D locations for the UAVs deployment and provides integer solutions with the generated columns very close to the optimum. Moreover, the deployment changes among time remains low in terms of number of UAVs and cost, to maintain connectivity and minimize the data collection delay to the base station.

We also have studied a problem arising when one will to recharge wireless sensor networks using drones and wireless power transfer; in [44] we consider the optimal energy replenishment problem (OERP). The goal is to operate a given number of flying drones in order to efficiently recharge wireless sensor nodes. We present a linear program that maximizes the amount of harvested energy to the sensors. We show that the model is solved to optimality in a few seconds for sensor networks with up to 50 nodes. The small number of available drones is shown to be optimally deployed at low altitude in order to efficiently recharge the batteries of at least half of the sensor nodes.

#### 7.1.6. Other results in wireless networks

#### 7.1.6.1. Backbone colouring and algorithms for TDMA scheduling

We investigate graph colouring models for the purpose of optimizing TDMA link scheduling in Wireless Networks. Inspired by the *BPRN*-colouring model recently introduced by Rocha and Sasaki, we introduce a new colouring model, namely the *BMRN*-colouring model, which can be used to model link scheduling problems where particular types of collisions must be avoided during the node transmissions.

In [64], we initiate the study of the BMRN-colouring model by providing several bounds on the minimum number of colours needed to BMRN-colour digraphs, as well as several complexity results establishing the hardness of finding optimal colourings. We also give a special focus on these considerations for planar digraph topologies, for which we provide refined results. Some of these results extend to the BPRN-colouring model as well.

#### 7.1.6.2. Gossiping with interference in radio chain networks

In [53], we study the problem of gossiping with interference constraint in radio chain networks. Gossiping (or total exchange information) is a protocol where each node in the network has a message and wants to distribute its own message to every other node in the network. The gossiping problem consists in finding the minimum running time (makespan) of a gossiping protocol and efficient algorithms that attain this makespan. The network is assumed to be synchronous, the time is slotted into steps, and each device is equipped with a half duplex interface; so, a node cannot both receive and transmit during a step. We use a binary asymmetric model of interference based on the distance in the communication digraph. We determine exactly the minimum number of rounds R needed to achieve a gossiping when transmission network is a dipath  $P_n$  on  $n \ge 3$  nodes and the interference distance is  $d_I = 1$ .

# 7.2. Graph Algorithms

**Participants:** Julien Bensmail, Jean-Claude Bermond, Nathann Cohen, David Coudert, Frédéric Giroire, Frédéric Havet, Fionn Mc Inerney, Nicolas Nisse, Stéphane Pérennes.

COATI is interested in the algorithmic aspects of Graph Theory. In general we try to find the most efficient algorithms to solve various problems of Graph Theory and telecommunication networks. We use Graph Theory to model various network problems. We study their complexity and then we investigate the structural properties of graphs that make these problems hard or easy.

#### 7.2.1. Complexity of graph problems

#### 7.2.1.1. Parameterized complexity of polynomial optimization problems (FPT in P)

Parameterized complexity theory has enabled a refined classification of the difficulty of NP-hard optimization problems on graphs with respect to key structural properties, and so to a better understanding of their true difficulties. More recently, hardness results for problems in P were established under reasonable complexity theoretic assumptions such as: Strong Exponential Time Hypothesis (SETH), 3SUM and All-Pairs Shortest-Paths (APSP). According to these assumptions, many graph theoretic problems do not admit truly subquadratic algorithms, nor even truly subcubic algorithms (Williams and Williams, FOCS 2010 [83] and Abboud *et al.* SODA 2015 [67]). A central technique used to tackle the difficulty of the above mentioned problems is fixed-parameter algorithms for polynomial-time problems with *polynomial dependency* in the fixed parameter (P-FPT). This technique was rigorously formalized by Giannopoulou et al. (IPEC 2015) [74], [75]. Following that, it was continued by Abboud *et al.* (SODA 2016) [68], by Husfeldt (IPEC 2016) [76] and Fomin *et al.* (SODA 2017) [73], using the treewidth as a parameter. Applying this technique to *clique-width*, another important graph parameter, remained to be done.

In [45] we study several graph theoretic problems for which hardness results exist such as cycle problems (triangle detection, triangle counting, girth), distance problems (diameter, eccentricities, Gromov hyperbolicity, betweenness centrality) and maximum matching. We provide hardness results and fully polynomial FPT algorithms, using clique-width and some of its upper-bounds as parameters (split-width, modular-width and  $P_4$ -sparseness). We believe that our most important result is an  $O(k^4 \cdot n + m)$ -time algorithm for computing a maximum matching where k is either the modular-width or the  $P_4$ -sparseness. The latter generalizes many algorithms that have been introduced so far for specific subclasses such as cographs,  $P_4$ -lite graphs,  $P_4$ -extendible graphs and  $P_4$ -tidy graphs. Our algorithms are based on preprocessing methods using modular decomposition, split decomposition and primeval decomposition. Thus they can also be generalized to some graph classes with unbounded clique-width.

#### 7.2.1.2. Revisiting Decomposition by Clique Separators

We study in [26] the complexity of decomposing a graph by means of clique separators. This common algorithmic tool, first introduced by Tarjan [79], allows to cut a graph into smaller pieces, and so, it can be applied to preprocess the graph in the computation of optimization problems. However, the bestknown algorithms for computing a decomposition have respective O(nm)-time and  $O(n^{(3+\alpha)/2}) = o(n^{2.69})$ time complexity, with  $\alpha < 2.3729$  being the exponent for matrix multiplication. Such running times are prohibitive for large graphs. In [26], we prove that for every graph G, a decomposition can be computed in  $O(T(G) + \min\{n^{\alpha}, \omega^2 n\})$ -time with T(G) and  $\omega$  being respectively the time needed to compute a minimal triangulation of G and the clique-number of G. In particular, it implies that every graph can be decomposed by clique separators in  $O(n^{\alpha} \log n)$ -time. Based on prior work from Kratsch and Spinrad [77], we prove in addition that decomposing a graph by clique-separators is as least as hard as triangle detection. Therefore, the existence of any  $o(n^{\alpha})$ -time algorithm for this problem would be a significant breakthrough in the field of algorithmic. Finally, our main result implies that planar graphs, bounded-treewidth graphs and bounded-degree graphs can be decomposed by clique separators in linear or quasi-linear time.

#### 7.2.1.3. Distance-preserving elimination orderings in graphs

For every connected graph G, a subgraph H of G is *isometric* if the distance between any two vertices in H is the same in H as in G. A *distance-preserving elimination ordering* of G is a total ordering of its vertex-set V(G), denoted  $(v_1, v_2, ..., v_n)$ , such that any subgraph  $G_i = G \setminus (v_1, v_2, ..., v_i)$  with  $1 \le i < n$  is isometric. This kind of ordering has been introduced by Chepoi in his study on weakly modular graphs [71]. In [27], we prove that it is NP-complete to decide whether such ordering exists for a given graph I even if it has diameter at most 2. Then, we prove on the positive side that the problem of computing a distance-preserving ordering when there exists one is fixed-parameter-tractable in the treewidth. Lastly, we describe a heuristic in order to compute a distance-preserving ordering when there exists one that we compare to an exact exponential time algorithm and to an ILP formulation for the problem.

#### 7.2.1.4. Complexity of computing strong pathbreadth

The strong pathbreadth of a given graph G is the minimum  $\rho$  such that G admits a Robertson and Seymour's path decomposition where every bag is the complete  $\rho$ -neighbourhood of some vertex in G. In [29] <sup>0</sup>, we prove that deciding whether a given graph has strong pathbreadth at most one is NP-complete. This answers negatively to a conjecture of Leitert and Dragan [78].

#### 7.2.1.5. Improving matchings in trees, via bounded-length augmentations

In [13] Due to a classical result of Berge, it is known that a matching of any graph can be turned into a maximum matching by repeatedly augmenting alternating paths whose ends are not covered. In a recent work, Nisse, Salch and Weber considered the influence, on this process, of augmenting paths with length at most k only. Given a graph G, an initial matching  $M \subseteq E(G)$  and an odd integer k, the problem is to find a longest sequence of augmenting paths of length at most k that can be augmented sequentially from M. They proved that, when only paths of length at most k = 3 can be augmented, computing such a longest sequence can be done in polynomial time for any graph, while the same problem for any  $k \ge 5$  is *NP*-hard. Although the latter result remains true for bipartite graphs, the status of the complexity of the same problem for trees is not known.

This work is dedicated to the complexity of this problem for trees. On the positive side, we first show that it can be solved in polynomial time for more classes of trees, namely bounded-degree trees (via a dynamic programming approach), caterpillars and trees where the nodes with degree at least 3 are sufficiently far apart. On the negative side, we show that, when only paths of length *exactlyk* can be augmented, the problem becomes *NP*-hard already for k = 3, in the class of planar bipartite graphs with maximum degree 3 and arbitrary large girth. We also show that the latter problem is *NP*-hard in trees when k is part of the input.

#### 7.2.2. Dynamics of formation of communities in social networks

We consider in [40] a community formation problem in social networks, where the users are either friends or enemies. The users are partitioned into conflict-free groups (i.e., independent sets in the conflict graph  $G^- = (V, E)$  that represents the enmities between users). The dynamics goes on as long as there exists any set of at most k users, k being any fixed parameter, that can change their current groups in the partition simultaneously, in such a way that they all strictly increase their utilities (number of friends i.e., the cardinality of their respective groups minus one). Previously, the best-known upper-bounds on the maximum time of convergence were  $O(|V|\alpha(G^-))$  for  $k \leq 2$  and  $O(|V|^3)$  for k = 3, with  $\alpha(G^-)$  being the independence number of  $G^-$ . Our first contribution in this paper consists in reinterpreting the initial problem as the study of a dominance ordering over the vectors of integer partitions. With this approach, we obtain for  $k \leq 2$  the tight upper-bound  $O(|V|\min \alpha(G^-), \sqrt{|V|})$  and, when  $G^-$  is the empty graph, the exact value of order  $\frac{(2|V|)^{3/2}}{3}$ . The time of convergence, for any fixed  $k \geq 4$ , was conjectured to be polynomial. In [40], we disprove this. Specifically, we prove that for any  $k \geq 4$ , the maximum time of convergence is an  $\Omega(|V|^{\Theta(\log |V|)})$ .

# 7.2.3. Application to bioinformatics

For a (possibly infinite) fixed family of graphs  $\mathcal{F}$ , we say that a graph *Goverlays* $\mathcal{F}$  on a hypergraph H if V(H) is equal to V(G) and the subgraph of G induced by every hyperedge of H contains some member of  $\mathcal{F}$  as a spanning subgraph. While it is easy to see that the complete graph on |V(H)| overlays  $\mathcal{F}$  on a hypergraph H whenever the problem admits a solution, the MINIMUM  $\mathcal{F}$ -OVERLAY problem asks for such a graph with at most k edges, for some given  $k \in \mathbb{N}$ . This problem allows to generalize some natural problems which may arise in practice. For instance, if the family  $\mathcal{F}$  contains all connected graphs, then MINIMUM  $\mathcal{F}$ -OVERLAY corresponds to the MINIMUM CONNECTIVITY INFERENCE problem (also known as SUBSET INTERCONNECTION DESIGN problem) introduced for the low-resolution reconstruction of macro-molecular assembly in structural biology, or for the design of networks.

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<sup>&</sup>lt;sup>0</sup>Work done while G. Ducoffe was a member of COATI and published this year.

In [23], we prove a strong dichotomy result regarding the polynomial vs. NP-complete status with respect to the considered family  $\mathcal{F}$ . Roughly speaking, we show that the easy cases one can think of (e.g. when edgeless graphs of the right sizes are in  $\mathcal{F}$ , or if  $\mathcal{F}$  contains only cliques) are the only families giving rise to a polynomial problem: all others are NP-complete. We then investigate the parameterized complexity of the problem and give similar sufficient conditions on  $\mathcal{F}$  that give rise to W[1]-hard, W[2]-hard or FPT problems when the parameter is the size of the solution. This yields an FPT/W[1]-hard dichotomy for a relaxed problem, where every hyperedge of H must contain some member of  $\mathcal{F}$  as a (non necessarily spanning) subgraph.

# 7.3. Games on Graphs

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We study several two-player games on graphs. Some of these games allow to model real-life applications. In the case of the Spy-game presented below, we propose a successful new approach by studying fractional relaxation of such games.

#### 7.3.1. Spy-game on graphs and eternal domination

In [24] we define and study the following two-player game on a graph G. Let  $k \in \mathbb{N}^*$ . A set of k guards is occupying some vertices of G while one spy is standing at some node. At each turn, first the spy may move along at most s edges, where  $s \in \mathbb{N}^*$  is his speed. Then, each guard may move along one edge. The spy and the guards may occupy the same vertices. The spy has to escape the surveillance of the guards, i.e., must reach a vertex at distance more than  $d \in \mathbb{N}$  (a predefined distance) from every guard. Can the spy win against k guards? Similarly, what is the minimum distance d such that k guards may ensure that at least one of them remains at distance at most d from the spy? This game generalizes two well-studied games: Cops and robber games (when s = 1) and Eternal Dominating Set (when s is unbounded).

In [24], we consider the computational complexity of the problem, showing that it is NP-hard (for every speed s and distance d) and that some variant of it is PSPACE-hard in DAGs. Then, we establish tight tradeoffs between the number of guards, the speed s of the spy and the required distance d when G is a path or a cycle.

In order to determine the smallest number of guards necessary for this task, we analyze in [25] the game through a Linear Programming formulation and the fractional strategies it yields for the guards. We then show the equivalence of fractional and integral strategies in trees. This allows us to design a polynomial-time algorithm for computing an optimal strategy in this class of graphs. Using duality in Linear Programming, we also provide non-trivial bounds on the fractional guard-number of grids and torus. We believe that the approach using fractional relaxation and Linear Programming is promising to obtain new results in the field of combinatorial games.

In [60] we pursue the study of the eternal domination game (which is equivalent to the spy game when s is unbounded and d = 0) on strong grids  $P_n \Box P_m$ . Cartesian grids  $P_n \Box P_m$  have been vastly studied with tight bounds existing for small grids such as  $k \times n$  grids for  $k \in \{2, 3, 4, 5\}$ . It was recently proven that  $\gamma_{all}^{\infty}(P_n \Box P_m) = \gamma(P_n \Box P_m) + O(n+m)$  where  $\gamma(P_n \Box P_m)$  is the domination number of  $P_n \Box P_m$  which lower bounds the eternal domination number. We prove that, for all  $n, m \in \mathbb{N}^*$  such that  $m \ge n$ ,  $\lceil \frac{nm}{9} \rceil + \Omega(n+m) = \gamma_{all}^{\infty}(P_n \boxtimes P_m) = \lceil \frac{nm}{9} \rceil + O(m\sqrt{n})$  (note that  $\lceil \frac{nm}{9} \rceil$  is the domination number of  $P_n \boxtimes P_m$ ).

#### 7.3.2. Metric dimension & localization

The questions that we study there are variant of the usual *Metric Dimension* problem in which one wishes to identify the vertices of a graph from the knowledge of the distances to a few points. This is motivated by localization problems, e.g., in cellular networks. few anchors.

In [19] we introduce a generalization of metric dimension based on a pursuit graph game that resembles the famous Cops and Robbers game. In this game, an invisible target is hidden at some vertex of a graph (at each turn, it may move to a neighbor). At every step,  $k \ge 1$  vertices of G can be probed which results in the knowledge of the distances between each of these vertices and the secret location of the target. We provide upper bounds on the related graph invariant  $\zeta(G)$ , defined as the least number of probes per turn needed to localize the robber on a graph G, for several classes of graphs (trees, bipartite graphs, etc). Our main result is that, surprisingly, there exists planar graphs of treewidth 2 and unbounded  $\zeta(G)$ . On a positive side, we prove that  $\zeta(G)$  is bounded by the pathwidth of G. We then show that the algorithmic problem of determining  $\zeta(G)$  is NP-hard in graphs with diameter at most 2. Finally, we show that at most one cop can approximate (arbitrary close) the location of the robber in the Euclidean plane. We further study this problem in [18] where, in particular, we prove that  $\zeta(G) \le 3$  in outer-planar graphs.

In [39], [56], [38], we address the sequential metric dimension when the invisible target is immobile. The objective of the game is to minimize the number of steps needed to locate the target whatever be its location. Precisely, given a graph G and two integers  $k, \ell \ge 1$ , the LOCALIZATION problem asks whether there exists a strategy to locate a target hidden in G in at most  $\ell$  steps and probing at most k vertices per step. We first show that, in general, this problem is NP-complete for every fixed  $k \ge 1$  (resp.,  $\ell \ge 1$ ). We then focus on the class of trees. On the negative side, we prove that the LOCALIZATION PROBLEM is NP-complete in trees when k and  $\ell$  are part of the input. On the positive side, we design a (+1)-approximation for the problem in n-node trees, *i.e.*, an algorithm that computes in time  $O(n \log n)$  (independent of k) a strategy to locate the target in at most one more step than an optimal strategy. This algorithm can be used to solve the LOCALIZATION PROBLEM in trees in polynomial time if k is fixed.

In [57] we try to understand the phenomena when one choose an orientation of an (undirected) graphs. Namely, we study, for particular graph families, the maximum metric dimension over all strongly-connected orientations, by exhibiting lower and upper bounds on this value. We first exhibit general bounds for graphs with bounded maximum degree. In particular, we prove that, in the case of subcubic *n*-node graphs, all strongly-connected orientations asymptotically have metric dimension at most  $\frac{n}{2}$ , and that there are such orientations having metric dimension  $\frac{2n}{5}$ . We then consider strongly-connected orientations of grids. For a torus with *n* rows and *m* columns, we show that the maximum value of the metric dimension of a strongly-connected Eulerian orientation is asymptotically  $\frac{nm}{2}$  (the equality holding when *n*, *m* are even, which is best possible). For a grid with *n* rows and *m* columns, we prove that all strongly-connected orientations asymptotically have metric dimension at most  $\frac{2nm}{3}$ , and that there are such orientations having metric dimension at most  $\frac{2nm}{3}$ , and that there are such orientations having metric dimension at most  $\frac{2nm}{3}$ .

#### 7.3.3. Orienting edges to fight fire in graphs

In [12], we investigate a new oriented variant of the Firefighter Problem. In the traditional Firefighter Problem, a fire breaks out at a given vertex of a graph, and at each time interval spreads to neighbouring vertices that have not been protected, while a constant number of vertices are protected at each time interval. In our version of the problem, the firefighters are able to orient the edges of the graph before the fire breaks out, but the fire could start at any vertex. We consider this problem when played on a graph in one of several graph classes, and give upper and lower bounds on the number of vertices that can be saved. In particular, when one firefighter graph, we present firefighting strategies that are provably optimal. We also provide lower bounds on the number of vertices that can be saved as a function of the chromatic number, of the maximum degree, and of the treewidth of a graph. For a sub-cubic graph, we show that the firefighters can save all but two vertices, and this is best possible.

#### 7.3.4. Network decontamination

The Network Decontamination problem consists in coordinating a team of mobile agents in order to clean a contaminated network. The problem is actually equivalent to tracking and capturing an invisible and arbitrarily fast fugitive. This problem has natural applications in network security in computer science or in robotics for search or pursuit-evasion missions. In this Chapter, we focus on networks modeled by graphs. Many different

objectives have been studied in this context, the main one being the minimization of the number of mobile agents necessary to clean a contaminated network. Another important aspect is that this optimization problem has a deep graph-theoretical interpretation. Network decontamination and, more precisely, graph searching models, provide nice algorithmic interpretations of fundamental concepts in the Graph Minors theory by Robertson and Seymour. For all these reasons, graph searching variants have been widely studied since their introduction by Breish (1967) and mathematical formalizations by Parsons (1978) and Petrov (1982). Our chapter [61] consists of an overview of algorithmic results on graph decontamination and graph searching.

## 7.3.5. Hyperopic Cops and Robbers

We introduce in [17] a new variant of the game of Cops and Robbers played on graphs, where the robber is invisible unless outside the neighbor set of a cop. The hyperopic cop number is the corresponding analogue of the cop number, and we investigate bounds and other properties of this parameter. We characterize the copwin graphs for this variant, along with graphs with the largest possible hyperopic cop number. We analyze the cases of graphs with diameter 2 or at least 3, focusing on when the hyperopic cop number is at most one greater than the cop number. We show that for planar graphs, as with the usual cop number, the hyperopic cop number is at most 3. The hyperopic cop number is considered for countable graphs, and it is shown that for connected chains of graphs, the hyperopic cop density can be any real number in [0, 1/2].

# 7.4. Graph theory

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COATI studies theoretical problems in graph theory. If some of them are directly motivated by applications, others are more fundamental.

#### 7.4.1. Interval number in cycle convexity

Recently, Araujo et al. [Manuscript in preparation, 2017] introduced the notion of Cycle Convexity of graphs. In their seminal work, they studied the graph convexity parameter called hull number for this new graph convexity they proposed, and they presented some of its applications in Knot theory. Roughly, the *tunnel* number of a knot embedded in a plane is upper bounded by the hull number of a corresponding planar 4-regular graph in cycle convexity. In [4], we go further in the study of this new graph convexity and we study the interval number of a graph in cycle convexity. This parameter is, alongside the hull number, one of the most studied parameters in the literature about graph convexities. Precisely, given a graph G, its *interval number* in cycle convexity, denoted by CCIHN(G), is the minimum cardinality of a set  $S \subseteq V(G)$  such that every vertex  $w \in V(G) \setminus S$  has two distinct neighbors  $u, v \in S$  such that u and v lie in same connected component of G[S], i.e. the subgraph of G induced by the vertices in S.

In [4] we provide bounds on CCIHN(G) and its relations to other graph convexity parameters, and explore its behaviour on grids. Then, we present some hardness results by showing that deciding whether  $CCIHN(G) \le k$  is NP-complete, even if G is a split graph or a bounded-degree planar graph, and that the problem is W[2]-hard in bipartite graphs when k is the parameter. As a consequence, we obtain that CCIHN(G) cannot be approximated up to a constant factor in the classes of split graphs and bipartite graphs (unless P = NP).

On the positive side, we present polynomial-time algorithms to compute CCIHN(G) for outerplanar graphs, cobipartite graphs and interval graphs. We also present fixed-parameter tractable (FPT) algorithms to compute it for (q, q - 4)-graphs when q is the parameter and for general graphs G when parameterized either by the treewidth or the neighborhood diversity of G.

Some of our hardness results and positive results are not known to hold for related graph convexities and domination problems. We hope that the design of our new reductions and polynomial-time algorithms can be helpful in order to advance in the study of related graph problems.

#### 7.4.2. Steinberg-like theorems for backbone colouring

A function  $f: V(G) \to \{1, ..., k\}$  is a (proper) k-colouring of G if  $|f(u) - f(v)| \ge 1$ , for every edge  $uv \in E(G)$ . The chromatic number $\chi(G)$  is the smallest integer k for which there exists a proper k-colouring of G. Given a graph G and a subgraph H of G, a circular q-backbone k-colouring f of (G, H) is a k-colouring of G such that  $q \le |c(u) - c(v)| \le k - q$ , for each edge  $uv \in E(H)$ . The circular q-backbone chromatic number of a graph pair (G, H), denoted  $\operatorname{CBC}_q(G, H)$ , is the minimum k such that (G, H) admits a circular q-backbone k-colouring. Steinberg conjectured that if G is planar and G contains no cycles on 4 or 5 vertices, then  $\chi(G) \le 3$ . If this conjecture is correct, then one could deduce that  $\operatorname{CBC}_2(G, H) \le 6$ , for any  $H \subseteq G$ . In [5], we first show that if G is a planar graph containing no cycle on 4 or 5 vertices and  $H \subseteq G$  is a forest, then  $\operatorname{CBC}_2(G, H) \le 6$ .

#### 7.4.3. Homomorphisms of planar signed graphs and absolute cliques

Homomorphisms are an important topic in graph theory, as example the chromatic number of a graph G is the minimum k such that G maps onto the complete graph  $K_k$ . A signed graph  $(G, \Sigma)$  is a (simple) graph with sign function  $\Sigma E(G) \to \{-1, 1\}$ . A closed-walk is unbalanced if it has an odd number of negative edges, it is balanced otherwise. Homomorphisms of signed graphs are mapping that preserve adjacency and balance of cycles. Naserasr, Rollova and Sopena (Journal of Graph Theory 2015) posed the important question of finding out the minimum size k such that any planar signed graph  $(G, \Sigma)$  admits a homomorphism to a signed graph with k vertices. The question can be seen as the counterpart of the 4 color theorem which implies that any palnar graph maps onto  $K_4$ . It is known that if this minimum value is equal to 10, then every planar signed graph maps to a particular unique signed graph  $(G, \Sigma)$  which does not admit any homomorphism to any signed graph  $(H, \Pi)$  with |V(H)| < |V(G)|. In [66] we characterize all underlying absolute signed planar graph having underlying graphs obtained by (repeated, finite) k-clique sums  $(k \leq 3)$  of underlying absolute signed planar graph having to  $(P^+9, \Gamma^+)$ . Based on this evidence, we conjecture that every planar signed graph admits a homomorphism to  $(P + 9, \Gamma^+)$ .

#### 7.4.4. Edge-partitioning a graph into paths: the Barát-Thomassen conjecture

In 2006, Barát and Thomassen conjectured that there is a function f such that, for every fixed tree T with t edges, every f(t)-edge-connected graph with its number of edges divisible by t has a partition of its edges into copies of T. We recently proved this conjecture with Merker [69].

The path case of the Barát-Thomassen conjecture (i.e  $\forall k, m = |E| \mod k = 0$  there exists f(k) such that if the connectivity of G is larger than f(k) then G can be partitionned into  $P_k$ ) has also been studied, notably by Thomassen [80], [81], [82], and had been solved by Botler, Mota, Oshiro and Wakabayashi [70]. In [15] we propose an alternative proof of the path case with a weaker hypothesis: Namely, we prove that there is a function f such that every 24-edge-connected graph with minimum degree f(k) has an edge-partition into paths of length k. We also show that 24 can be dropped to 4 when the graph is Eulerian.

#### 7.4.5. Some Aspects of Arbitrarily Partitionable Graphs

An *n*-graph *G* is arbitrarily partitionable (AP) if, for every partition of *n* as  $n = n_1 + ... + n_p$ , there is a partition  $(V_1, ..., V_p)$  of V(G) such that for  $i = 1, ..., pG[V_i]$  is connected and  $|V_i| = n_i$ . The property of being AP is related to other well-known graph notions, such as perfect matchings and Hamiltonian cycles (obviously Hamiltonian graph is AP), with which it shares several properties. In [65] This work we studying two aspects of AP graphs.

On the one hand, we consider the algorithmic aspects. We first establish the *NP*-hardness of the problem of partitioning a graph into connected subgraphs following a given sequence, for various new graph classes of interest. We then prove that the problem of deciding whether a graph is AP is *NP*-hard for several classes of graphs, confirming a conjecture of Barth and Fournier.

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On the other hand, we consider the weakening of APness to sufficient conditions for Hamiltonicity. While previous works have suggested that such conditions can sometimes indeed be weakened, we point out cases for which this is not true. This is done by considering conditions for Hamiltonicity involving squares of graphs, and claw- and net-free graphs.

#### 7.4.6. Incident Sum problems and the 1-2-3 Conjecture

How can one distinguish the adjacent vertices of a graph through an edge-weighting? In the last decades, this question has been attracting increasing attention, which resulted in the active field of distinguishing labelings. One of its most popular problems is the one where neighbours must be distinguishable via their incident sums of weights. An edge-weighting verifying this is said to be *proper*. The popularity of this notion arises mainly due to the influence of the famous 1-2-3 Conjecture (posed by Karoński, Łuczak and Thomason), which claims that proper weightings with weights in  $\{1, 2, 3\}$  exist for graphs with no isolated edge.

The questions that we study aim at solving or at progressing toward the solution of the 1-2-3 conjecture and similar problems.

In [8] we study locally irregular decompositions of sub-cubic graphs. A graph G is locally irregular if every two adjacent vertices of G have different degrees (this corresponds to a uniform weight). A locally irregular decomposition of G is a partition  $E_1, \dots, E_k$  of the edge set E(G) such that each  $G[E_i]$  is locally irregular. Not all graphs admit locally irregular decompositions, but for those who are decomposable, it was conjectured by Baudon, Bensmail, Przybyło and Woźniak that the decomposition uses at most 3 locally irregular graphs. Towards that conjecture, it was recently proved by Bensmail, Merker and Thomassen that every decomposable graph decomposes into at most 328 locally irregular graphs. Our work focuses on the case of sub-cubic graphs, which form an important family of graphs in this context, as all non-decomposable graphs are sub-cubic. As a main result, we prove that decomposable sub-cubic graphs decompose into at most 5 locally irregular graphs, and at most 4 when the maximum average degree is less than  $\frac{12}{5}$ . We then consider weaker decomposition, where subgraphs can also include regular connected components, and prove the relaxations of the conjecture above for sub-cubic graphs.

In [9] we pursue recent works generalizing "Neighbour Sum problems" (e.g. the well-known 1-2-3 Conjecture, or the notion of locally irregular decomposition) to digraphs. We introduce and study several variants of the 1-2 Conjecture for digraphs and for every such variant, we state conjectures concerning the number of weights necessary to obtain a desired total-weighting in any digraph. We verify some of these conjectures, while we obtain close results towards the solution of the ones that are still open.

In [10] we study a variant of the classical 1-2-3 Conjecture. This conjecture asks whether every graph but  $K_2$  can be 3-edge-weighted so that every two adjacent vertices u and v can be distinguished via the sum of their incident weights, that is the incident sums of u and v differ by at least 1. In this work we investigate the consequences on the 1-2-3 Conjecture of requiring a stronger distinction condition, that is requiring the incident sums to differ by at least 2. Our conjecture is that every graph but  $K_2$  admits a 5-edge-weighting permitting to distinguish the adjacent vertices in this stronger way. We prove this conjecture for several classes of graphs, including bipartite graphs and cubic graphs. We then consider algorithmic aspects, and show that it is *NP*-complete to determine the smallest k such that a given bipartite graph admits such a k-edge-weighting. In contrast, we show that the same problem can be solved in polynomial time when the graph is a tree.

In [11] we prove a 1-2-3-4 result for the 1-2-3 Conjecture in 5-regular graphs. Currently the best-known result toward te 1-2-3 conjecture is due to Kalkowski, Karoński and Pfender, who proved that it holds when relaxed to 5-edge-weightings. Their proof builds upon a weighting algorithm designed by Kalkowski for a total version of the problem (.i.e in our context total means that both the vertices and the edges are assigned weights). Our work, present new mechanisms for using Kalkowski's algorithm in the context of the 1-2-3 Conjecture. As a main result we prove that every 5-regular graph admits a 4-edge-weighting that permits to distinguish adjacent vertices.

In [63] we investigate another aspect of edge weighting that allow to distinguish adjacent vertices (we shall call them *proper*). Namely we study the minimum number of distinct neighbourhood sums we can produce using such proper weightings. Clearly, this minimum number is bounded below by the chromatic number  $\chi(G)$ 

of G. When using weights in Z, we show that we can always produce proper edge-weightings generating  $\chi(G)$  distinct sums but in the peculiar case where G is a balanced bipartite graph, in which case exactly  $\chi(G) + 1$  distinct sums have to be generated. When using k consecutive weights 1, ..., k, we provide both lower and upper bounds, as a function of the maximum degree  $\Delta$ , on the maximum least number of sums that can be generated for a graph with maximum degree  $\Delta$ . For trees, which, in general, admit neighboursum-distinguishing 2-edge-weightings, we prove that this maximum, when using weights 1 and 2, is of order  $2 \log_2 \Delta$ . Finally, we also establish the NP-hardness of several decision problems related to these questions.

The 1-2-3 Conjecture has recently been investigated from a decompositional angle, via so-called locally irregular decompositions, which are edge-partitions into locally irregular subgraphs. Through several recent studies, it was shown that this concept is quite related to the 1-2-3 Conjecture. However, the full connection between all those concepts was not clear. In [55], we propose an approach that generalizes all concepts above, involving coloured weights and sums. As a consequence, we get another interpretation of several existing results related to the 1-2-3 Conjectures, to which we give some support.

#### 7.4.7. Identifying codes

For G a graph or a digraph, let id(G) be the minimum size of an identifying code of G if one exists, and  $id(G) = +\infty$  otherwise. For a graph G, let idor(G) be the minimum of id(D) overall orientations D of G. In [20], we give some lower and upper bounds on idor(G). In particular, we show that  $idor(G) \le 3/2id(G)$  for every graph G. We also show that computing idor(G) is NP-hard, while deciding whether  $idor(G) \le |V(G)| - k$  is polynomial-time solvable for every fixed integer k.

# 7.5. Digraph theory

Participants: Julien Bensmail, Frédéric Havet, Nicolas Nisse, William Lochet.

We are putting an effort on understanding better directed graphs (also called *digraphs*) and partitioning problems, and in particular colouring problems. We also try to better the understand the many relations between orientations and colourings. We study various substructures and partitions in (di)graphs. For each of them, we aim at giving sufficient conditions that guarantee its existence and at determining the complexity of finding it.

#### 7.5.1. Constrained ear decompositions in graphs and digraphs

Ear decompositions of graphs are a standard concept related to several major problems in graph theory like the Traveling Salesman Problem. For example, the Hamiltonian Cycle Problem, which is notoriously NPcomplete, is equivalent to deciding whether a given graph admits an ear decomposition in which all ears except one are trivial (i.e. of length 1). On the other hand, a famous result of Lovász states that deciding whether a graph admits an ear decomposition with all ears of odd length can be done in polynomial time. In [59], we study the complexity of deciding whether a graph admits an ear decomposition with prescribed ear lengths. We prove that deciding whether a graph admits an ear decomposition with all ears of length at most is polynomial-time solvable for all fixed positive integer. On the other hand, deciding whether a graph admits an ear decomposition without ears of length in F is NP-complete for any finite set F of positive integers. We also prove that, for any  $k \ge 2$ , deciding whether a graph admits an ear decomposition with all ears of length 0 mod k is NP-complete. We also consider the directed analogue to ear decomposition, which we call handle decomposition, and prove analogous results : deciding whether a digraph admits a handle decomposition with all handles of length at most is polynomial-time solvable for all positive integer; deciding whether a digraph admits a handle decomposition without handles of length in F is NP-complete for any finite set F of positive integers (and minimizing the number of handles of length in F is not approximable up to  $n(1-\varepsilon)$ ); for any k > 2, deciding whether a digraph admits a handle decomposition with all handles of length 0 mod k is NP-complete. Also, in contrast with the result of Lovász, we prove that deciding whether a digraph admits a handle decomposition with all handles of odd length is NP-complete. Finally, we conjecture that, for every set A of integers, deciding whether a digraph has a handle decomposition with all handles of length in A is NP-complete, unless there exists  $h \in \mathbf{N}$  such that  $A = \{1, \dots, h\}$ .

#### 7.5.2. Substructures in digraphs

We study substructures in digraphs. We study all kind of substructures: subdigraphs (induced or not), subdivision, immersion, minors, etc. We are both interested in the algorithmic point of view, that is determining the complexity of finding a (fixed or given) substructure in a given graph, and the structural point of view, that is finding sufficient conditions to guarantee the existence of a substructure.

In [32], we study the algorithmic complexity of the problem of deciding if a digraph contains a subdivision of a fixed digraph F. Up to 5 exceptions, we completely classify for which 4-vertex digraphs F, the F-subdivision problem is polynomial-time solvable and for which it is NP-complete. While all NP-hardness proofs are made by reduction from some version of the 2-linkage problem in digraphs, some of the polynomial-time solvable cases involve relatively complicated algorithms.

In [25], [22] we study conditions under which a digraph contain a subdivision of an oriented cycle. An oriented cycle is an orientation of a undirected cycle. We first show that for any oriented cycle C, there are digraphs containing no subdivision of C (as a subdigraph) and arbitrarily large chromatic number. In contrast, we show that for any C a cycle with two blocks, every strongly connected digraph with sufficiently large chromatic number contains a subdivision of C. We prove a similar result for the antidirected cycle on four vertices (in which two vertices have out-degree 2 and two vertices have in-degree 2). We study the existence of more general structures than cycles. A  $(k_1 + k_2)$ -bispindle is the union of  $k_1(x, y)$ -dipaths and  $k_2(y, x)$ dipaths, all these dipaths being pairwise internally disjoint. The above-mentioned results on cycle with two blocks [25] can be restated as follows: for every (1, 1)-bispindle B, there exists an integer k such that every strongly connected digraph with chromatic number greater than k contains a subdivision of B. In [21], we investigate generalizations of this result by first showing constructions of strongly connected digraphs with large chromatic number without any (3,0)-bispindle or (2,2)-bispindle. We then consider (2,1)-bispindles. Let  $B(k_1, k_2; k_3)$  denote the (2, 1)-bispindle formed by three internally disjoint dipaths between two vertices x, y, two (x, y)-dipaths, one of length  $k_1$  and the other of length  $k_2$ , and one (y, x)-dipath of length  $k_3$ . We conjecture that for any positive integers  $k_1$ ,  $k_2$ ,  $k_3$ , there is an integer  $g(k_1, k_2, k_3)$  such that every strongly connected digraph with chromatic number greater than  $g(k_1, k_2, k_3)$  contains a subdivision of  $B(k_1, k_2; k_3)$ . As evidence, we prove this conjecture for  $k_2 = 1$  (and  $k_1$ ,  $k_3$  arbitrary).

In [36], we prove the existence of a function h(k) such that every simple digraph with minimum outdegree greater than h(k) contains an immersion of the transitive tournament on k vertices. This solves a conjecture of Devos, McDonald, Mohar and Scheide [72].

In [3], we study  $\chi$ -bounded families of oriented graphs. A famous conjecture of Gyárfás and Sumner states for any tree T and integer k, if the chromatic number of a graph is large enough, either the graph contains a clique of size k or it contains T as an induced subgraph. We present some results and open problems about extensions of this conjecture to oriented graphs. In particular, we conjecture that for every oriented star S and integer k, if the chromatic number of a digraph is large enough, either the digraph contains a clique of size k or it contains S as an induced subgraph. As an evidence, we prove that for any oriented star S, every oriented graph with sufficiently large chromatic number contains either a transitive tournament of order 3 or S as an induced subdigraph. We then study for which sets  $\mathcal{P}$  of orientations of  $P_4$  (the path on four vertices) similar statements hold. We establish some positive and negative results.

#### 7.5.3. Partitions of digraphs

We also study partitions of digraphs. Again we are interested in the algorithmic point of view, that is determining the complexity of finding a partition satisfying some properties in a digraph, and the structural point of view, that is finding sufficient conditions to guarantee the existence of such a partition.

For a given 2-partition  $(V_1, V_2)$  of the vertices of a (di)graph G, we study in [7] properties of the spanning bipartite subdigraph  $B_G(V_1, V_2)$  of G induced by those arcs/edges that have one end in each  $V_i$ ,  $i \in \{1, 2\}$ . We determine, for all pairs of non-negative integers  $k_1, k_2$ , the complexity of deciding whether G has a 2-partition  $(V_1, V_2)$  such that each vertex in  $V_i$  (for  $i \in \{1, 2\}$ ) has at least  $k_i$  (out-)neighbours in  $V_{3-i}$ . We prove that it is NP-complete to decide whether a digraph D has a 2-partition  $(V_1, V_2)$  such that each vertex in  $V_1$  has an outneighbour in  $V_2$  and each vertex in  $V_2$  has an in-neighbour in  $V_1$ . The problem becomes polynomially solvable if we require D to be strongly connected. We give a characterization of the structure of NP-complete instances in terms of their strong component digraph. When we want higher in-degree or out-degree to/from the other set the problem becomes NP-complete even for strong digraphs. A further result is that it is NP-complete to decide whether a given digraph D has a 2-partition  $(V_1, V_2)$  such that  $B_D(V_1, V_2)$  is strongly connected. This holds even if we require the input to be a highly connected Eulerian digraph.

The dichromatic number  $\vec{\chi}(D)$  of a digraph D is the least number k such that the vertex set of D can be partitioned into k parts each of which induces an acyclic subdigraph. Introduced by Neumann-Lara in 1982, this digraph invariant shares many properties with the usual chromatic number of graphs and can be seen as the natural analog of the graph chromatic number. In [14], we study the list dichromatic number of digraphs, giving evidence that this notion generalizes the list chromatic number of graphs. We first prove that the list dichromatic number and the dichromatic number behave the same in many contexts, such as in small digraphs (by proving a directed version of Ohba's Conjecture), tournaments, and random digraphs. We finally give a Brooks-type upper bound on the list dichromatic number of digraphs.

# **DIANA Project-Team**

# 6. New Results

#### **6.1. Service Transparency**

#### 6.1.1. An Intelligent Sampling Framework for Controlled Experimentation and QoE Modeling

Participants: Muhammad Jawad Khokhar, Nawfal Abbasi Saber, Thierry Spetebroot, Chadi Barakat.

For internet applications, measuring, modeling and predicting the quality experienced by end users as a function of network conditions is challenging. A common approach for building application specific Quality of Experience (QoE) models is to rely on controlled experimentation. For accurate QoE modeling, this approach can result in a large number of experiments to carry out because of the multiplicity of the network features, their large span (e.g., bandwidth, delay) and the time needed to setup the experiments themselves. However, most often, the space of network features in which experimentations are carried out shows a high degree of similarity in the training labels of QoE. This similarity, difficult to predict beforehand, amplifies the training cost with little or no improvement in QoE modeling accuracy. So, in this work, funded by ANR BottleNet and IPL BetterNet, we aim to exploit this similarity, and propose a methodology based on active learning, to sample the experimental space intelligently, so that the training cost of experimentation is reduced. We validate our approach for the case of YouTube video streaming QoE modeling from out-of-band network performance measurements, and perform a rigorous analysis of our approach to quantify the gain of active sampling over uniform sampling. We first develop the methodology for an offline case where a pool of scenarios to experiment with is available. Then, we present an online variant that does not require a pool of scenarios, but finds automatically and in an online manner the best scenarios to experiment with. This latter variant outperforms the offline variant both in terms of accuracy and computation complexity. It is published in [22]. The overall methodology and its specification to both the offline and the online cases are published in [15].

# 6.1.2. A Methodology for Performance Benchmarking of Mobile Networks for Internet Video Streaming

Participants: Muhammad Khokhar, Thierry Spetebroot, Chadi Barakat.

Video streaming is a dominant contributor to the global Internet traffic. Consequently, gauging network performance w.r.t. the video Quality of Experience (QoE) is of paramount importance to both telecom operators and regulators. Modern video streaming systems, e.g. YouTube, have huge catalogs of billions of different videos that vary significantly in content type. Owing to this difference, the QoE of different videos as perceived by end users can vary for the same network Quality of Service (QoS). In this work, funded by ANR BottleNet and IPL BetterNet, we present a methodology for benchmarking performance of mobile operators w.r.t Internet video that considers this variation in QoE. We take a data-driven approach to build a predictive model using supervised machine learning (ML) that takes into account a wide range of videos and network conditions. To that end, we first build and analyze a large catalog of YouTube videos. We then propose and demonstrate a framework of controlled experimentation based on active learning to build the training data for the targeted ML model. Using this model, we then devise YouScore, an estimate of the percentage of YouTube videos that may play out smoothly under a given network condition. Finally, to demonstrate the benchmarking utility of YouScore, we apply it on an open dataset of real user mobile network measurements to compare performance of mobile operators for video streaming. This work is published in [21] and its extension to more sophisticated QoE models that consider other factors than interruptions is ongoing.

#### 6.1.3. On the Cost of Measuring Traffic in a Virtualized Environment

Participants: Karyna Gogunska, Chadi Barakat.

The current trend in application development and deployment is to package applications and services within containers or virtual machines. This results in a blend of virtual and physical resources with complex network interconnection schemas mixing virtual and physical switches along with specific protocols to build virtual networks spanning over several servers. While the complexity of this setup is hidden by private/public cloud management solutions, e.g. OpenStack, this new environment constitutes a challenge when it comes to monitor and debug performance related issues. In this work carried out in collaboration with the Signet team of I3S with the support of the UCN@Sophia Labex, we introduce the problem of measuring traffic in a virtualized environment and focus on one typical scenario, namely virtual machines interconnected with a virtual switch. For this scenario, we assess the cost of continuously measuring the network traffic activity of the machines. Specifically, we seek to estimate the competition that exists to access the physical resources (e.g., CPU) of the physical server between the measurement task and the legacy application activity. This work was published in the IEEE Cloudnet 2018 conference [20] where it was awarded the Best Student Award. The collaboration with I3S is pursued towards a controlled configuration and deployment of measurements tools in a way to limit their impact on the legacy data plane of virtualized environments.

#### 6.1.4. ElectroSmart

Participants: Arnaud Legout, Mondi Ravi, David Migliacci, Abdelhakim Akodadi, Yanis Boussad.

We are currently evaluating the relevance to create a startup for the ElectroSmart project. We are quite advanced in the process and the planned creation is June 2019. There is a "contrat de transfer" ready between Inria and ElectroSmart to transfer the PI from Inria to the ElectroSmart company (when it will be created). Arnaud Legout the future CEO of the company obtained the "autorisation de création d'entreprise" from Inria. ElectroSmart has been incubated in PACA Est in December 2018.

The three future co-founder of ElectroSmart (Arnaud Legout, Mondi Ravi, David Migliacci) are following the Digital Startup training from Inria/EM Lyon. This training helped formalize and improve the product market fit and the business model. We are also preparing the iLab competition.

The business model of ElectroSmart is to create an affiliation strategy to help companies selling product to reduce EMF exposure to find potential clients. Indeed, ElectroSmart users represent a highly qualified database of people concerned by EMF exposure. This database is invaluable to these companies as it is an emerging market and it is hard for these companies to make efficient marketing campaigns. The benefit for the ElectroSmart users is to have access to negotiated and validated solutions to reduce their EMF exposure. We are currently validating this market. We started our first affiliation campaign in December 2018 with the Spartan company that sells radiation blocking boxers. We already have two more planned campaigns in 2019, with a goal of 5 campaigns in 2019.

# 6.2. Open Network Architecture

#### 6.2.1. Controller load in SDN networks

#### Participant: Damien Saucez.

In OpenFlow, a centralized programmable controller installs forwarding rules into switches to implement policies. However, this flexibility comes at the expense of extra overhead in signalling and number of rules to install. The community considered that it was essential to install all rules and strictly respect routing requirements, hence working on making extra fast and large memory switches and controllers. Instead we took an opposite direction and came with a new vision that leverages the SDN concept and considers the network as a black box where tailored rules should be used only for network traffic that really matters while for the rest a good-enough (sub-optimal but cheap) default behaviour should be enough. In the past, we applied this vision to limit the needed memory on network switches in [7]. Lately, we proposed solutions to limit the number of exchanged messages between the switches and the controller. More precisely, in [19], we developed a distributed sampling adaptive algorithm that allows switches to locally decide if they can contact the controller or if instead they should make their own decision locally. Numerical evaluation and emulation in Mininet demonstrate the benefit of the approach. The results were published in IEEE INFOCOM 2018, April 2018.

#### 6.2.2. Resilient Service Function Chains in virtual networks

Participants: Ghada Moualla, Damien Saucez, Thierry Turletti.

Virtualization of network functions has led to the whole new concept of Service Function Chaining (SFC) that aims at building on the fly network services by deploying them in the Cloud. A vast literature proposes techniques to build virtual service chains and map them into physical infrastructure to maximize performance while reducing costs. However, the resiliency of chains is not investigated. However, such service chains are used for critical services like e-health or autonomous transportation systems and thus require high availability. Respecting some availability level is hard in general, but it becomes even harder if the operator of the service is not aware of the physical infrastructure that will support the service, which is the case when SFCs are deployed in multi-tenant data centers. With this work, we propose algorithms to solve the placement of topology-oblivious SFC demands such that placed SFCs respect availability constraints imposed by the tenant. In order to be practically usable, i.e., without knowledge on future demands, we leverage the structural properties of multi-tier data-center topologies such as Fat-Tree or Sine and Leaf topologies to build fast yet efficient online algorithms. We explored two radically different approaches: a deterministic one and a stochastic one and results show that both can be used in very large scale data-centers (i.e., 40k nodes or more) and our simulation results show that the algorithms are able to satisfy as many demands as possible by spreading the load between the replicas and enhancing the network resources utilization [23].

Initial results were published in IEEE International Conference on Cloud Networking 2018, October 2018.

#### 6.2.3. Privacy preserving distributed services

Participants: Damien Saucez, Yevhenii Semenko, Alberto Zirondelli.

Blockchains are expected to help in reducing dependency on centralized platforms (e.g., Uber, Airbnb). With this internship, we have designed a protocol to make a fully distributed, secured, and privacy protecting taxi service – a distributed version of Uber. The analytical study shows that in such system the privacy protection comes with an important overhead in network communications which raises reasonable doubt on the feasibility of actually using fully distributed platforms in an "internet-scale environment" even though our implementation on Android phones shows that it is technically possible to build such systems. This work is done in collaboration with the GREDEG  $^{0}$ , that is evaluating the incentives for users to move to fully distributed platforms that are privacy preserving but that require the users to play an active role in the system.

#### 6.2.4. P4Bricks: Enabling multiprocessing using Linker-based network data plane architecture

Participants: Hardik Soni, Thierry Turletti, Walid Dabbous.

Packet-level programming languages such as P4 usually require to describe all packet processing functionalities for a given programmable network device within a single program. However, this approach monopolizes the device by a single large network application program, which prevents possible addition of new functionalities by other independently written network applications. We propose P4Bricks, a system which aims to deploy and execute multiple independently developed and compiled P4 programs on the same reconfigurable hardware device. P4Bricks is based on a Linker component that merges the programmable parsers/deparsers and restructures the logical pipeline of P4 programs by refactoring, decomposing and scheduling the pipelines' tables. It merges P4 programs according to packet processing semantics (parallel or sequential) specified by the network operator and runs the programs on the stages of the same hardware pipeline, thereby enabling multiprocessing. We present the initial design of our system with an ongoing implementation and study P4 language's fundamental constructs facilitating merging of independently written programs [34], [12].

#### 6.2.5. Applications in ITS Message Dissemination

#### Participants: Thierry Turletti.

<sup>&</sup>lt;sup>0</sup>Groupe de Recherche en Droit, Economie, Gestion, a research center related to both the CNRS and the University of Nice-Sophia Antipolis and dealing with economic, managerial and legal aspects. See http://unice.fr/laboratoires/gredeg in French.

We build upon our prior work on D2-ITS, a flexible and extensible framework to dynamically distribute network control to enable message dissemination in Intelligent Transport Systems (ITS), and extend it with handover and load balancing capabilities. More specifically, D2-ITS' new handover feature allows a controller to automatically "delegate" control of a vehicle to another controller as the vehicle moves. Control delegation can also be used as a way to balance load among controllers and ensure that required application quality of service is maintained. We showcase D2-ITS' handover and load-balancing features using the Mininet-Wifi network simulator/emulator. Our preliminary experiments show D2-ITS' ability to seamlessly handover control of vehicles as they move. This work has been presented at the 27th International Conference on Computer Communications and Networks (ICCCN 2018), Jul 2018, Hangzhou, China [17].

#### 6.2.6. Low Cost Video Streaming through Mobile Edge Caching: Modelling and Optimization

#### Participants: Luigi Vigneri, Chadi Barakat.

Caching content at the edge of mobile networks is considered as a promising way to deal with the data tsunami. In addition to caching at fixed base stations or user devices, it has been recently proposed that an architecture with public or private transportation acting as mobile relays and caches might be a promising middle ground. While such mobile caches have mostly been considered in the context of delay tolerant networks, in this work done in collaboration with Eurecom with the support of the UCN@Sophia Labex, we argue that they could be used for low cost video streaming without the need to impose any delay on the user. Users can prefetch video chunks into their playout buffer from encountered vehicle caches (at low cost) or stream from the cellular infrastructure (at higher cost) when their playout buffer empties while watching the content. Our main contributions are: (i) to model the playout buffer in the user device and analyze its idle periods which correspond to bytes downloaded from the infrastructure; (ii) to optimize the content allocation to mobile caches, to minimize the expected number of non-offloaded bytes. We perform trace-based simulations to support our findings showing that up to 60 percent of the original traffic could be offloaded from the main infrastructure. These contributions were published in IEEE Transactions on Mobile Computing [16]. The part specifying the framework to a chunk-based scenario by accounting for partial storage of videos in vehicles was published in [25].

#### 6.2.7. Cost Optimization of Cloud-RAN Planning and Provisioning for 5G Networks

#### Participants: Osama Arouk, Thierry Turletti.

We propose a network planning and provisioning framework that optimizes the deployment cost in C-RAN based 5G networks. Our framework is based on a Mixed Integer Quadratically Constrained Programming (MIQCP) model that optimizes "virtualized" 5G service chain deployment cost while performing adequate provisioning to address user demand and performance requirements. We use two realistic scenarios to showcase that our framework can be applied to different types of deployments and discuss the computational cost and scalability of our solution. This work has been presented at the IEEE International Conference on Communications, in May 2018, at Kansas City, MO, United States [18].

#### 6.2.8. Slice Orchestration for Multi-Service Disaggregated Ultra Dense RANs

#### Participants: Osama Arouk, Thierry Turletti.

Ultra Dense Networks (UDNs) are a natural deployment evolution for handling the tremendous traffic increase related to the emerging 5G services, especially in urban environments. However, the associated infrastructure cost may become prohibitive. The evolving paradigm of network slicing can tackle such a challenge while optimizing the network resource usage, enabling multi-tenancy and facilitating resource sharing and efficient service-oriented communications. Indeed, network slicing in UDN deployments can offer the desired degree of customization in both vanilla Radio Access Network (RAN) designs, but also in the case of disaggregated multi-service RANs. We propose a novel multi-service RAN environment, i.e., RAN runtime, capable to support slice orchestration procedures and to enable flexible customization of slices as per tenant needs. Each network slice can exploit a number of services, which can either be dedicated or shared between multiple slices over a common RAN. The novel architecture we present concentrates on the orchestration and management systems. It interacts with the RAN modules, through the RAN runtime, via a number of new interfaces

enabling a customized dedicated orchestration logic for each slice. We present results for a disaggregated UDN deployment where the RAN runtime is used to support slice-based multi-service chain creation and chain placement, with an auto-scaling mechanism to increase the performance. This work has been published in IEEE Communications Magazine [13].

# **6.3. Experimental Evaluation**

#### 6.3.1. nepi-ng: an efficient experiment control tool in R2lab

Participants: Thierry Parmentelat, Thierry Turletti, Walid Dabbous, Mohamed Naoufal Mahfoudi.

Experimentation is an essential step for realistic evaluation of wireless network protocols. The evaluation methodology entails controllable environment conditions and a rigorous and efficient experiment control and orchestration for a variety of scenarios. Existing experiment control tools such as OMF often lack in efficiency in terms of resource management and rely on abstractions that hide the details about the wireless setup. We propose nepi-ng, an efficient experiment control tool that leverages job oriented programming model and efficient single-thread execution of parallel programs using asyncio. nepi-ng provides an efficient and modular fine grain synchronization mechanism for networking experiments with light software dependency footprint. This work has been presented at the 12th ACM International Workshop on Wireless Network Testbeds, Experimental evaluation & CHaracterization (WINTECH) in November 2018 at New Delhi, India [24].

#### 6.3.2. Using nepi-ng for Mesh Networks Experiments

Participants: Thierry Parmentelat, Thierry Turletti, Mohamed Naoufal Mahfoudi, Walid Dabbous.

We describe a demonstration run on R2lab, an open wireless testbed located in an anechoic chamber at Inria Sophia Antipolis. The demonstration consists in easily deploying a Wi-Fi mesh network. The nodes provisioning, configuration and the scenario orchestration and control are automatically done using the neping experiment orchestration tool. A performance comparison of two wireless mesh routing protocols in presence of controlled interference is shown. This demo has been presented at the 12th ACM International Workshop on Wireless Network Testbeds, Experimental evaluation & CHaracterization (WINTECH) in November 2018 at New Delhi, India [32].

#### 6.3.3. R2Lab Testbed Evaluation for Wireless Mesh Network Experiments

Participants: Farzaneh Pakzad, Thierry Turletti, Thierry Parmentelat Mohamed Naoufal Mahfoudi, Walid Dabbous.

We have provided critical evaluations of new potential testbeds for the evaluation of SDN-based WMNs. We evaluated the R2Lab wireless testbed platform at Inria Sophia Antipolis, France. This testbed has 37 customisable wireless devices in an anechoic chamber for reproducible research in wireless WiFi and 4G/5G networks. Our work presents the first initial evaluation of the testbed for wireless multi-hop experiments, using traditional WMN routing protocols. Our results demonstrate the potential for SDN experiments. We believe this is an important contribution in its own right, since experimental validation is a key research methodology in this context, and trust in the validity of experimental results is absolutely critical.

# **FOCUS Project-Team**

# 6. New Results

# 6.1. Service-Oriented Computing

**Participants:** Mario Bravetti, Maurizio Gabbrielli, Saverio Giallorenzo, Claudio Guidi, Ivan Lanese, Cosimo Laneve, Fabrizio Montesi, Davide Sangiorgi, Gianluigi Zavattaro, Stefano Pio Zingaro.

#### 6.1.1. Orchestrations and choreographies

The practice of programming distributed systems is extremely error-prone, due to the complexity in correctly implementing separate components that, put together, enact an agreed protocol. Usage of contracts and session types in orchestration languages guarantees correct communication [22]. Asynchronous subtyping for binary session types has been thought to be decidable for 8 years, before we proved in previous work it to be undecidable. We have now highlighted some practically-relevant fragments of session types where asynchronous subtyping is indeed decidable [14].

We also studied practical aspects of choreographies, that is multiparty contracts. On the one hand we extended the classical proof of correctness of the projection of a choreography on one participant, which is the cornerstone of the theory of choreographies. Indeed, the classical proof considers projection to a model based on channels in the CCS style, while practice mainly relies on correlation sets. We bridged this gap by giving a correctness proof towards a real-world execution model based on correlation sets [31].

We then studied how to apply choreographies for cross-organizational system integration. More precisely, we proposed a software development process to build integrations composed by distributed, independent connectors whose global behaviour is correct by construction [30]. Choreographies and choreography projection are at the heart of the proposed development process.

#### 6.1.2. Microservices

We continued the study of microservice-oriented computing started in past years, in particular by using our microservice-oriented language Jolie. We focused, in particular, on the use of Jolie in an Internet of Things (IoT) setting [28]. Technically, a key feature of Jolie is that it supports in a uniform way multiple service-oriented communication protocols such as HTTP and SOAP. We extended Jolie in order to support, uniformly as well, also lightweight protocols such as MQTT and CoAP, which are largely used in IoT. These are very different from service-oriented protocols which are point-to-point and based on TCP since MQTT is publish-subscribe while CoAP is based on UDP.

#### 6.2. Models for Reliability

Participant: Ivan Lanese.

#### 6.2.1. Reversibility

We have continued the study of reversibility started in the past years, concentrating on contracts and debugging, and applying the results related to debugging to the Erlang programming language. Concerning contracts, in [12] we further studied the retractable contracts that we defined in previous work. The main novelty consists in showing how retractable contracts can be obtained by taking standard contracts, making them reversible using the general approach presented by Phillips and Ulidowski [44], and then applying suitable control policies.

Concerning debugging, we highlighted in [18] the general approach that can be used to build a causalconsistent reversible debugger for a given language. We then instantiated this general approach to a relevant subset of the language Erlang, first defining uncontrolled and controlled reversible semantics for it [16], and then building an actual causal-consistent reversible debugger called CauDEr [32].

# 6.3. Probabilistic Systems and Resource Control

**Participants:** Martin Avanzini, Mario Bravetti, Raphaelle Crubillé, Ugo Dal Lago, Francesco Gavazzo, Davide Sangiorgi, Gabriele Vanoni, Akira Yoshimizu.

#### 6.3.1. Probabilistic Rewriting and Computation

In Focus, we are interested in studying probabilistic higher-order programming languages and, more generally, the fundamental properties of probabilistic computation when placed in an interactive scenario, for instance concurrency. One of the most basic but nevertheless desirable properties of programs is of course termination. Termination can be seen as a minimal guarantee about the time complexity of the underlying program. When probabilistic choice comes into play, termination can be defined by stipulating that a program is terminating if its probability of convergence is 1, this way giving rise to the notion of *almost sure termination*. Alternatively, a probabilistic program is said to be *positively* almost surely terminating if its average runtime is finite. The latter condition easily implies the former. Termination, already undecidable for deterministic (universal) programming languages, remains so in the presence of probabilistic choice, even becoming provably harder.

The Focus team has been the first in advocating the use of types to guarantee probabilistic termination, in the form of a sized-type system. In 2018, Focus has produced another work along these lines, based on intersection types [23]. In the usual, pure, lambda-calculus, various notions of terminating terms can be characterised by way of intersection types, in such a way that the class of terminating terms *coincides* with the one of typable terms. The presence of probabilistic choices together with the aforementioned recursion theoretical limitations prevents the same scenario to happen in probabilistic lambda-calculi, i.e., lambda-calculi endowed with some form of probabilistic choice. Nevertheless, Breuvart and Dal Lago proved that capturing the probability of termination in an approximate way by means of intersection types is indeed possible [23].

In 2018, we have also been active in laying out a novel foundation for *probabilistic abstract reduction systems* (*probabilistic ARSs*). ARSs constitute a general framework to study fundamental properties of computations, such as termination or confluence. These properties are intricately related to the well-definedness of functions, and consequently, play key roles in the formal study of programming languages. Specifically, in collaboration with Yamada, Avanzini and Dal Lago [20] introduced a new notion of probabilistic computation by means of a reduction relation over multidistributions. This relation enables the seamless combination of non-deterministic and probabilistic choice, thereby, considerably simplifying earlier notions of reduction semantics by means of schedulers and Markov chains. On top of this, a partially flawed characterisation of positive almost sure termination by means of Lyapunov ranking functions, initially due to Bournez and Garnier, could be clarified. Moreover, the *interpretation method*, which is maybe the most fundamental technique to investigate termination and runtime complexity of term rewrite systems, could be lifted to probabilistic systems.

Finally, we have been able to propose a novel and natural way of giving the reduction semantics for Markovian process algebras [13], a model of concurrent interaction which is particularly appropriate to the performance analysis of concurrent systems.

#### 6.3.2. Complexity Analysis of Functional Programs

A research topic which lies at the core of Focus since its inception is the complexity analysis of functional programs, through tools like implicit complexity and linear logic. During 2018, we have published an extended version of a paper in which we proved that the most general form of ramified recursion, a key tool in term rewriting, remains sound for polynomial time computation, although requiring some nontrivial machinery based on sharing and memoisation [11]. We have also started to investigate along a new and promising research direction concerning the efficient implementation of functional programming languages through randomised strategies. We have shown that even the simplest strategy is nontrivial for the pure, untyped lambda-calculus [25], being in certain cases more efficient than both innermost and outermost strategies.

#### 6.3.3. Reasoning About Effectful and Concurrent Programs

Pure functional programs are relatively easy to reason about due to referential transparency, a property inherent to functional programs that renders their semantics close to the one of mathematical expressions.

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Quite recently, functional programming has found its way into main stream programming languages. Thus functional programming is *combined* with various forms of computational effects, such as exceptions, state, or even nondeterministic choice. Since a couple of years, we are interested in studying the impact of effects on the metatheory of functional programming languages, with an eye to coinductive methodologies akin to those employed in concurrency, coinduction *in primis*. In 2018, Francesco Gavazzo has extended some of our previous work about a generic approach to behavioural equivalences for higher-order effectual languages to *metrics*, themselves a much more natural way to compare programs in many cases (e.g., in the presence of probabilistic choice). His contribution has been published in the top conference in logic in computer science in 2018 [29].

# 6.4. Verification Techniques

Participants: Mario Bravetti, Adrien Durier, Daniel Hirschkoff, Ivan Lanese, Cosimo Laneve, Davide Sangiorgi.

We analyze sensible properties of concurrent systems such as deadlock freedom, and proof techniques for deriving behavioural equalities and preorders on processes.

#### 6.4.1. Deadlock detection

We have continued the work on deadlock detection of previous years, on languages of concurrent objects. Thus in [33] we have applied and refined previous techniques so to handle multi-threaded programs with reentrant locks. For this we have defined a simple calculus featuring recursion, threads and synchronizations that guarantee exclusive access to objects. We detect deadlocks by associating an abstract model to programs and we define an algorithm for verifying that a problematic object dependency (e.g. a circularity) between threads will not be manifested.

In [15] we give two different notions of deadlock for systems based on active objects and futures. One is based on blocked objects and conforms with the classical definition of deadlock. The other one is an extended notion of deadlock based on blocked processes which is more general than the classical one. We introduce a technique to prove deadlock freedom in which an abstract version of the program is translated into Petri nets. Extended deadlocks, and then also classical deadlock, can be detected via checking reachability of a certain forms of marking.

#### 6.4.2. Proof techniques based on unique solutions

We study bisimilarity, a behavioural equivalence whose success is much due to the associated bisimulation proof method. In particular, we discuss different proof methods, based on unique solution of equations or of special forms of inequations called contractions, and inspired by Milner's theorem on unique solution of equations. The techniques are at least as powerful as the bisimulation proof method and its up-to context enhancements. The techniques can be transferred onto other behavioural equivalences, possibly contextual and non-coinductive. This enables a coinductive reasoning style on such equivalences. An overview paper on these techniques is [19].

The paper [36] discusses a rather comprehensive formalisation of the core of the theory of CCS in the HOL theorem prover (HOL4), with a focus towards the theory of unique solutions of contractions. (The formalisation consists of about 20,000 lines of proof scripts in Standard ML.) Some refinements of the theory itself are obtained. In particular we remove the constraints on summation, which must be weakly-guarded, by moving to rooted contraction, that is, the coarsest precongruence contained in the contraction preorder.

In [26] we apply the above techniques to study Milner's encoding of the call-by-value  $\lambda$ -calculus into the  $\pi$ -calculus. We show that, by tuning the encoding to two subcalculi of the  $\pi$ -calculus (Internal  $\pi$  and Asynchronous Local  $\pi$ ), the equivalence on  $\lambda$ -terms induced by the encoding coincides with Lassen's eager normal-form bisimilarity, extended to handle  $\eta$ -equality. As behavioural equivalence in the  $\pi$ -calculus we consider contextual equivalence and barbed congruence. We also extend the results to preorders.

On a different, but related, strand of work [17], we study the tree structures that result when writing callby-name functions as processes, and give general conditions under which this representation produces Lévy-Longo Trees and Böhm Trees, the best known tree structures on the lambda-calculus.

# 6.5. Computer Science Education

Participants: Michael Lodi, Simone Martini.

We study why and how to teach computer science principles (nowadays often referred to as "computational thinking", CT), in particular in the context of K-12 education (students aged approximately from 5 to 18). We study philosophical, sociological and historical motivations to teach computer science at all school levels. Furthermore, we study what concepts and skills related to computer science are not barely technical abilities, but have a general value for all students. Finally, we try to find/produce/evaluate suitable materials (tools, languages, lesson plans...) to teach these concepts, taking into account: difficulties in learning CS concepts (particularly programming); stereotypes about computer science (particularly gender-related issues); teacher training (particularly non-specialist teachers).

#### 6.5.1. Computational thinking and constructionism

In the last ten years, the expression "computational thinking" has been used to talk about the introduction of CS in K-12 education. The expression was originally used in the 1980s by Seymour Papert, a pioneer in Math education using programming (he is the principal inventor of the LOGO programming language). We analysed [37] the original context in which the expression originated: the constructionist learning theory, that promotes an active way of learning by constructing meaningful computational artifacts. Papert aimed to teach Math and Physics, but we think CS too is a breeding ground for applying constructionist practices like creative learning, iterative and incremental development, learning by doing, learning by trial and error, project-based learning [35].

# 6.5.2. CS in the school curriculum

As there is no established practice in teaching CS, academics should facilitate the introduction of CS principles in the school curriculum, to avoid misconceptions and to focus mainly on scientific principles, rather than on technical aspects. Within a CINI (Italian National Interuniversity Consortium for Informatics) group, we designed a proposal [27] for CS teaching in Italian K-10 schools, that focuses on CS principles, and gives space to the use of digital technologies only as tools for self-expression through computation. When introducing a new discipline, often misconceptions arise. In a large sample of primary teachers, we investigate [38], [24] the ideas about the "buzzword" *coding*, that is more and more used to talk about CS at school. Only 60% of teachers correctly linked "coding" to "programming" (some of them implicitly), and many misconceptions (e.g. "coding is only for children", or "coding is the transversal use of computational thinking at school", "programming is only for professionals") were found. After defining a curriculum, one should also provide some materials to concretely teach the discipline and ensure learning objectives will be achieved. We presented [21] the structure of a nationwide initiative by the Italian Ministry of Education: Problem Solving Olympics (OPS). Preliminary analysis of students' results in the last five editions suggests the competition fosters learning of computational thinking knowledge and skills.

#### 6.5.3. Growth mindset and teacher training

Every person holds an idea (mindset) about intelligence: someone thinks it is a fixed trait, like eye colour (fixed mindset), while others believe it can grow like muscles (growth mindset). The latter is beneficial for students to have better results, particularly in STEM disciplines, and to not being influenced by stereotypes. Computer science is a subject that can be affected by fixed ideas ("geek gene"), and some (small) studies showed it can induce fixed ideas. Teachers' mindset directly affects students' one. By contrast, applying constructionists approaches seems to foster a growth mindset. In facts, we found a statistically significative, albeit little, increase of pre-service primary teacher's growth mindset after a "creative computing and computational thinking" course [34].

# 6.6. Constraint Programming

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Participants: Maurizio Gabbrielli, Liu Tong.

In Focus, we sometimes make use of constraint solvers (e.g., cloud computing, service-oriented computing). Since a few years we have thus began to develop tools based on constraints and constraint solvers.

In this area a *portfolio solver* combines a variety of different constraint solvers for solving a given problem. This fairly recent approach enables to significantly boost the performance of single solvers, especially when multicore architectures are exploited. In [10] we give a brief overview of the portfolio solver sunny-cp, and we discuss its performance in the MiniZinc Challenge —the annual international competition for CP solvers —where it won two gold medals in 2015 and 2016.

# **INDES Project-Team**

# 5. New Results

# 5.1. Information Flow Security

We have pursued our study on information flow security policies and enforcements. We have followed two main axes.

**Impossibility of Precise and Sound Termination Sensitive Security Enforcements** An information flow policy is termination sensitive if it imposes that the termination behavior of programs is not influenced by confidential input. Termination sensitivity can be statically or dynamically enforced. On one hand, existing static enforcement mechanisms for termination sensitive policies are typically quite conservative and impose strong constraints on programs like absence of while loops whose guard depends on confidential information. On the other hand, dynamic mechanisms can enforce termination sensitive policies in a less conservative way. Secure Multi-Execution (SME), one of such mechanisms, was even claimed to be sound and precise in the sense that the enforcement mechanism will not modify the observable behavior of programs that comply with the termination sensitive policy. However, termination sensitivity is a subtle policy, that has been formalized in different ways. A key aspect is whether the policy talks about actual termination, or observable termination.

We have proved that termination sensitive policies that talk about actual termination are not enforceable in a sound and precise way. For static enforcements, the result follows directly from a reduction of the decidability of the problem to the halting problem. However, for dynamic mechanisms the insight is more involved and requires a diagonalization argument.

In particular, our result contradicts the claim made about SME. We correct these claims by showing that SME enforces a subtly different policy that we call indirect termination sensitive noninterference and that talks about observable termination instead of actual termination. We construct a variant of SME that is sound and precise for indirect termination sensitive noninterference. Finally, we also show that static methods can be adapted to enforce indirect termination sensitive information flow policies (but obviously not precisely) by constructing a sound type system for an indirect termination sensitive policy.

This study is described in [16].

#### A Better Facet of Dynamic Information Flow Control

Multiple Facets (MF) is a dynamic enforcement mechanism which has proved to be a good fit for implementing information flow security for JavaScript. It relies on multi executing the program, once per each security level or view, to achieve soundness. By looking inside programs, MF encodes the views to reduce the number of needed multi-executions.

In this year, we have published a paper [15], where we have extended Multiple Facets in three directions. First, we propose a new version of MF for arbitrary lattices, called Generalised Multiple Facets, or GMF. GMF strictly generalizes MF, which was originally proposed for a specific lattice of principals. Second, we propose a new optimization on top of GMF that further reduces the number of executions. Third, we strengthen the security guarantees provided by Multiple Facets by proposing a termination sensitive version that eliminates covert channels due to termination.

# 5.2. JavaScript Implementation

We have pursued the development of Hop.js and our study on efficient JavaScript implementation. We have followed three main axes.

#### Implementing Hop.js

Hop.js supports full ECMAScript 5 but it still lack many of the new features ECMAScript 2016 has introduced and now that are now well established in ECMAScript 2017. During the year, we have implemented many of these features (iterators, destructuring assignments, modules, etc.). Few constructs remain missing and hopefully will be added to the system by the end of the year (map, set, and proxies). Completing full ECMAScript 2017 is important as we now see more and more packages using these new features being made available and we consider that maintaining the ability to use all these publicly available resources is a prerequisite to a wide Hop.js adoption. We also consider that this is an important asset for Hop.js users, in particular, for the Denimbo company, an Inria startup using Hop.js extensively.

#### Ahead-of-time JavaScript compilation

Hop.js differs from most JavaScript implementations by many aspects because contrary to all fast and popular JavaScript engines that use just-in-time compilation, Hop.js relies on static compilation, *a.k.a.*, ahead-of-time (AOT) compilation. It is an alternative approach that can combine good speed and lightweight memory footprint, and that can accommodate read-only memory constraints that are imposed by some devices and some operating systems. Unfortunately the highly dynamic nature of JavaScript makes it hard to compile statically and all existing AOT compilers have either gave up on good performance or full language support.

Indeed, JavaScript is hard to compile, much harder than languages like C, Java, and even harder than Scheme and ML two other close functional languages. This is because a JavaScript source code accepts many more possible interpretations than other languages do. It forces JavaScript compilers to adopt a defensive position by generating target codes that can cope with all the possible, even unlikely, interpretations because general compilers can assume very little about JavaScript programs. The situation is worsened further by the *raise as little errors as possible* principle that drives the design of the language. JavaScript functions are not required to be called with the declared number of arguments, fetching an unbound property is permitted, assigning undeclared variables is possible, etc.

All these difficulties are considered serious enough to prevent classic static compilers to deliver efficient code for a language as dynamic and as flexible as JavaScript. We do not share this point of view. We think that by carefully combining classical analyses, by developing new ones when needed, and by crafting a compiler where the results of the high-level analyses are propagated up to the code generation, it is possible for AOT compilation to be in the same range of performance as fast JIT compilers. This is what we attempt to demonstrate with this study. Of course, our ambition is not to produce a compiler strictly as fast as the fastest industrial JavaScript implementations. This would require much more engineering strength than what we can afford. Instead, we only aim at showing that static compilation can have performances reasonably close to those of fastest JavaScript implementations. *Reasonably close* is of course a subjective notion, that everyone is free to set for himself. For us, it means a compiler showing half the performances of the fastest implementations.

The version of the Hop.js AOT compiler we have developed during the year contains new typing analyses and heuristics that compensate for the lack of information JavaScript source codes contain. A first analysis, named *occurrence typing*, that elaborates on top of older techniques developed for the compilation of the Scheme programming language, extracts as much as possible syntactic information directly out of the source code. This analysis alone would give only rough approximations of the types used by the program but its main purpose is to feed the compiler with sufficient information so that it can deploys more efficient supplemental analyses. Probably the most original one is the analysis that we have named *hint typing* or *which typing* that consists in assigning types to variables and to function arguments according to the efficiency of the generated code. In other words, the *which typing* assign types for which the compiler will be able to deliver its best code instead of assigning types that might denote all the possible values variables and arguments may have during all possible executions. We have shown that these *whiched* types correspond very frequently to the implicit *intentional* types programmers had in mind when they wrote their programs. These analyses and the optimizations they enable are implemented in Hop.js version 3.2.0 available on the Inria pages and from Github. They are described in [17] paper.

**Property caches**: Property caches are a well-known technique invented over 30 years ago to improve dynamic object accesses. They have been adapted to JavaScript, which they have greatly contributed to accelerate.

However, this technique is applicable only when some constraints are satisfied by the objects, the properties, and the property access sites. We have started a study to try to improve it on two common usage patterns: *prototype accesses* and *megamorphic accesses*. We have built a prototypical implementation in Hop.js that has let us measure the impact of the technique we propose. We have observed that they effectively complement traditional caches and that they reduce cache misses and consequently accelerate execution. Moreover, they do not cause a slowdown in the handling of the other usage patterns. We are now at completing this study by polishing the implementation and by publishing a paper exposing and evaluating the new techniques.

# 5.3. Web Reactive Programming

During the year, we have continued our effort in designing and implementing the HipHop.js programming language, we have applied it to interactive music composition, and we have studied security of reactive systems.

#### HipHop.js

Web applications react to many sort of events. Let them be GUI events, multimedia events, or network events on client code or IO and system events on the server, they are all triggered asynchronously. JavaScript, the hegemonic programming language of the Web, handles them using low level constructs based on *listeners*, a synonym for *callback*. To improve on the so-called *callback hell*, the recent versions of the language have proposed new constructs that raise the programming abstraction level (promises and async/await). They enable a programming style, closer to traditional sequential programming, which helps developing and maintaining applications. However, the improvements they propose rely exclusively on syntactic extensions. They do not change the programming model. For that reason, complex orchestration problems that imply all sorts of synchronization, preemption, and parallelism remain as complex to program as before. We think that orchestration should be reconsidered more globally and from the ground. The solution we propose consists in embedding a DSL specialized on orchestration inside the traditional Web development environment, in our case, Hop.js, the Web programming language that the team develop.

The orchestration DSL we propose is called HipHop.js. It is a reactive synchronous language. More precisely, it is an adaptation of the Esterel programming language to the Web. The motivations for choosing Esterel are diverse. First, and most important, Esterel is powerful enough to handle all the orchestration patterns we are considering. Second, the team, via its partnership with Colège de France, has high expertise in the design and development of Esterel-like languages, which constitutes a highly valuable asset for our development.

Esterel is powerful enough to handle all the orchestration patterns we are considering but Esterel has been designed and developed in a context baring no resemblance with the Web. Esterel was considering static execution models while the Web assumes permanent evolutions and modifications of the running programs. Esterel was considering sequential imperative languages for its embedding, while the Web is considering dynamic functional languages (i.e., JavaScript). Esterel was assuming static execution contexts where *a-priori* validity proof were enforced before hand while the Web assumes highly dynamic runtime executions so that only dynamic verifications are doable. For all these reasons, adapting Esterel and transforming it to form HipHop.js has needed a deep revamping and a deep paradigm shift.

During the year of 2018, we have finalized and completed the design of the language that is now almost stabilized. It follows previous version developed in C. Vidal's PhD studies [13], [18]. The version 0.3.x has been made available at the URL http://hop-dev.inria.fr. It has been used to implement our first orchestration demanding applications, in particular, an interactive music composition application. Our next steps will consist in completing the design and implementation of the language and a minimal development environment without which only experts can use the system. We of course also need to publicize the system and describe its design and internal in various academic publications.

#### Interactive music composition: the Skini platform

In the sixties, the philosopher Umberto Eco, and musicians such as K. Stockausen, K. Penderescki, L. Berio questioned about the relationship between composers, musicians, and the way we perceive music. Eco used the wording "Open Work", and showed that, the vision of the world evolved from a static world to a more

blurred perception. According to this new perception and in a shift comparable to the evolution of physics from Copernic to Einstein, some contemporary artists tried to express this complexity through works where the performer and the audience have a concrete impact on the work. Since the sixties, the development of audience participation for collaborative music production has become a more and more active field. Thanks to the large device market and web based technology development such as web audio API, "Open Work" got a broader meaning with systems allowing individual interaction. Nevertheless it is still difficult to find systems proposing frameworks dedicated to music composition of interactive performances with a clear composition scheme and ease of use. This is our motivation for developing a framework, called Skini, designed for composing, simulating, and executing interactive performances. Skini is based on elementary music patterns, automatic control of the patterns activation made possible thanks to Hop and Hiphop. Skini was first used for a concert that took place at the very end of 2017 in the contemporary Musical Festival of Nice (MANCA) followed in 2018 by performances during the "Portes ouvertes" of Inria, the "Fête de la Science" and the Synchron conference.

In 2018: The Skini's user interface has been revamped. We have tried several interfaces for the pattern activation and focused on a simple one in order to make the interface more intuitive and fluid. We have added an important feature called the "distributed sequencer", which allows the audience not only to activate patterns but also to create them. We have added a new level of interaction, the scrutator, which allows global actions by the audience on the orchestration. The complete system is now synchronized with an external Midi clock. We have developed a first version of stand alone Midi control of the pattern. The system has followed the evolution of the Hiphop syntax and now implements the last version for the control of orchestration. We improved the synchronisation system and the processes for implementing the orchestration.

# 5.4. Session Types

Session types describe communication protocols between two or more participants by specifying the sequence of exchanged messages, together with their functionality (sender, receiver and type of carried data). They may be viewed as the analogue, for concurrency and distribution, of data types for sequential computation. Originally conceived as a static analysis technique for an enhanced version of the  $\pi$ -calculus, session types have now been embedded into a range of functional, concurrent, and object-oriented programming languages.

We have pursued our work on session types along three main directions.

#### **Multiparty Reactive Sessions**

Ensuring that communication-centric systems interact according to an intended protocol is an important but difficult problem, particularly for systems with some reactive or timed components. To rise to this challenge, we have studied the integration of session-based concurrency and Synchronous Reactive Programming (SRP).

Synchronous reactive programming (SRP) is a well-established programming paradigm whose essential features are logical instants, broadcast events and event-based preemption. This makes it an ideal vehicle for the specification and analysis of reactive systems. *Session-based concurrency* is the model of concurrent computation induced by session types, a rich typing discipline designed to specify the structure of interactions.

In this work, we propose a process calculus for multiparty sessions enriched with features from SRP. In this calculus, protocol participants may broadcast messages, suspend themselves while waiting for a message, and also react to events.

Our main contribution is a session type system for this calculus, which enforces session correctness in terms of communication safety and protocol fidelity, and also ensures a time-related property, which we call input timeliness, which entails livelock-freedom. Our type system departs significantly from existing ones, specifically as it captures the notion of "logical instant" typical of SRP. This work is currently under submission.

#### **Reversible Sessions with Flexible Choices**

*Reversibility* has been an active trend of research for the last fifteen years. A reversible computation is a computation that has the ability to roll back to a past state. Allowing computations to reverse is a means to improve system flexibility and reliability. In the setting of concurrent process calculi, reversible computations have been first studied for CCS, then for the  $\pi$ -calculus, and only recently for session calculi.

Following up on our previous work on concurrent reversible sessions [29], we studied a simpler but somewhat "more realistic" calculus for concurrent reversible multiparty sessions, equipped with a flexible choice operator allowing for different sets of participants in each branch of the choice. This operator is inspired by the notion of *connecting action* recently introduced by Hu and Yoshida to describe protocols with optional participants. We argue that this choice operator allows for a natural description of typical communication protocols. Our calculus also supports a compact representation of the history of processes and types, which facilitates the definition of rollback. Moreover, it implements a fine-tuned strategy for backward computation. We present a session type system for the calculus and show that it enforces the expected properties of session fidelity, forward progress and backward progress. This work has been accepted for journal publication.

#### **Multiparty sessions with Internal Delegation**

We have investigated a new form of delegation for multiparty session calculi. Usually, delegation allows a session participant to appoint a participant in another session to act on her behalf. This means that delegation is inherently an inter-session mechanism, which requires session interleaving. Hence delegation falls outside the descriptive power of global types, which specify single sessions. As a consequence, properties such as deadlock-freedom or lock-freedom are difficult to ensure in the presence of delegation. Here we adopt a different view of delegation, by allowing participants to delegate tasks to each other within the same multiparty session. This way, delegation occurs within a single session (internal delegation) and may be captured by its global type. To increase flexibility in the use of delegation, our calculus uses connecting communications, which allow optional participants in the branches of choices. By these means, we are able to express conditional delegation. We present a session type system based on global types with internal delegation, and show that it ensures the usual safety properties of multiparty sessions, together with a progress property. This work is under submission.

# 5.5. Measurement and Detection of Web Tracking

#### Detecting Web Trackers via Analyzing Invisible Pixels

The Web has become an essential part of our lives: billions are using Web applications on a daily basis and while doing so, are placing *digital traces* on millions of websites. Such traces allow advertising companies, as well as data brokers to continuously profit from collecting a vast amount of data associated to the users.

Web tracking has been extensively studied over the last decade. To detect tracking, most of the research studies and user tools rely on *consumer protection lists*. EasyList [23] and EasyPrivacy [24] (EL&EP) are the most popular publicly maintained blacklist of know advertising and tracking domains, used by the popular browser extensions AdBlock Plus [20] and uBlockOrigin [28]. Disconnect [22] is another very popular list for detecting domains known for tracking, used in Disconnect browser extension [21] and in integrated tracking protection of Firefox browser [25]. Relying on EL&EP or Disconnect became the *de facto* approach to detect third-party tracking requests in privacy and measurement community. However it is well-known that these lists detect only known tracking and ad-related requests, and a tracker can easily avoid this detection by registering a new domain or changing the parameters of the request.

In this work, to detect trackers, we propose a new technique based on the analysis of invisible pixels <sup>0</sup>. These images are routinely used by trackers in order to send information or third-party cookies back to their servers: the simplest way to do it is to create a URL containing useful information, and to dynamically add an image HTML tag into a webpage. Since invisible pixels do not provide any useful functionality, we consider them *perfect suspects for tracking*.

<sup>&</sup>lt;sup>0</sup>By "invisible pixels" we mean 1x1 pixel images or images without content.

By using an Inria cluster and setting up a distributed crawler, we have collected a dataset of invisible pixels from 829,349 webpages. By analyzing this dataset, we observed that invisible pixels are widely used: more than 83% of pages incorporate at least one invisible pixel.

Overall, we made the following key contributions:

- We define a new classification of Web tracking behaviors based on the analysis of invisible pixels. By analyzing behavior associated to the delivery of invisible pixels, we propose a new fine-grained classification of tracking behaviors, that consists of 8 categories of tracking. To our knowledge, we are the first to analyse tracking behavior based on invisible pixels that are present on 83% of the webpages.
- We apply our classification to a full dataset and uncover new collaborations between third-party domains. We detect new relationships between third-party domains beyond basic cookie syncing detected in the past. In particular, we discovered that *first to third party cookie syncing* is the most prevalent tracking behavior performed by 50,812 distinct domains. Finally, we find that 76.23% of requests responsible for tracking originate from loading other resources than invisible images. To our knowledge, we are the first to discover a highly prevalent first to third party syncing behavior detected on 51.54% of all crawled domains.
- We show that the consumer protection lists cannot be considered as ground truth to identify trackers. We find out that the browser extensions based on EasyList and EasyPrivacy (EL&EP) and Disconnect each miss 22% of tracking requests we detect. Moreover, if we combine all the lists, 238,439 requests originated from 7,773 domains are unknown to these lists and hence still track users on 5,098 webpages even if tracking protection is installed. We also detect instances of cookie syncing in domains unknown to these lists and therefore likely unrelated to advertising. To our knowledge, we are the first to detect that EL&EP and also Disconnect lists used in majority of Web Tracking detection literature are actually missing tracking requests to 7,773 distinct domains.

This working paper [19] is currently under submission at an international conference.

#### A survey on Browser Fingerprinting

This year, we have conducted a survey on the research performed in the domain of browser fingerprinting, while providing an accessible entry point to newcomers in the field. We explain how this technique works and where it stems from. We analyze the related work in detail to understand the composition of modern fingerprints and see how this technique is currently used online. We systematize existing defense solutions into different categories and detail the current challenges yet to overcome.

A *browser fingerprint* is a set of information related to a user's device from the hardware to the operating system to the browser and its configuration. *Browser fingerprinting* refers to the process of collecting information through a web browser to build a fingerprint of a device. Via a script running inside a browser, a server can collect a wide variety of information from public interfaces called Application Programming Interface (API) and HTTP headers. An API is an interface that provides an entry point to specific objects and functions. While some APIs require a permission to be accessed like the microphone or the camera, most of them are freely accessible from any JavaScript script rendering the information collection trivial. Contrarily to other identification techniques like cookies that rely on a unique identifier (ID) directly stored inside the browser, browser fingerprinting is qualified as completely *stateless*. It does not leave any trace as it does not require the storage of information inside the browser.

The goal of this work is twofold: first, to provide an accessible entry point for newcomers by systematizing existing work, and second, to form the foundations for future research in the domain by eliciting the current challenges yet to overcome. We accomplish these goals with the following contributions:

- A thorough survey of the research conducted in the domain of browser fingerprinting with a summary of the framework used to evaluate the uniqueness of browser fingerprints and their adoption on the web.
- An overview of how this technique is currently used in both research and industry.

- A taxonomy that classifies existing defense mechanisms into different categories, providing a highlevel view of the benefits and drawbacks of each of these techniques.
- A discussion about the current state of browser fingerprinting and the challenges it is currently facing on the science, technological, business, and legislative aspects.

This work has been submitted for publication at an international journal.

#### Measuring Uniqueness of Browser Extensions and Web Logins

Web browser is the tool people use to navigate through the Web, and privacy research community has studied various forms of *browser fingerprinting*. Researchers have shown that a user's browser has a number of inherent "physical" characteristics that can be used to uniquely identify her browser and hence to track it across the Web. Fingerprinting of users' devices is similar to physical biometric traits of people, where only physical characteristics are studied.

Similar to previous demonstrations of user uniqueness based on their behavior, *behavioral characteristics*, such as browser settings and the way people use their browsers can also help to uniquely identify Web users. For example, a user installs web browser extensions she prefers, such as AdBlock, LastPass, or Ghostery to enrich her Web experience. Also, while browsing the Web, she logs in her preferred social networks, such as Gmail, Facebook or LinkedIn. In this work, we study *users' uniqueness* based on their behavior and preferences on the Web: we analyze how unique are Web users based on their *browser extensions and logins*.

In this work, we performed the first large-scale study of user uniqueness based on browser extensions and Web logins, collected from more than 16,000 users who visited our website https://extensions.inrialpes.fr/. Our experimental website identifies installed Google Chrome extensions via Web Accessible Resources. and detects websites where the user is logged in by methods that rely on URL redirection and CSP violation reports. Our website is able to detect the presence of 13K Chrome extensions (the number of detected extensions varied monthly between 12, 164 and 13, 931), covering approximately 28% of all free Chrome extensions <sup>0</sup>. We also detect whether the user is connected to one or more of 60 different websites. Our main contributions are:

- A large scale study on *how unique users are based on their browser extensions and website logins*. We discovered that 54.86% of users that have installed at least one detectable extension are unique; 19.53% of users are unique among those who have logged into one or more detectable websites; and 89.23% are unique among users with at least one extension and one login. Moreover, we discover that 22.98% of users could be uniquely identified by web logins, even if they disable JavaScript.
- We study the privacy dilemma on Adblock and privacy extensions, that is, *how well these extensions protect their users against trackers and how they also contribute to uniqueness*. We evaluate the statement "the more privacy extensions you install, the more unique you are" by analyzing how users' uniqueness increases with the number of privacy extensions she installs; and by evaluating the tradeoff between the privacy gain of the blocking extensions such as Ghostery [26] and Privacy Badger [27].

We furthermore show that browser extensions and web logins can be exploited to fingerprint and track users by only checking a limited number of extensions and web logins. We have applied an advanced fingerprinting algorithm [30] that carefully selects a limited number of extensions and logins. For example, we show that 54.86% of users are unique based on all 16,743 detectable extensions. However, by testing 485 carefully chosen extensions we can identify more than 53.96% of users. Besides, detecting 485 extensions takes only 625ms.

Finally, we give suggestions to the end users as well as website owners and browser vendors on how to protect the users from the fingerprinting based on extensions and logins.

This paper has been published at at WPES international workshop affiliated with ACM CCS 2018 [14].

<sup>&</sup>lt;sup>0</sup>The list of detected extensions and websites are available on our website: https://extensions.inrialpes.fr/faq.php

# **Neo Project-Team**

# 7. New Results

# 7.1. Stochastic Modeling

**Participants:** Eitan Altman, Konstantin Avrachenkov, Mandar Datar, Swapnil Dhamal, Alain Jean-Marie, Albert Sunny.

#### 7.1.1. Markov chains with restart/jumps

In [7], K. Avrachenkov together with A. Piunovskiy and Y. Zhang (Univ. of Liverpool, UK) consider a discretetime Markov process with restart. At each step the process either with a positive probability restarts from a given distribution, or with the complementary probability continues according to a Markov transition kernel. The main contribution of this work is an explicit expression for the expectation of the hitting time (to a given target set) of the process with restart. The formula is convenient when considering the problem of optimization of the expected hitting time with respect to the restart probability. The results with are illustrated with two examples in uncountable and countable state spaces and with an application to network centrality.

Then, in [19], K. Avrachenkov and I. Bogdanov (HSE, Russia) study the relaxation time in the random walk with jumps. The random walk with jumps combines random walk based sampling with uniform node sampling and improves the performance of network analysis and learning tasks. They derive various conditions under which the relaxation time decreases with the introduction of jumps.

## 7.1.2. Markov modeling of Lasers

A. Jean-Marie has continued the investigation of Markov models of Lasers at several levels of physical accuracy, in conjunction with F. Philippe, L. Chusseau and A. Vallet (Univ. Montpellier and CNRS). In [17], a Markov model of relatively low complexity, the "Canonical Markov Model" (CMM), is built on the basis of a time-scale decomposition of physical phenomena. This simplified model is validated by comparison with a "microscopic Markov model" previously existing. Thanks to its smaller state space, simulations with the CMM are orders of magnitude faster, and numerical investigation of stationary and transient features become possible. As an example, the focus is put in [17], [39] on the Laser "threshold", a phenomenon related to sojourn of the CMM in states where no light is emitted. Simulations and numerical solutions reveal the existence of a bi-modal distribution for the particles for a certain range of parameters, thereby predicting a certain instability of the Laser for these values. Investigations continue with a quantification of the intensity of "flashes" through the computation of hitting times in the CMM.

#### 7.1.3. The marmoteCore platform

The development of marmoteCore (see Section 6.1) has been pursued by A. Jean-Marie. The software library is now being used in NEO's research projects such as [17] or queuing models supporting the analysis of Green Data Centers. marmoteCore provides the classes necessary to represent the state space of Markov models, from the elementary bricks that are interval or rectangular domains, simplices, or binary sequences. From there, the user easily programs the construction of probability transition matrices or infinitesimal generators. Structural analysis methods allow to identify recurrent and transient classes, and to compute the period of the model. Numerous methods allow the Monte Carlo simulation of the chain, the computation of transient and stationary distributions, as well as hitting times. In conjunction with E. Hyon (Univ. Paris-Nanterre), extensions of the core of the software are being programmed for Markov Decision Processes and Stochastic Games.

#### 7.1.4. Blockchain mining

S. Dhamal, T. Chahed (Telecom SudParis), W. Ben-Ameur (Telecom SudParis), E. Altman, A. Sunny, and S. Poojary (UAPV, the Univ. of Avignon) have studied a stochastic game framework for distributed computing settings such as blockchain mining in [42]. A continuous-time Markov chain model, where players arrive and depart according to a stochastic process, is proposed, and their investment strategies are determined based on the state of the system. Two scenarios are analyzed, based on whether the rate of problem getting solved is dependent on or independent of the computational power invested by the players. The equilibrium strategies are shown to follow a threshold policy when this rate is proportional to the total invested power, while the players are shown to invest proportionally to the reward-cost ratio when this rate is independent of the invested power. The effects of arrival and departure rates on the players' utilities are quantified using simulations.

The paper extends the game theoretic modeling and analysis of the static case (fixed number of miners) done in [18] by E. Altman in collaboration with A. Reiffers-Masson (IISc, India), D. Sadoc Menasché (UFRJ), M. Datar and S. Dhamal, and C. Touati (Inria Grenoble Rhône-Alpes).

# 7.2. Queueing Theory

Participants: Sara Alouf, Konstantin Avrachenkov, Alain Jean-Marie, Dimitra Politaki.

## 7.2.1. Multiclass processor sharing and random order scheduling policies

In [2], K. Avrachenkov and T. Bodas (LAAS-CNRS) consider a single server system serving a multiclass population. Some popular scheduling policies for such system are the discriminatory processor sharing (DPS), discriminatory random order service (DROS), generalized processor sharing (GPS) and weighted fair queueing (WFQ). In this work, the authors propose two classes of policies, namely MPS (Multi-class Processor Sharing) and MROS (Multi-class Random Order Service), that generalize the four policies mentioned above. For the special case when the multi-class population arrive according to Poisson processes and have independent and exponential service requirement with parameter  $\mu$ , they show that the tail of the sojourn time distribution for a class i customer in a system with the MPS policy is a constant multiple of the tail of the sojourn time distribution in a system with the DPS (GPS) scheduling policy is a constant multiple of the tail of the waiting time distribution in a system with the DROS (respectively WFQ) policy.

## 7.2.2. The marmoteCore-Q tool

Using the marmoteCore platform, a tool called marmoteCore-Q has been developed by D. Politaki under the supervision of S. Alouf and A. Jean-Marie for the simulation of a family of queueing models based on the general BMAP/PH/c queue with impatience and resubmissions. There exist many special cases of this queue for which analytical results are known. Examples are: the M/M/1 queue and its finite capacity version, the M/M/c/K queue, the M/PH/1 and M/PH/ $\infty$  queues, the M<sup>X</sup>/M/1 and M<sup>X</sup>/M/ $\infty$  queues. Such examples are used to validate the implementation of the marmoteCore-Q tool.

# 7.3. Random Graph and Matrix Models

Participants: Konstantin Avrachenkov, Maximilien Dreveton.

In [5], K. Avrachenkov, together with A. Kadavankandy (CentraleSupélec) and N. Litvak (Univ. of Twente, The Netherlands), analyse a mean-field model of Personalized PageRank on the Erdös-Rényi random graph containing a denser planted Erdös-Rényi subgraph. They investigate the regimes where the values of Personalized PageRank concentrate around the mean-field value. They also study the optimization of the damping factor, the only parameter in Personalized PageRank. Their theoretical results help to understand the applicability of Personalized PageRank and its limitations for local graph clustering.

# 7.4. Data Analysis and Learning

Participant: Konstantin Avrachenkov.

# 7.4.1. Unsupervised learning

In [6], K. Avrachenkov, together with A. Kondratev, V. Mazalov (Petrozavodsk State Univ., Russia) and D. Rubanov (Amadeus), applied game-theoretic methods for community detection in networks. The traditional methods for detecting community structure are based on selecting dense subgraphs inside the network. Here the authors propose to use the methods of cooperative game theory that highlight not only the link density but also the mechanisms of cluster formation. Specifically, they suggest two approaches from cooperative game theory: the first approach is based on the Myerson value, whereas the second approach is based on hedonic games. Both approaches allow to detect clusters with various resolutions. However, the tuning of the resolution parameter in the hedonic games approach is particularly intuitive. Furthermore, the modularity-based approach and its generalizations as well as ratio cut and normalized cut methods can be viewed as particular cases of the hedonic games. Finally, for approaches based on potential hedonic games a very efficient computational scheme using Gibbs sampling is suggested.

#### 7.4.2. Semi-supervised learning

Graph Semi-supervised learning (gSSL) aims to classify data exploiting two initial inputs: firstly, the data are structured in a network whose edges convey information on the proximity, in a wide sense, of two data points (e.g. correlation or spatial proximity) and, second, there is a partial information on some nodes, which have previously been labelled. Thus, the classification problem is usually a balance between two terms: one diffusing the information from the labelled points to the unlabelled ones through the network and another one that constrains the solution to be similar, on the labelled nodes, to the given labels. In practice, popular SSL methods as Standard Laplacian (SL), Normalized Laplacian (NL) or PageRank (PR), exploit those operators defined on graphs to spread the labels and, from a random walk perspective, the classification of a given point is given the maximum of the expected number of visits from one class. Anomalous diffusion can alter the way a graph is "explored" and, therefore, it can alter classification performance. In a nushell, Lévy flights/walks are a way to create superdiffusive regimes: the customary rule for their ignition is to allow the walkers to perform non-local jumps, whose length is distributed according to a fat-tailed probability density function with diverging second moment. Mathematically speaking, there have been several attempts to convert the Lévy flight phenomenon on networks and, in the context of gSSL, K. Avrachenkov in conjunction with S. De Nigris, E. Bautista, P. Abry and P. Gonçalves, settled in [38] for the use of fractional operators. In this SSL context, the authors cast those operators in the SSL problem in each different incarnation (SL, PR and NL) and investigated the beneficial effect of such a procedure for classification.

In [13], K. Avrachenkov, together with A. Kadavankandy (CentraleSupélec), L. Cottatellucci (EURECOM) and R. Sundaresan (IISc, India), tackle the problem of hidden community detection. We consider Belief Propagation (BP) applied to the problem of detecting a hidden Erdös-Rényi (ER) graph embedded in a larger and sparser ER graph, in the presence of side-information. We derive two related algorithms based on BP to perform subgraph detection in the presence of two kinds of side-information. The first variant of side-information consists of a set of nodes, called cues, known to be from the subgraph. The second variant of side-information consists of a set of nodes that are cues with a given probability. It was shown in past works that BP without side-information fails to detect the subgraph correctly when a so-called effective signal-to-noise ratio (SNR) parameter falls below a threshold. In contrast, in the presence of non-trivial side-information, we show that the BP algorithm achieves asymptotically zero error for any value of a suitably defined phase-transition parameter. We validate our results on synthetic datasets and a few real world networks.

# 7.4.3. Supervised learning

Graphlets are defined as k-node connected induced subgraph patterns. For instance, for an undirected graph, 3-node graphlets include closed triangles and open triangles. The number of each graphlet, called graphlet count, is a signature which characterizes the local network structure of a given graph. Graphlet count plays a prominent role in network analysis of many fields, most notably bioinformatics and social science. However, computing exact graphlet count is inherently difficult and computational expensive because the number of graphlets grows exponentially large as the graph size and/or graphlet size grow. To deal with this difficulty, many sampling methods were proposed to estimate graphlet count with bounded error. Nevertheless, these

methods require large number of samples to be statistically reliable, which is still computationally demanding. Intuitively, learning from historic graphs can make estimation more accurate and avoid many repetitive counting to reduce computational cost. Based on this idea, in [29] K. Avrachenkov, together with X. Liu, J. Chen and J. Lui (CUHK, Hong Kong), propose a convolutional neural network (CNN) framework and two preprocessing techniques to estimate graphlet count. Extensive experiments on two types of random graphs and real world biochemistry graphs show that their framework can offer substantial speedup on estimating graphlet count of new graphs with high accuracy.

# 7.5. Game Theory

Participants: Eitan Altman, Swapnil Dhamal.

## 7.5.1. Resource allocation polytope games

S. Dhamal, W. Ben-Ameur, T. Chahed (both from Telecom SudParis), and E. Altman have studied two-player resource allocation polytope games in [24]. The strategy of a player is considered to be restricted by the strategy of the other player, with common coupled constraints. In the context of such games, novel notions of independent optimal strategy profile and common contiguous set are introduced. Necessary and sufficient conditions are derived for the game to have a unique pure strategy Nash equilibrium. Given an instance of the game, an efficient algorithm is presented to compute the price of anarchy. Under reasonable conditions, the price of stability is shown to be 1. A paradox is shown that higher budgets may lead to worse outcomes.

# **7.6.** Applications in Telecommunications

**Participants:** Zaid Allybokus, Sara Alouf, Eitan Altman, Konstantin Avrachenkov, Swapnil Dhamal, Alain Jean-Marie, Giovanni Neglia, Dimitra Politaki.

# 7.6.1. Caching

A fundamental brick of the information-centric architectures proposed for Internet evolution is in-network caching, i.e. the possibility for the routers to store locally the contents and directly serve future requests. This has raised a new interest in the performance of networks of caches. Since 2012, there has been a significant research activity in NEO on this topic. Our work raised the attention of researchers at Akamai Technologies (the world leader in Content Delivery Networks). In real caching systems the hit rate is often limited by the speed at which contents can be retrieved by the Hard-Disk Drive (HDD) (this is the so-called *spurious misses*' problem). Akamai researchers asked us to design an algorithm to solve this problem. In [43] G. Neglia and D. Tsigkari, together with D. Carra (Univ. of Verona, Italy), M. Feng, V. Janardhan (Akamai Technologies, USA), and P. Michiardi (EURECOM) have proposed a simple randomized caching policy that makes optimal use of the RAM to minimize the load on the HDD and then the number of spurious misses. Moreover, experiments in Akamai CDN have shown that our policy reduces the HDD load by an additional 10% in comparison to the (highly optimized) baseline policy currently employed by Akamai. In [15] a subset of the same authors (G. Neglia, D. Carra, P. Michardi) have shown that the same approach can be adapted to minimize any miss cost function as far as the cost is additive over the misses.

More recently, we moved to consider the problem of caches' coordination in a dense cellular network scenario, where caches are deployed at base stations (BSs) and a user can potentially retrieve the content from multiple BSs. In this setting, the optimal content placement problem is NP-hard even when the goal is simply to maximize the hit ratio. Most of the existing literature has proposed heuristics assuming that content popularities are static and known, but in reality their estimation can be very difficult at the scale of the geographical area covered by a BS. In [14] E. Leonardi (Politecnico di Torino, Italy) and G. Neglia have introduced a class of simple and fully distributed caching policies, which require neither direct communication among BSs, nor a priori knowledge of content popularity (strongly deviating from the assumptions of existing policies and piggybacking an additional information bit to each content request. How to achieve coordination for more complex performance metrics (e.g. the retrieval time or fairness) is still an open research problem that is now the PhD subject of G. Iecker, co-supervised by G. Neglia and T. Spyropoulos (EURECOM).

## 7.6.2. Modeling and workload characterization of data center clusters

There are many challenges faced when modeling computing clusters. In such systems, jobs to be executed are submitted by users. These jobs may generate a large number of tasks. Some tasks may be executed more than once while other may abandon before execution. D. Politaki, S. Alouf, F. Hermenier (Nutanix), and A. Jean-Marie have developed a multi-server queueing system with abandonments and resubmissions to model computing clusters. To capture the correlations observed in real workload submissions, a Batch Markov Arrival Process is considered. The service time is assumed to have a phase-type distribution. This model has not been analyzed in the literature. The distributions of the interarrivals and the service times found in the Google Cluster Data have been characterized and compared with fitted distributions. The authors findings support the model assumptions. Ongoing work investigates the approaches that can be adopted to overcome the technical challenges found in the performance evaluation of the computing clusters. In particular, the developed tool marmoteCore-Q (see §7.2.2) will be used.

To understand the essential characteristics of a computing cluster for modelling purposes, the same authors have looked into two datasets consisting of job scheduler logs. The first dataset comes from a Google cluster and is publicly available (https://github.com/google/cluster-data). The second dataset has been collected from the internal computing cluster of Inria Sophia-Antipolis Méditerrannée. After a preliminary analysis and sanitizing of each dataset, a numerical analysis is performed to characterize the different stochastic processes taking place in the computing cluster. In particular, the authors characterize the impatience process, the resubmission process, the arrival process (batch sizes and correlations) and the service time, considering the impact of the scheduling class and of the execution type.

#### 7.6.3. Software Defined Networks (SDN)

The performance of computer networks relies on how bandwidth is shared among different flows. Fair resource allocation is a challenging problem particularly when the flows evolve over time. To address this issue, bandwidth sharing techniques that quickly react to the traffic fluctuations are of interest, especially in large scale settings with hundreds of nodes and thousands of flows. In this context, K. Avrachenkov and Z. Allybokus, together with J. Leguay (Huawei Research) and L. Maggi (Nokia Bell Labs), in [1] propose a distributed algorithm based on the Alternating Direction Method of Multipliers (ADMM) that tackles the multi-path fair resource allocation problem in a distributed SDN control architecture. Their ADMM-based algorithm continuously generates a sequence of resource allocation solutions converging to the fair allocation while always remaining feasible, a property that standard primal-dual decomposition methods often lack. Thanks to the distribution of all computer intensive operations, they demonstrate that large instances can be handled at scale.

## 7.6.4. Impulsive control of G-AIMD dynamics

Motivated by various applications from Internet congestion control to power control in smart grids and electric vehicle charging, in [20] K. Avrachenkov together with A. Piunovskiy and Y. Zhang (Univ. of Liverpool, UK) study Generalized Additive Increase Multiplicative Decrease (G-AIMD) dynamics under impulsive control in continuous time with the time average alpha-fairness criterion. They first show that the control under relaxed constraints can be described by a threshold. Then, they propose a Whittle-type index heuristic for the hard constraint problem. They prove that in the homogeneous case the index policy is asymptotically optimal when the number of users is large.

#### 7.6.5. Application of Machine Learning to optimal resource allocation in cellular networks

In [9], E. Altman in collaboration with A. Chattopadhyay and B. Błaszczyszyn (from Inria DYOGENE team) consider location-dependent opportunistic bandwidth sharing between static and mobile downlink users in a cellular network. In order to provide higher data rate to mobile users, the authors propose to provide higher bandwidth to the mobile users at favourable times and locations, and provide higher bandwidth to the static users in other times. They formulate the problem as Markov decision process (MDP) where the perstep reward is a linear combination of instantaneous data volumes received by static and mobile users. The transition structure of this MDP is not known in general. They thus propose a learning algorithms based on

stochastic approximation with one and with two time scales. The results are extended to address the issue of fair bandwidth sharing between the two classes of users.

To optimize routing of flows in datacenters, SDN controllers receive a packet-in message whenever a new flow appears in the network. Unfortunately, flow arrival rates can peak to millions per second, impairing the ability of controllers to treat them on time. Flow scheduling copes with this by segmenting the traffic between elephant and mice flows and by treating elephant flows in priority, as they disrupt short lived TCP flows and create bottlenecks. In [21], E. Altman in collaboration with F. De Pellegrini (UAPV), L. Maggi (Huawei), A. Massaro (FBK Trento), D. Saucez (Inria DIANA team) and J. Leguay (Huawei Research) propose a stochastic approximation based learning algorithm called SOFIA and able to perform optimal online flow segmentation. Extensive numerical experiments characterize the performance of SOFIA.

#### 7.6.6. Forecast Scheduling

With the age of big data and with geo-localisation measurements available, the precision in predicting the mobility of users increases, and hence also that of the prediction of channel conditions. In [35], E. Altman in collaboration with H. Zaaraoui, S. Jema, Z. Altman (Orange Labs) and T. Jimenez (UAPV) propose a convex optimization approach to Forecast Scheduling which makes use of current and future predicted channel conditions to obtain an optimal alpha fair schedule. They further extend the model in [34] to take into account different types of random events such as arrival and departure of users and uncertainties in the mobile trajectories. Simulation results illustrate the significant performance gain achieved by the Forecast Scheduling algorithms in the presence of random events.

# 7.6.7. Fairness in allocation to users with different time constraints

E. Altman and S. Ramanath (IIT Bombay, India) study in [31] how to allocate resources fairly when different users have different time constraints for using the resources. They formulate this as a Markov Decision Process (MDP) for a two user case and provide a Dynamic Program (DP) solution. Simulation results in an LTE framework are provided to support the theoretical claims.

# 7.7. Applications in Social Networks

Participants: Eitan Altman, Konstantin Avrachenkov, Swapnil Dhamal, Giovanni Neglia.

#### 7.7.1. Fairness in Online Social Network Timelines

Facebook News Feed personalization algorithm has a significant impact, on a daily basis, on the lifestyle, mood and opinion of millions of Internet users. Nonetheless, the behavior of such algorithm lacks transparency, motivating measurements, modeling and analysis in order to understand and improve its properties. E. Altman and G. Neglia, together with other researchers from THANES team (E. Hargreaves and D. Menasché from UFRJ, A. Reiffers-Masson from IIsc, and E. Altman) and with the journalist C. Agosti (Univ. of Amsterdam), have proposed a reproducible methodology encompassing measurements, an analytical model and a fairness-based News Feed design. The model leverages the versatility and analytical tractability of time-to-live (TTL) counters to capture the visibility and occupancy of publishers over a News Feed. Measurements from 2018 Italian political election are used to parameterize and to validate the expressive power of the proposed model. Then, we have conducted a what-if analysis to assess the visibility and occupancy bias incurred by users against a baseline derived from the model. Our results indicate that a significant bias exists and it is more prominent at the top position of the News Feed. In addition, we have found that the bias is non-negligible even for users that are deliberately set as neutral with respect to their political views, motivating the proposal of a novel and more transparent fairness-based News Feed design. This is a very recent research direction, but it has already led to 4 publications [36], [27], [28], [12] with a *best paper award* for [36].

### 7.7.2. Sampling online social networks

In the framework of network sampling, random walk (RW) based estimation techniques provide many pragmatic solutions while uncovering the unknown network as little as possible. Despite several theoretical advances in this area, RW based sampling techniques usually make a strong assumption that the samples are in stationary regime, and hence are impelled to leave out the samples collected during the burn-in period. In [4] K. Avrachenkov, together with V.S. Borkar (IIT Bomaby, India), A. Kadavankandy (CentraleSupélec) and J.K. Sreedharan (Purdue Univ., USA), propose two sampling schemes without burn-in time constraint to estimate the average of an arbitrary function defined on the network nodes, for example, the average age of users in a social network. The central idea of the algorithms lies in exploiting regeneration of RWs at revisits to an aggregated super-node or to a set of nodes, and in strategies to enhance the frequency of such regenerations either by contracting the graph or by making the hitting set larger. Our first algorithm, which is based on reinforcement learning (RL), uses stochastic approximation to derive an estimator. This method can be seen as intermediate between purely stochastic Markov chain Monte Carlo iterations and deterministic relative value iterations. The second algorithm, which we call the Ratio with Tours (RT)-estimator, is a modified form of respondent-driven sampling (RDS) that accommodates the idea of regeneration. We study the methods via simulations on real networks. We observe that the trajectories of RL-estimator are much more stable than those of standard random walk based estimation procedures, and its error performance is comparable to that of respondent-driven sampling (RDS) which has a smaller asymptotic variance than many other estimators. Simulation studies also show that the mean squared error of RT-estimator decays much faster than that of RDS with time. The newly developed RW based estimators (RL- and RT-estimators) allow to avoid burn-in period, provide better control of stability along the sample path, and overall reduce the estimation time.

#### 7.7.3. Crawling ephemeral content

In [3], K. Avrachenkov and V.S. Borkar (IIT Bombay, India) consider the task of scheduling a crawler to retrieve from several sites their ephemeral content. This is content, such as news or posts at social network groups, for which a user typically loses interest after some days or hours. Thus development of a timely crawling policy for ephemeral information sources is very important. The authors first formulate this problem as an optimal control problem with average reward. The reward can be measured in terms of the number of clicks or relevant search requests. The problem in its exact formulation suffers from the curse of dimensionality and quickly becomes intractable even with a moderate number of information sources. Fortunately, this problem admits a Whittle index, a celebrated heuristics which leads to problem decomposition and to a very simple and efficient crawling policy. The authors derive the Whittle index for a simple deterministic model and provide its theoretical justification. They also outline an extension to a fully stochastic model.

# 7.7.4. Posting behavior

In [32], E. Altman in collaboration with A. Reiffers-Masson (IISc, India), Y. Hayel and G. Marrel (UAPV) consider a "generalized" fractional program in order to solve a popularity optimization problem in which a source of contents controls the topics of her contents and the rate with which posts are sent to a time line. The objective of the source is to maximize its overall popularity in an Online Social Network (OSN). The authors propose an efficient algorithm that converges to the optimal solution of the Popularity maximization problem.

## 7.7.5. Recommendation system for OSNs

When a user interested in a service/item, visits an online web-portal, it provides description of its interest through initial search keywords. The system recommends items based on these keywords. The user is satisfied if it finds the item of its choice and the system benefits, otherwise the user explores an item from the list. In [33], E. Altman in collaboration with K. Veeraruna, S. Memon, M. Hanawal and R. Devanand (IEOR IIT Bombay, India), develop algorithms that efficiently utilize user responses to recommended items and find the item of user's interest quickly. The authors first derive optimal policies in the continuous Euclidean space and adapt the same to the space of discrete items.

## 7.7.6. Opinion dynamics

S. Dhamal, W. Ben-Ameur, T. Chahed (both from Telecom SudParis), and E. Altman have studied the problem of optimally investing in nodes of a social network, wherein two camps attempt to maximize adoption of their respective opinions by the population. In [11], several settings are analyzed, namely, when the influence of a camp on a node is a concave function of its investment on that node, when one of the camps has uncertain information regarding the values of the network parameters, when a camp aims at maximizing competitor's investment required to drive the overall opinion of the population in its favor, and when there exist common coupled constraints concerning the combined investment of the two camps on each node. In [23], the possibility of campaigning in multiple phases is explored, where the final opinion of a node in a phase acts as its initial bias for the next phase. A further intricate setting where a camp's influence on a node also depends on the node's initial bias, is analyzed in [22]. Extensive simulations are conducted on real-world social networks for all the considered settings.

### 7.7.7. Information diffusion under practical models

S. Dhamal has studied the effectiveness of adaptive seeding in multiple phases under the independent cascade model of information diffusion, in [25]. The effect on the mean and standard deviation of the extent of diffusion is observed, with an explanation of how adaptive seeding reduces uncertainty in diffusion. The other aspects studied are: how the number of phases impacts the effectiveness of diffusion, how the diffusion progresses phase-by-phase, and how to optimally split the total seeding budget across phases. Another study [26] generalizes the linear threshold model to account for multiple product features, and presents an integrated framework for product marketing using multiple channels: mass media advertisement, recommendations using social advertisement, and viral marketing using social networks. An approach for allocating budget among these channels is proposed.

# 7.8. Applications to Energy

Participant: Giovanni Neglia.

#### 7.8.1. Smart grids

Balancing energy demand and production is becoming a more and more challenging task for energy utilities because of the larger penetration of renewable energies, more difficult to predict and control. While the traditional solution is to dynamically adapt energy production to follow the time-varying demand, a new trend is to drive the demand itself. We have first considered the direct control of inelastic home appliances, whose energy consumption cannot be shaped, but simply deferred. Our solution does not suppose any particular intelligence at the appliances, the actuators are rather smart plugs, simple devices with communication capabilities that can be inserted between appliances' plugs and power sockets and are able to interrupt/reactivate power flow. During previous years we have considered both closed-loop and open-loop control of such devices in order to satisfy a probabilistic bound on the aggregated power consumption. Recently, G. Neglia, together with L. Giarré (Univ. di Modena e Reggio Emilia, Italy), I. Tinnirello and G. Di Bella (Univ. di Palermo, Italy) have considered a mixed approach [16]. They have been able to quantify the trade-off between the amount of controlled power and delays experienced by the users to evaluate to which scale this solution should be deployed.

We have also looked at Demand-Response (DR) programs, whereby users of an electricity network are encouraged by economic incentives to re-arrange their consumption in order to reduce production costs. Several recent works proposed DR mechanisms relying on a macroscopic description of the population that does not model individual choices of users. In [8], G. Neglia, together with A. Benegiamo (EURECOM/Inria) and P. Loiseau (EURECOM) has shown that these macroscopic models hide important assumptions that can jeopardize the mechanisms' implementation (such as the ability to make personalized offers and to perfectly estimate the demand that is moved from a timeslot to another). Then, starting from a microscopic description that explicitly models each user's decision, they have introduced new DR mechanisms with various assumptions on the provider's capabilities. Contrarily to previous studies, they have found that 1) the resulting

optimization problems are complex and can be solved numerically only through heuristics, 2) the savings from DR mechanisms are significantly lower than those suggested by previous studies.

# **GRAPHDECO Project-Team**

# 6. New Results

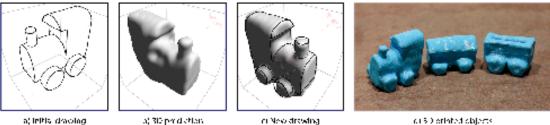
# 6.1. Computer-Assisted Design with Heterogeneous Representations

## 6.1.1. 3D Sketching using Multi-View Deep Volumetric Prediction

Participants: Johanna Delanoy, Adrien Bousseau.

Drawing is the most direct way for people to express their visual thoughts. However, while humans are extremely good are perceiving 3D objects from line drawings, this task remains very challenging for computers as many 3D shapes can yield the same drawing. Existing sketch-based 3D modeling systems rely on heuristics to reconstruct simple shapes, require extensive user interaction, or exploit specific drawing techniques and shape priors. Our goal is to lift these restrictions and offer a minimal interface to quickly model general 3D shapes with contour drawings. While our approach can produce approximate 3D shapes from a single drawing, it achieves its full potential once integrated into an interactive modeling system, which allows users to visualize the shape and refine it by drawing from several viewpoints (Figure 4). At the core of our approach is a deep convolutional neural network (CNN) that processes a line drawing to predict occupancy in a voxel grid. The use of deep learning results in a flexible and robust 3D reconstruction engine that allows us to treat sketchy bitmap drawings without requiring complex, hand-crafted optimizations. While similar architectures have been proposed in the computer vision community, our originality is to extend this architecture to a multiview context by training an updater network that iteratively refines the prediction as novel drawings are provided.

This work is a collaboration with Mathieu Aubry from Ecole des Ponts ParisTech and Alexei Efros and Philip Isola from UC Berkeley. The work was published in Proceedings of the ACM on Computer Graphics and Interactive Techniques and presented at the ACM SIGGRAPH I3D Symposium on Interactive Computer Graphics and Games [12].



seen from an other viewpoint

and updated prediction

Figure 4. Our sketch-based modeling system can process as little as a single perspective drawing (a) to predict a volumetric object (b). Users can refine this prediction and complete it with novel parts by providing additional drawings from other viewpoints (c). This iterative sketching workflow allows quick 3D concept exploration and rapid prototyping (d).

# 6.1.2. Procedural Modeling of a Building from a Single Image Participant: Adrien Bousseau.

Creating a virtual city is demanded for computer games, movies, and urban planning, but it takes a lot of time to create numerous 3D building models. Procedural modeling has become popular in recent years to overcome this issue, but creating a grammar to get a desired output is difficult and time consuming even for expert users. In this paper, we present an interactive tool that allows users to automatically generate such a grammar from a single image of a building. The user selects a photograph and highlights the silhouette of the target building as input to our method. Our pipeline automatically generates the building components, from large-scale building mass to fine-scale windows and doors geometry. Each stage of our pipeline combines convolutional neural networks (CNNs) and optimization to select and parameterize procedural grammars that reproduce the building elements of the picture. In the first stage, our method jointly estimates camera parameters and building mass shape. Once known, the building mass enables the rectification of the facades, which are given as input to the second stage that recovers the facade layout. This layout allows us to extract individual windows and doors that are subsequently fed to the last stage of the pipeline that selects procedural grammars for windows and doors. Finally, the grammars are combined to generate a complete procedural building as output. We devise a common methodology to make each stage of this pipeline tractable. This methodology consists in simplifying the input image to match the visual appearance of synthetic training data, and in using optimization to refine the parameters estimated by CNNs. We used our method to generate a variety of procedural models of buildings from existing photographs.

The work was published in Computer Graphics Forum, presented at Eurographics 2018 [15].

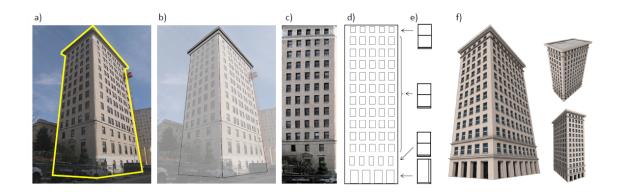


Figure 5. (a) Given an image and a silhouette of a building, (b) our approach automatically estimates the camera parameters and generates a building mass grammar as a first step. Then, (c) the facade image is rectified, and (d) the facade grammar is generated. (e) For each window non-terminal, the best window grammar is selected by maximum vote. (f) Finally the output grammar is constructed and a corresponding 3D geometry is generated.

#### 6.1.3. OpenSketch: A Richly-Annotated Dataset of Product Design Sketches

Participants: Yulia Gryaditskaya, Frédéric Durand, Adrien Bousseau.

We collected a dataset of more than 400 product design sketches, representing 12 man-made objects drawn from two different view points by 7 to 15 product designers of varying expertise. Together with industrial design teachers, we distilled a taxonomy of the methods designers use to accurately sketch in perspective and used it to label each stroke of the 214 sketches drawn from one of the two viewpoints. We registered each sketch to its reference 3D model by annotating sparse correspondences. We made an analysis of our annotated sketches, which reveals systematic drawing strategies over time and shapes. We also developed several applications of our dataset for sketch-based modeling and sketch filtering. We will distribute our dataset under the Creative Commons CC0 license to foster research in digital sketching.

This work is a collaboration with Mark Sypesteyn, Jan Willem Hoftijzer and Sylvia Pont from TU Delft, Netherlands. It is currently under review.

#### 6.1.4. Line Drawing Vectorization using a Global Parameterization

Participants: Tibor Stanko, Adrien Bousseau.

Despite the progress made in recent years, automatic vectorization of line drawings remains a difficult task. For drawings containing noise, holes and oversketched strokes, the main challenges are the correct classification of curve junctions, filling the missing information, and clustering multiple strokes corresponding to a single curve. We propose a new line drawing vectorization method, which addresses the above challenges in a global manner. Inspired by the quad meshing literature, we compute a global parametrization of the input drawing, such that nearby strokes are mapped to a single straight line in the parametric domain, while junctions are mapped to straight line intersections. The vectorization is obtained by following the straight lines in the parametric domain, and mapping them back to the original space. This allows us to process both clean and sketchy drawings.

This work is an ongoing collaboration with David Bommes from University of Bern, Mikhail Bessmeltsev from University of Montreal, and Justin Solomon from MIT.

#### 6.1.5. Image-Space Motion Rigidification for Video Stylization

Participants: Johanna Delanoy, Adrien Bousseau.

Existing video stylization methods often retain the 3D motion of the original video, making the result look like a 3D scene covered in paint rather than the 2D painting of a scene. In contrast, traditional hand-drawn animations often exhibit simplified in-plane motion, such as in the case of cut-out animations where the animator moves pieces of paper from frame to frame. Inspired by this technique, we propose to modify a video such that its content undergoes 2D rigid transforms. To achieve this goal, our approach applies motion segmentation and optimization to best approximate the input optical flow with piecewise-rigid transforms, and re-renders the video such that its content follows the simplified motion. The output of our method is a new video and its optical flow, which can be fed to any existing video stylization algorithm.

This work is a collaboration with Aaron Hertzmann from Adobe Research. It is currently under review.

#### 6.1.6. Computational Design of Tensile Structures

### Participants: David Jourdan, Adrien Bousseau.

Tensile structures are architectural shapes made of stretched elastic material that can be used to create largespan roofs. Their elastic properties make it quite challenging to obtain a specific shape, and the final shape of a tensile structure is usually found rather than imposed. We created a design tool for tensile structures that, unlike existing software, lets the user specify the shape they want and finds the closest fit.

This work is an ongoing collaboration with Melina Skouras from IMAGINE (Inria Rhone Alpes). A preliminary version was presented at JFIG (Journées Françaises d'Informatique Graphique) 2018.

# 6.2. Graphics with Uncertainty and Heterogeneous Content

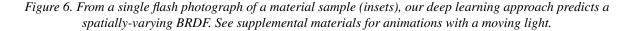
#### 6.2.1. Single-Image SVBRDF Capture with a Rendering-Aware Deep Network

Participants: Valentin Deschaintre, Aittala Miika, Frédéric Durand, George Drettakis, Adrien Bousseau.

Texture, highlights, and shading are some of many visual cues that allow humans to perceive material appearance in single pictures. Yet, recovering spatially-varying bi-directional reflectance distribution functions (SVBRDFs) from a single image based on such cues has challenged researchers in computer graphics for decades. We tackle lightweight appearance capture by training a deep neural network to automatically extract and make sense of these visual cues. Once trained, our network is capable of recovering per-pixel normal, diffuse albedo, specular albedo and specular roughness from a single picture of a flat surface lit by a hand-held flash. We achieve this goal by introducing several innovations on training data acquisition and network design. For training, we leverage a large dataset of artist-created, procedural SVBRDFs which we sample and render under multiple lighting directions. We further amplify the data by material mixing to cover a wide diversity of shading effects, which allows our network to work across many material classes. Motivated by the observation that distant regions of a material sample often offer complementary visual cues, we design a network that combines an encoder-decoder convolutional track for local feature extraction with a fully-connected track for global feature extraction and propagation. Many important material effects are view-dependent, and as such ambiguous when observed in a single image. We tackle this challenge by defining the loss as a differentiable SVBRDF similarity metric that compares the *renderings* of the predicted maps against renderings of the ground truth from several lighting and viewing directions. Combined together, these novel ingredients bring clear improvement over state of the art methods for single-shot capture of spatially varying BRDFs.

The work was published in ACM Transactions on Graphics and presented at SIGGRAPH 2018 [13], and was cited by several popular online ressources (https://venturebeat.com/2018/08/15/researchers-develop-ai-that-can-re-create-real-world-lighting-and-reflections/, https://www.youtube.com/watch?v=UkWnExEFADI).





#### 6.2.2. Material Acquisition using an Arbitrary Number of Inputs

Participants: Valentin Deschaintre, Aittala Miika, Frédéric Durand, George Drettakis, Adrien Bousseau.

Single-image material acquisition methods try to solve the very ill-posed problem of appearance to parametric BRDF. We explore different acquisition configurations to solve the most important ambiguities while still focusing on convenience of acquisition. Our main exploration directions are multiple lights and view angles over multiple pictures. This is possible thanks to the use of deep learning and in-line input data rendering, allowing us to easily explore a wide variety of configurations simultaneously. We also specialize our network architecture to make the most of an arbitrary number of input, provided in any order.

#### 6.2.3. Exploiting Repetitions for Image-Based Rendering of Facades

Participants: Simon Rodriguez, Adrien Bousseau, Frédéric Durand, George Drettakis.

Street-level imagery is now abundant but does not have sufficient capture density to be usable for Image-Based Rendering (IBR) of facades. We presented a method that exploits repetitive elements in facades – such as windows – to perform data augmentation, in turn improving camera calibration, reconstructed geometry and overall rendering quality for IBR. The main intuition behind our approach is that a few views of several instances of an element provide similar information to many views of a single instance of that element. We first select similar instances of an element from 3-4 views of a facade and transform them into a common coordinate system (Fig. 7 (a)), creating a "platonic" element. We use this common space to refine the camera calibration of each view of each instance (Fig. 7 (b)) and to reconstruct a 3D mesh of the element with multi-view stereo, that we regularize to obtain a piecewise-planar mesh aligned with dominant image contours (Fig. 7 (c)). Observing the same element under multiple views also allows us to identify reflective areas – such as glass panels – (Fig. 7 (d)) which we use at rendering time to generate plausible reflections using an environment map. We also combine information from multiple viewpoints to augment our initial set of views of the elements (Fig. 7 (e)). Our detailed 3D mesh, augmented set of views, and reflection mask enable image-based rendering of much higher quality than results obtained using the input images directly(Fig. 7 (f)).

The work was published in Computer Graphics Forum, presented at the Eurographics Symposium on Rendering 2018 [16].

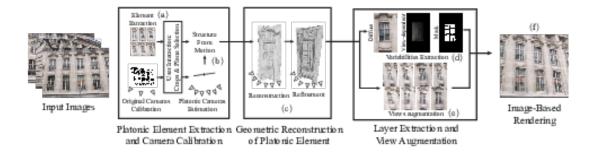


Figure 7. Overview of our technique for Image-Based Rendering of facades.

# 6.2.4. Plane-Based Multi-View Inpainting for Image-Based Rendering in Large Scenes Participants: Julien Philip, George Drettakis.

Image-Based Rendering (IBR) allows high-fidelity free-viewpoint navigation using only a set of photographs and 3D reconstruction as input. It is often necessary or convenient to remove objects from the captured scenes, allowing a form of scene editing for IBR. This requires multi-view inpainting of the input images. Previous methods suffer from several major limitations: they lack true multi-view coherence, resulting in artifacts such as blur, they do not preserve perspective during inpainting, provide inaccurate depth completion and can only handle scenes with a few tens of images. Our approach addresses these limitations by introducing a new multiview method that performs inpainting in intermediate, locally common planes. Use of these planes results in correct perspective and multi-view coherence of inpainting results. For efficient treatment of large scenes, we present a fast planar region extraction method operating on small image clusters. We adapt the resolution of inpainting to that required in each input image of the multi-view dataset, and carefully handle image resampling between the input images and rectified planes. We show results on large indoors and outdoors environments.

The work was presented at the ACM SIGGRAPH I3D Symposium on Interactive Computer Graphics and Games [19].

#### 6.2.5. Deep Blending for Free-Viewpoint Image-Based Rendering

Participants: Julien Philip, George Drettakis.

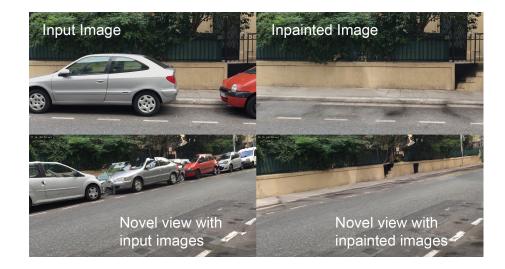


Figure 8. Our plane-based multi-view inpainting method allows us to remove cars in this large urban scene.

Free-viewpoint image-based rendering (IBR) is a standing challenge. IBR methods combine warped versions of input photos to synthesize a novel view. The image quality of this combination is directly affected by geometric inaccuracies of multi-view stereo (MVS) reconstruction and by view- and image-dependent effects that produce artifacts when contributions from different input views are blended. We present a new deep learning approach to blending for IBR, in which we use held-out real image data to learn blending weights to combine input photo contributions. Our Deep Blending method requires us to address several challenges to achieve our goal of interactive free-viewpoint IBR navigation. We first need to provide sufficiently accurate geometry so the Convolutional Neural Network (CNN) can succeed in finding correct blending weights. We do this by combining two different MVS reconstructions with complementary accuracy vs. completeness tradeoffs. To tightly integrate learning in an interactive IBR system, we need to adapt our rendering algorithm to produce a fixed number of input layers that can then be blended by the CNN. We generate training data with a variety of captured scenes, using each input photo as ground truth in a held-out approach. We also design the network architecture and the training loss to provide high quality novel view synthesis, while reducing temporal flickering artifacts. Our results demonstrate free-viewpoint IBR in a wide variety of scenes, clearly surpassing previous methods in visual quality, especially when moving far from the input cameras.

This work is a collaboration with Peter Hedman and Gabriel Brostow from University College London and True Price and Jan-Michael Frahm from University of North Carolina at Chapel Hill. It was published in ACM Transactions on Graphics and presented at SIGGRAPH Asia 2018 [14].

#### 6.2.6. Thin Structures in Image Based Rendering

Participants: Theo Thonat, Abdelaziz Djelouah, Frédéric Durand, George Drettakis.

This work proposes a novel method to handle thin structures in Image-Based Rendering (IBR), and specifically structures supported by simple geometric shapes such as planes, cylinders, etc. These structures, e.g. railings, fences, oven grills etc, are present in many man-made environments and are extremely challenging for multi-view 3D reconstruction, representing a major limitation of existing IBR methods. Our key insight is to exploit multi-view information to compute multi-layer alpha mattes to extract the thin structures. We use two multi-view terms in a graph-cut segmentation, the first based on multi-view foreground color prediction and the second ensuring multi-view consistency of labels. Occlusion of the background can challenge reprojection error calculation and we use multi-view median images and variance, with multiple layers of thin structures.

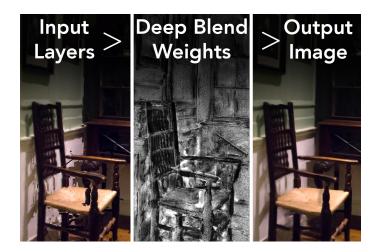


Figure 9. Deep Blending for Free-Viewpoint Image-Based Rendering

Our end-to-end solution uses the multi-layer segmentation to create per-view mattes and the median colors and variance to extract a clean background. We introduce a new multi-pass IBR algorithm based on depth-peeling to allow free-viewpoint navigation of multi-layer semi-transparent thin structures. Our results show significant improvement in rendering quality for thin structures compared to previous image-based rendering solutions.

The work was published in the journal Computer Graphics Forum, and was presented at the Eurographics Symposium on Rendering (EGSR) 2018 [17].



Figure 10. Thin structures are present in many environments, both indoors and outdoors (far left). Our solution extracts multi-view mattes together with clean background images and geometry (center). These elements are used by our multi-layer rendering algorithm that allows free-viewpoint navigation, with significantly improved quality compared to previous solutions (right).

# 6.2.7. Multi-Scale Simulation of Nonlinear Thin-Shell Sound with Wave Turbulence

Participants: Gabriel Cirio, George Drettakis.

Thin shells – solids that are thin in one dimension compared to the other two – often emit rich nonlinear sounds when struck. Strong excitations can even cause chaotic thin-shell vibrations, producing sounds whose energy spectrum diffuses from low to high frequencies over time – a phenomenon known as wave turbulence. It is all these nonlinearities that grant shells such as cymbals and gongs their characteristic "glinting" sound. Yet, simulation models that efficiently capture these sound effects remain elusive. In this project, we proposed a

physically based, multi-scale reduced simulation method to synthesize nonlinear thin-shell sounds. We first split nonlinear vibrations into two scales, with a small low-frequency part simulated in a fully nonlinear way, and a high-frequency part containing many more modes approximated through time-varying linearization. This allows us to capture interesting nonlinearities in the shells' deformation, tens of times faster than previous approaches. Furthermore, we propose a method that enriches simulated sounds with wave turbulent sound details through a phenomenological diffusion model in the frequency domain, and thereby sidestep the expensive simulation of chaotic high-frequency dynamics. We show several examples of our simulations, illustrating the efficiency and realism of our model, see Fig. 11.

This work is a collaboration with Ante Qu from Stanford, Eitan Grinspun and Changzi Zheng from Columbia. This work was published at ACM Transactions on Graphics, and presented at SIGGRAPH 2018 [11].

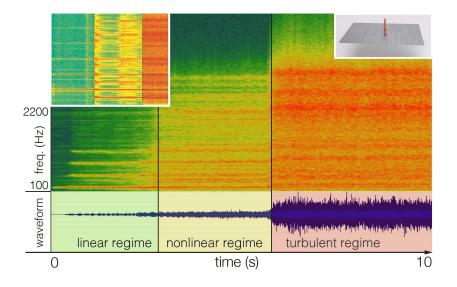


Figure 11. Thin-shell bifurcation. We excite a thin plate with increasing forces (the red arrow in the top-right inset) and simulate its dynamical responses). As the force increases, its vibration bifurcates, changing from linear vibration (left) to nonlinear (middle), and finally moving into a turbulent regime (right). This spectrogram is generated without any wave turbulence enrichment, indicating that model is able to capture chaos, albeit in low frequencies. We note that this spectrogram is qualitatively close to spectrograms from physical experiments, shown in the top-left inset (Image courtesy of Cyril Touzé).

#### 6.2.8. Learning to Relight Multi-View Photographs from Synthetic Data

Participants: Julien Philip, George Drettakis.

We introduce an image relighting method that allows users to alter the lighting in their photos given multiple views of the same scene. Our method uses a deep convolutional network trained on synthetic photorealistic images. The use of a 3D reconstruction of the surroundings allows to guide the relighting process.

This ongoing project is a collaboration with Tinghui Zhou and Alexei A. Efros from UC Berkeley, and Michael Gharbi from Adobe research.

# 6.2.9. Exploiting Semantic Information for Street-level Image-Based Rendering Participants: Simon Rodriguez, George Drettakis.

Following our work on facade rendering (Sec. 6.2.3), this ongoing project explores the use of semantic segmentation to inform Image-Based Rendering algorithms. In particular, we plan to devise algorithms that adapt to different types of objects in the scene (cars, buildings, trees).

## 6.2.10. Casual Video Based Rendering of Stochastic Phenomena

Participants: Theo Thonat, Miika Aittala, Frédéric Durand, George Drettakis.

The goal of this work is to extend traditional Image Based Rendering to capture subtle motions in real scenes. We want to allow free-viewpoint navigation with casual capture, such as a user taking photos and videos with a single smartphone or DSLR camera, and a tripod. We focus on stochastic time-dependent textures such as leaves in the wind, water or fire, to cope with the challenge of using unsynchronized videos.

This ongoing work is a collaboration with Sylvain Paris from Adobe Research.

## 6.2.11. Cutting-Edge VR/AR Display Technologies

Participant: Koulieris Georgios.

Near-eye (VR/AR) displays suffer from technical, interaction as well as visual quality issues which hinder their commercial potential. We presented a tutorial that delivered an overview of cutting-edge VR/AR display technologies, focusing on technical, interaction and perceptual issues which, if solved, will drive the next generation of display technologies. The most recent advancements in near-eye displays were presented providing (i) correct accommodation cues, (ii) near-eye varifocal AR, (iii) high dynamic range rendition, (iv) gaze-aware capabilities, either predictive or based on eye-tracking as well as (v) motion-awareness (Fig. 12). Future avenues for academic and industrial research related to the next generation of AR/VR display technologies were analyzed.

This work is a collaboration with Kaan Akşit (NVIDIA), Christian Richardt (University of Bath), Rafal Mantiuk (University of Cambridge) and Katerina Mania (Technical University of Crete). The work was presented at IEEE VR 2018, 18-22 March, Reutlingen, Germany [18].



Figure 12. We presented novel display technologies, including but not limited to (left-to-right) varifocal augmented reality displays, body-tracking displays and focus-tunable displays.

# **GRAPHIK Project-Team**

# 7. New Results

# 7.1. Ontology Mediated Query Answering

**Participants:** Jean-François Baget, Meghyn Bienvenu, Efstathios Delivorias, Michel Leclère, Marie-Laure Mugnier, Federico Ulliana.

Ontolology-mediated query answering (OMQA) is the issue of querying data while taking into account inferences enabled by ontological knowledge. This gives rise to *knowledge bases*, composed of a factbase (in database terms: an instance that contains incomplete data) and an ontology. Answers to queries are logically entailed from the knowledge base. Two families of formalisms for representing and reasoning with the ontological component have been considered in this context: *description logics* (DLs) and *existential rules* (aka Datalog+, or tuple-generating dependencies in database theory). Both frameworks correspond to fragments of first-order logic, which are incomparable in general but closely related in the context of OMQA: indeed, most DLs considered for OMQA, known as lighthweight DLs, are naturally translated into specific classes of existential rules. Importantly, the foundational work carried by the knowledge representation community led to the definition of several W3C standards for Semantic Web languages, namely the family of OWL 2 ontology languages, which can be used in combination with the RDF(S) Semantic Web language. This paradigm is also supported by commercial systems, such as Oracle.

Techniques for query answering under existential rules mostly rely on the two classical ways of processing rules, namely forward chaining and backward chaining. In forward chaining (also known as the *chase* in databases), the rules are applied to enrich the factbase and query answering can then be solved by evaluating the query against the *saturated* factbase (as in a classical database system, i.e., with forgetting the ontological knowledge). The backward chaining process can be divided into two steps: first, the query is *rewritten* using the rules into a first-order query (typically a union of conjunctive queries, but possibly a more compact form); then the rewritten query is evaluated against the factbase (again, as in a classical database system). Some classes of existential rules and lightweight description logics ensure the termination of the chase and/or query rewriting, but not all.

## 7.1.1. Revisiting the Chase

The interest for existential rules in the OMQA context brought again to light a fundamental tool in database theory, namely the chase. Several chase variants are known: they all yield logically equivalent results, but differ on how they handle redundancies possibly caused by the introduction of unknown individuals (often called nulls). Briefly, detecting redundancies leads to smaller saturated factbases, and prevents some infinite chase sequences, but it is costly. Given a chase variant, the (all-instances) chase termination problem takes as input a set of existential rules and asks if this set of rules ensures the termination of the chase for any factbase. It is well-known that this problem is undecidable for all known chase variants.

Hence, a crucial issue is whether chase termination becomes decidable for some known subclasses of existential rules. We considered *linear* existential rules, a simple yet important subclass of existential rules that generalizes inclusion dependencies. We showed the decidability of the (all-instances) chase termination problem on linear rules for three main chase variants, namely *semi-oblivious, restricted* and *core* chase. The restricted chase is the most used variant of the chase, however it is notoriously tricky to study because the order in which rule applications are performed matters. Indeed, for the same factbase, some restricted chase sequences may terminate, while others may not. To obtain these results, we introduced a novel approach based on so-called derivation trees and a single notion of forbidden pattern. Besides the theoretical interest of an unified approach and new proofs, we provided the first positive decidability results concerning the termination of the restricted chase, proving that chase termination on linear existential rules is decidable for both versions of the problem: Does *every* chase sequence terminate? Does *some* chase sequence terminate? [37] [27] (also to appear at ICDT 2019).

As part of Stathis Delivorias' PhD thesis, we considered the related problem of *boundedness*, which asks if a given set of existential rules is bounded, i.e., whether there is a predefined upper bound on the depth of the chase, independently from any factbase. This problem is already undecidable in the specific case of datalog rules (whose head has no existential variables). However, knowing that a set of rules is bounded for some chase variant does not help much in practice if the bound is unknown. Hence, we investigated the decidability of the k-boundedness problem, which asks whether a given set of rules is bounded by an integer k. We proved that k-boundedness is decidable for three main chase variants, namely the oblivious, semi-oblivious and restricted chase [23].

We investigated the combination of existential rules and answer set programming. The combination of the two formalisms requires to extend existential rules with nonmonotonic negation and to extend ASP with existential variables. To this aim, we introduced the syntax and semantics of existential non-monotonic rules using skolemization which join together the two frameworks. Building on our previous work published at ECAI and NMR, we presented syntactic conditions that ensure the termination of the chase for existential rules and discussed extension of these results in the nonmonotonic case [13].

# 7.1.2. Complexity of Ontology-Mediated Query Rewriting

Extending our previous work published at LICS, we carried out a systematic study on two fundamental problems in ontology-mediated query answering, in the context of the description logic OWL 2 QL. This dialect of the W3C standard ontology language OWL 2 is aimed towards efficient query answering on large data and ensures that every conjunctive ontology-mediated-query (OMQ) is rewritable into a first-order query. The first problem is the *succintness* of first-order rewritings of OMQs, which consists in understanding how difficult it is to built rewritings for queries in some OMQ class, and in particular to determine whether OMQs in the class have polynomial-size rewritings. The second problem is the *complexity* of OMQ answering. We classified OMQs according to the shape of their conjunctive queries (treewidth, the number of leaves) and the existential depth of their ontologies. For each of these classes, we determined the combined complexity of OMQ answering, and whether all OMQs in the class have polynomial-size first-order, positive existential and nonrecursive datalog rewritings. We obtained the succinctness results using hypergraph programs, a new computational model for Boolean functions, which makes it possible to connect the size of OMQ rewritings and circuit complexity [14].

#### 7.1.3. Ontology-Based Data Access

In the above settings, data is supposed to be stored in a factbase built on the same vocabulary as the ontology. We now consider a more general setting, often called *Ontology-Based Data Access (OBDA)*, in which data is stored in one or several databases, which were generally built independently from the ontology. Hence, the ontological level acts as a mediating level, and a new component, namely *mappings*, allows to transfer the answers to queries over the data into facts expressed in the ontology vocabulary. Mappings may be triggered to actually materialize the factbase, but such materialization may be not possible nor desirable, in which case the factbase remains virtual.

OBDA is the core setting we consider in the Inria Project Lab iCODA on data journalism (https://project. inria.fr/icoda/). As part of Maxime Buron's PhD thesis (co-supervision shared between CEDAR and GraphIK teams), we investigate several frameworks and query answering techniques in the OBDA setting. We consider the Semantic Web language RDFS to express the (possibly virtual) factbase and the core ontology, RDF rules that include classical RDF entailment rules but possibly richer ontological knowledge, expressive mappings (namely global-local-as-view mappings, whereas most existing work in the area is restricted to global-as-view mappings), and queries which, in the spirit of RDF, can interrogate both the ontology and the data at the same time. In particular, we proposed a new way of answering queries by a reduction to database query rewriting with views [21]. Software development and experiments are under progress.

We also pursued our work on inconsistency-tolerant query answering, revisiting existing complexity results obtained for OMQA in the wider context of OBDA, i.e., considering mappings. We formalized the problem and performed a detailed analysis of the data complexity of inconsistency-tolerant OBDA for ontologies formulated in data-tractable description logics, considering different semantics, notions of repairs and classes of GAV mappings. Our results imply that adding plain GAV mappings to the OMQA framework does not affect data complexity of inconsistency-tolerant query answering, but considering mappings with negated atoms leads to higher complexity [20].

Note that the latter work can also be seen as a contribution to maxi-consistent reasoning (see Section 7.2.2).

# 7.2. Reasoning with Inconsistency

**Participants:** Meghyn Bienvenu, Pierre Bisquert, Patrice Buche, Abdelraouf Hecham, Madalina Croitoru, Jérôme Fortin, Rallou Thomopoulos, Bruno Yun.

When reasoning about inconsistent logical KBs, one has to deploy reasoning mechanisms that do not follow the classical logical inference. This is due to the fact that, in classical logic, falsum implies everything. Alternative reasoning techniques are therefore needed in order to make sense of such KBs. In this section we present our results using two main classes of such techniques: defeasible reasoning and maxi-consistent reasoning.

#### 7.2.1. Defeasible Reasoning

Defeasible reasoning is used to evaluate claims or statements in an inconsistent setting where the rules encoding the ontological knowledge may contradict each other. Unfortunately, there is no universally valid way to reason defeasibly. An inherent characteristic of defeasible reasoning is its systematic reliance on a set of intuitions and rules of thumb, which have been long debated between logicians. For example, could an information derived from a contested claim be used to contest another claim (i.e., ambiguity handling)? Could "chains" of reasoning for the same claim be combined to defend against challenging statements (i.e., team defeat)? Is circular reasoning allowed? Etc. We got interested in the task of a data engineer looking to select what existing tool to use to perform defeasible reasoning. To this end we proposed the first benchmark in the literature for first-order logic defeasible reasoning tools profiling and showed how to use the proposed benchmark in order to categorize existing tools based on their semantics (e.g. ambiguity handling), logical language (e.g. existential rules) and expressiveness (e.g. priorities) [25]. Furthermore, we proposed a new logical formalism called Statement Graphs (SGs) that captures the state-of-the-art defeasible reasoning features via a flexible labelling function [24].

#### 7.2.2. Maxi-Consistent Reasoning

We now consider reasoning with inconsistent knowledge bases, when making the assumption that the ontological knowledge (here expressed by rules) is reliable, hence inconsistencies come from the data (or factbase), which may contradict ontological knowledge. We consider maximally consistent subsets of the factbase as the basis for inference (in short, "maxi-consistent" reasoning).

Repair semantics. One of the main challenges of reasoning with inconsistency is handling the inherent inconsistency that might occur amongst independently built data sources partially describing the same knowledge of interest. Inconsistency-tolerant semantics consider all maximally consistent subsets of a factbase, called repairs, that they manipulate using a modifier of these repairs (e.g. saturating them by the rules) and an inference strategy (e.g. answers have to be found in all repairs). However, using all repairs might be inappropriate for certain applications that would rather focus on particular data sources. For instance, when considering more reliable sources (i.e., sensor information, provenance data etc.) one could focus on repairs using mostly facts from such sources. When there is no given preference order on sources, we propose to use an intrinsic preference on facts based on their participation in inconsistencies, which generates a preference of repairs (i.e., those that contain less controversial facts are preferred). This led us to define a novel framework that takes into consideration the inconsistency on the facts and restricts the set of repairs to the "best" with respect to inconsistency values. We showed the significance and the practical interest of our approach using the real data collected in the framework of the Pack4Fresh project for reducing food wastes. During this project, we collected data using an online poll from a set of professionals of the food industry, including wholesalers, quality managers, floorwalkers and warehouse managers, about food packagings and their characteristics. The framework was able to rank the repairs efficiently and the results were then analysed and evaluated by experts from the packaging industry [35].

*Argumentation.* Argumentation is a reasoning under inconsistency technique, that allows to build arguments and attacks over an inconsistent data. The arguments represent the various inferences one can make. The attacks capture the inconsistency between the different pieces of knowledge. The set of arguments and the corresponding set of attacks is referred to as an argumentation framework (AF). AFs are visually represented using a directed graph where the nodes represent the arguments and the directed edges the attacks between the arguments. Classically, reasoning with argumentation systems consists of finding the maximal sets of arguments that (1) are not attacking each other and (2) defend themselves (as a group) from all incoming attacks. Such sets are called extensions.

Argumentation as a reasoning method over logic knowledge bases has the added value of providing better explanations to users than classical methods. However, one drawback of logic based argumentation frameworks is the large number of arguments generated. We provided a methodology for filtering semantically redundant arguments adapted for knowledge bases without rules or knowledge bases with rules. In the first case of knowledge bases without rules, we use the observation that free facts (i.e., facts that are not touched by any negative constraints) induce an exponential growth on the argumentation graph without any impact on its underlying structure. Therefore, we first generate the argumentation graph corresponding to the knowledge base without the free facts and then redo the whole graph including the arguments of the free facts in an efficient manner. In the second case, of the knowledge bases with rules, we introduce a new structure for the arguments and the attacks. In this new structure, we have significantly less arguments [28] (extended in [31]).

Furthermore, we provided a tool called Dagger that allows a knowledge engineer to (1) input a KB in a commonly used format and then (2) generate, (3) visualise or (4) export the argumentation graph [30]. Using the tool we were able to provide the first benchmark of logic based argumentation graphs in the litterature [32].

An alternative to the extension based semantics explained above are the ranking based semantics used mainly in the case where arguments are seen as abstract entities (and not necessarily logic derivation). There is a difference in the output format between these two approaches: when using a ranking based semantics, the output is a ranking on the arguments; in the case of extension based semantics, the output is a set of extensions. While the ranking and the scores (which are present in many ranking based semantics) allow to better assess the acceptability degree of each individual argument, the question "what are the different points of view of the argumentation framework?" stays unanswered when using a ranking based semantics. We have proposed a modular framework that is generic enough to be able to accommodate various application scenarios. In this case, one important property of the framework lies in its versatility and its capacity to yield different results according to various instantiations [33].

# 7.3. Decision Support Systems Applied to Agronomy

**Participants:** Pierre Bisquert, Patrice Buche, Abdelraouf Hecham, Madalina Croitoru, Jérôme Fortin, Rallou Thomopoulos, Bruno Yun.

High-level decision-making needs to take into account the often-conflicting interests of different stakeholders with the goal of finding solutions to provide trade-offs and build consensus towards the adoption of socalled win-win solutions. In order to enrich the deliberation process we have proposed several complementary approaches that combine various methods for an unified approach towards decision making. This has been applied in practical domains as explained below.

First, in [17] we presented a systematic method to assess possible options, based on the complementarity of argumentation modeling and system dynamics (SD) simulation, in conjunction with field experimentation. Taking advantage of the argument analysis, SD simulations are used to: 1) compare different cultural strategies available to farmers in current operating, market and regulatory conditions; 2) propose plausible what-if scenarios anticipating technological progress, and exploring the impact of adopting potential incentives and dissuasive regulatory measures.

Second, voting theory has been applied at the service of decision making. We employed Computational Social Choice (CSC) and Argumentation Framework (AF) as a combination to propose socially fair decisions which take into account both (1) the involved agents' preferences and (2) the justifications behind these preferences. Furthermore we implemented a software tool for decision-making which is composed of two main systems, i.e., the social choice system and the deliberation system [16]. This work was evaluated in practice [18]. Note that the use of argumentation in practice, when not considering fully formalised domains is very challenging. This specifically concerns decision support systems as shown in [34] where we focused on the following research question: "How to define an attack relation for argumentative decision making in socio-economic systems?" To address this question we proposed three kinds of attacks that could be defined in the context of a specific application (packaging selection) and studied how the non-computer-science experts evaluated, against a given set of decision tasks, each of these attacks.

# **HEPHAISTOS Project-Team**

# 7. New Results

# 7.1. Robotics

## 7.1.1. Analysis of Cable-driven parallel robots

Participants: Alain Coulbois, Artem Melnyk, Jean-Pierre Merlet [correspondant], Yves Papegay.

We have continued the analysis of suspended CDPRs for control and design purposes. This analysis is heavily dependent on the behavior of the cable. Three main models can be used: *ideal* (no deformation of the cable due to the tension, the cable shape is a straight line between the attachments points), *elastic* (cable length changes according to the tension to which it is submitted, straight line cable shape) and sagging (cable shape is not a line as the cable is submitted to its own mass). The different models leads to very different analysis with a complexity increasing from ideal to sagging. All cables exhibit sagging but the sagging effect is often neglected if the CDPR is relatively small while it definitively cannot be neglected for large CDPRs. The most used sagging model is the Irvine model [19]. This is a non algebraic planar model with the upper attachment point of the cable is supposed to be grounded: it provides the coordinates of the lowest attachment point B of the cable if the cable length  $L_0$  at rest and the force applied at this point are known. It takes into account both the elasticity and deformation of the cable due to its own mass. A drawback of this model is that we will be more interested in a closed-form of the  $L_0$  for a given pose of B (for the inverse kinematics of CDPR) and in alternate form of the model that will provide constraint on the force components (for the direct kinematics). We have proposed new original formulations of the Irvine model in [15] (best paper award of the Eucomes conference) and have shown that their use drastically improve the solving time for both the inverse and direct kinematics (i.e finding all possible solutions for both problems) that are required for CDPRs control. Still the solving time of the direct kinematics is too large for the real-time direct kinematics and in that case only the current pose of the platform is of interest. For that purpose it is of interest to add sensors on the robot beside the measurement of cable lengths in order to improve the solving time by using additional constraints and possibly ending up with a single solution. But these measurements are uncertain although we may assume that the measurement errors are bounded. It is necessary to determine these error bounds for a practical use of these measurement and we have conducted an experimental investigation of various additional measurements [12]: a mechanical system for measuring the angle of the cable plane with respect to a reference axis, cable angulation with accelerometers glued on the cable, a "poor man lidar" on the platform for optically determining several cables angulation, accelerometers on the platform and cable tensions with strain gauges while the pose of the platform was estimated accurately by using a metrology arm and laser range-meters. This investigation has shown that:

- the friction in the mechanical system leads to large errors for the cable plane angle (up to 30 degrees). For later measure we have bypassed this system
- even for small and medium-sized CDPRs the sagging effect cannot be neglected for estimating cable angulation
- accelerometers on the cable and the lidar system have a good accuracy (between 1 and 5 degrees)
- cable tension measurement is very approximate even with high accuracy strain gauges and cannot be used for control purposes.

We have also continued to investigate calculation of planar cross-sections of the workspace for CDPR with sagging cables, i.e. when 4 of the 6 platform pose parameters are fixed leaving only 2 free parameters. Brand new algorithms have been developed, based on a continuation approach [12],[13]. The main idea is that almost everywhere the workspace border is a one-dimensional variety so that if one of the free parameters is fixed, then a pose on the border should satisfy a square equation system constituted of the kinematic equations and the constraints equations (e.g. that a cable length is equal to a given maximum limit). Pose on the border are obtained by choosing an arbitrary pose that has an inverse kinematic solution that satisfy the constraints in the workspace and then moves incrementally along one of the free axis using a certified Newton scheme for finding the inverse kinematics solution until the constraint equations are almost satisfied in which case the certified Newton scheme is used to determine exactly (i.e with an arbitrary accuracy) a pose that lies on the border. Then a continuation scheme is used to find new poses on the border until we reach a pose at which a new set of constraints is satisfied i.e. a starting point for a new border arc. The border is then composed of several polygonal arcs that approximate the real border. The scheme is devised so that we completely master the difference between the real workspace area and the region defined by the polygonal approximation of the border. If necessary we may reduce this difference by adding new vertices on the border polygon. An important point is that the constraints define border arcs but also singularity curves (i.e. pose at which the direct kinematics equations are singular) and a specific continuation scheme has been developed to determine those arcs. Indeed the cancellation of the determinant of the jacobian of the direct kinematic equations is part of the equations that are satisfied on this type of border arc but this determinant cannot be obtained in closedform. Consequently we have devised a certified Newton scheme that just require to evaluate the determinant and its derivatives at a given pose. A consequence of the existences of such arcs is that the workspace may have several *aspects* i.e. workspace region that can be reached only for a given inverse kinematics solution and is unreachable for the other one(s).

#### 7.1.2. Cable-Driven Parallel Robots for large scale additive manufacturing

Participants: Jean-Pierre Merlet, Yves Papegay [correspondant].

Easy to deploy and to reconfigure, dynamically efficient in large workspaces even with payloads, cable-driven parallel robots are very attractive for solving displacement and positioning problems in architectural building at large scale seems to be a good alternative to crane and industrial manipulators in the area of additive manufacturing. We have co-founded in 2015 years ago the XtreeE (www.xtreee.eu) start-up company that is currently one of the leading international actors in large-scale 3D concrete printing.

We have been contacted this year by artists interested in mimicking the 3D additive manufacturing process on a large scale with glass micro-beads for a live art performance to be held in 2019 (www.lestanneries.fr/exposition/monuments-larmes-prince). We have been working on the design of the robotics system, namely a cables parallel robots with autonomous refilling capabilities.

## 7.1.3. Robotized ultrasound probe

#### Participant: Jean-Pierre Merlet.

In collaboration with the EPIONE project we have started investigation the development of a portable robotized cardiac ultrasound probe that may be used while performing an effort test. A first step, somewhat surprising was the necessity to instrument an existing probe in order to determine what are the forces that the doctor exert on the probe during an investigation and the maximal angulation of the probe (apparently this data has not been measured beforehand). We add an accelerometer (for measuring the angle) and a force sensor in a 3D-printed covering of the probe and recorded the data during several experiments. We were then planing to develop a small, portable 3 d.o.f. rotational parallel robot whose range of motion was within the maximum angles that has been determined experimentally and was able to sustain the force exerted by the doctor. Unfortunately there was not a general consensus between the doctors and the company manufacturing the probe on the number of d.o.f. that was requested for the robot (which clearly have a drastic influence on the mechanical design and on the dimensional synthesis of the robot) so that the project is on stand-by.

#### 7.1.4. Parallel robot performances and uncertainties

Participants: Jean-Pierre Merlet, Hiparco Lins Vieira [correspondant].

The purpose of this study, which is the PhD subject of H. Lins Vieira, is to develop interval analysis-based algorithm for determining if some performance requirements for parallel robots (e.g. on workspace, accuracy, load lifting ability) can be guaranteed in spite of the unavoidable manufacturing and control uncertainties of the system.

# 7.2. Assistance

We are still going on in building a framework for customizable and modular assistive robotics including hardware, software and communication and medical monitoring. The development of our platforms shows that we are now able to identify problematic issues for end-users, helpers and the medical community and to propose appropriate hardware/software solutions. But the most time consuming part of our work is related to evaluation and therefore experimentation: this involves legal/ethical issues (for which we have contributed [5]), participation of the medical community (for evaluation and recruitment) and heavy administrative management. Clearly we are lacking of permanent staff as we have long term objectives that cannot be fulfilled only with PhD or post-doc students. We need also engineers during specific periods (for hardware development and experimentation) but over a longer time than the one or two years currently proposed by Inria.

## 7.2.1. Rehabilitation in an immersive environment

Participants: Artem Melnyk, Jean-Pierre Merlet, Yves Papegay [correspondant], Ting Wang.

Rehabilitation is a tedious and painful process and it is difficult to assess its trend. Using an immersive environment has shown to increase the patient motivation but is not sufficient regarding rehabilitation efficiency. First the visual feedback (event 3D) is not sufficient to provide a full immersive feeling as body motion is not involved. Controlling body motion is also very important for therapists that currently must continuously correct the patient pose so that the rehabilitation exercise is the most efficient. We propose to add motion generators in the environment to reinforce realism (thereby increasing patient motivation) but also to allow therapists to use these generators to control the body pose so that they will be able to repeat rehabilitation exercises in a controlled context. Furthermore these generators are instrumented to provide information on the body pose and additional external sensors complete these measurements for rehabilitation assessment. We have developed 3 types of motions generators: one 6 d.o.f. motion base, a CDPR that is able to lift a patient and 2 multipurpose lifting columns.

When starting this project we were planning to use Inria-Sophia immersive room, hence allowing us to focus on the rehabilitation station. Unfortunately this room is no more available. This year we have developed a 2D renderer that has been connected to a flexible software platform allowing the various agents to exchange messages. We have been able to build a first version of our rehabilitation platform using a treadmill as exercise tool and columns to animate the treadmill (figure 1). For measuring the gait pattern we are using a planar lidar for detecting the leg motions, a kinect for detecting the motion of a skeleton and a distance sensor that measure the body motion with respect to the head of the treadmill. Figures 2 and 3 show an extract of the measurements obtained during a typical walk. It may be seen that the lidar data are very clean and allows one to estimate the mean position of the leg as a function of time (from which we will be able to deduce the number of steps, velocities of the leg, ...). Kinect data are much more noisy although that a fusion with the lidar data and the distance data will allows us to detect significant trunk motion. A typical walk of 3mn provides approximately 20 Mo of data.

Note that we are not using wearable sensors (although they are available: accelerometers for the arms and legs, shoes with pressure sensor and accelerometers): this is voluntary as our contacts with the medical community have indicated that many patients will not be comfortable with wearable sensors. In the same manner we have experimented having a headset instead of the screen but it appears that visualization is very disturbing and uncomfortable. Subject safety is ensured: during the exercise the subject must keep a push button pressed and when released the treadmill stop immediately. An emergency stop button is also available for the operator. Furthermore the system has been designed to provide various supports for avoiding fall and is surrounded by soft carpets.

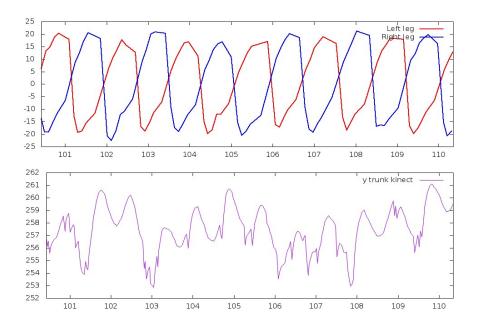


Figure 2. An extract of the legs motions in the walking direction as measured by the lidar and the trunk forward/backward motion estimated by the kinect

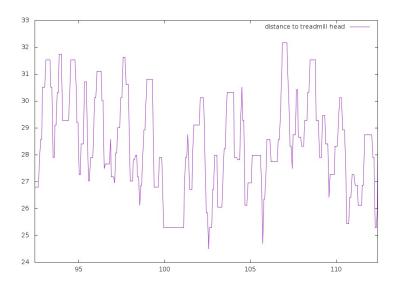


Figure 3. An extract of the trunk forward/backward motions as measured by the distance sensor in the head of the treadmill

The rehabilitation station for walking analysis on a treadmill in various walking condition is now almost fully functional and reliable. The next step will start of the beginning of 2019 with an experiment involving a cohort of voluntary subjects of Inria in order to obtain a significant amount of data. A statistical analysis of these data will then be performed in order to examine if synthetic and medically pertinent indicators (besides classical indicators such a number of steps, velocity, ...) may be obtained. The next step will involve repeating this experiment with pathological patients from Centre Héliomarin de Vallauris, most probably at the end of 2019. Meanwhile we will integrate our motion base as another element of the rehabilitation station with the purpose of equilibrium analysis, using a sea landscape as virtual environment with fans providing a realistic simulation of winds.

# 7.3. Smart Environment for Human Behaviour Recognition

**Participants:** Alain Coulbois, Aurélien Massein, Yves Papegay, Odile Pourtallier [correspondant], Eric Wajnberg.

The general aim of this research activity focuses on long term indoor monitoring of frail persons. In particular we are interested in early detection of daily routine and activity modifications. These modifications may indicate health condition alteration of the person and may require further medical or family care. Note that our work does not aim at detecting brutal modifications such as faintness or fall.

In our research we envisage both individual and collective housing such as rehabilitation center or retirement home.

Our work relies on the following leading ideas :

- We do not base our monitoring system on wearable devices since it appears that they may not be well accepted and worn regularly,
- Privacy advocates adequacy between the monitoring level needed by a person and the detail level of the data collected. We therefore strive to design a system fitted to the need of monitoring of the person.
- In addition to privacy concern, intrusive feature of video led us not to use it.

The main aspect that grounds this work is the ability to locate a person or a group in their indoor environment. We focus our attention to the case where several persons are present in the environment. As a matter of fact the single person case is less difficult.

This year we have focused our attention in several aspects : improvement of the hardware of the experimental monitoring system and tools for handling and analyzing the data gathered.

The PhD work about optimal location of sensors in a smart environments has been defended in november, defining new metrics on set of sensors and new methods <sup>0</sup>.

## 7.3.1. Hardware

Two monitoring systems have been installed. The first one in the first floor of EHPAD Valrose in Nice, and a second one in Institut Claude Pompidou in Nice. Both systems are composed of multi sensors barriers that provide raw data from which we deduce the time and direction of its crossing by a person.

For the second experimental system the analysis of the first data have shown that the system was not reliable enough while the data themselves were not satisfactory because of the specificity of the building (large corridors, large waiting room, picture windows and the number of sensors installed (77). We have worked on the hardware of the system (redundant power supply, better orientation of barriers, better communication system) to improve the gathered data.

<sup>&</sup>lt;sup>0</sup>Design of Instrumented Environment for Human Monitoring, defended on 12/26/2018

#### 7.3.2. Tools for handling data and data analysis

We have developed a simulation program, written in C and using the GTK library, that generates barrierevents (i.e. crossing time, direction of crossing, speed of crossing). This program is based on Monte Carlo procedures simulating the displacement of both elderly and caregivers in the EHPAD environment equipped with movement detectors. The code can simulate up to 20 persons and randomly draws room-to-room movements according to the walking speed of each individual (caregivers walk at a faster pace than elderly), and counts the locations and time coordinates of each movement event identified by the detectors. The figure 4 gives a view of the graphic interface. Such a simulation program, and the results produced, will provide basic training data to reconstruct patient movements from the information collected by the activity detectors.

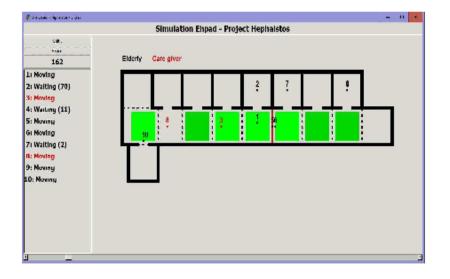


Figure 4. Simulation tool for event detection analysis

Another scientific activities were based on the development of diagnostic tools (also written in C) to visualize (and thus to check and to interpret) events identified by each detector in such equipped environment. Finally, another activity – that is still under development – is to analyze statistically gait data obtained through the event detection. In this case, the goal is to build a series of relevant statistical descriptive parameters that will be used to describe, identify and compare gait features and pathology in medically assisted environments. This last part is developed used the R software.

In the two installed system data are collected continuously during the all day and a large number of barrier crossing is observed. We are currently comparing raw and simulated data before moving on with a statistical analysis.

# **STARS Project-Team**

# 7. New Results

# 7.1. Introduction

This year Stars has proposed new results related to its three main research axes : perception for activity recognition, semantic activity recognition and software engineering for activity recognition.

## 7.1.1. Perception for Activity Recognition

**Participants:** François Brémond, Juan Diego Gonzales Zuniga, Abhijit Das, Antitza Dancheva, Furqan Muhammad Khan, Michal Koperski, Thi Lan Anh Nguyen, Remi Trichet, Ujjwal Ujjval, Srijan Das, Vikas Thamizharasan, Monique Thonnat.

The new results for perception for activity recognition are:

- Late Fusion of multiple convolutional layers for pedestrian detection (see 7.2)
- Deep Learning applied on Embedded Systems for People Tracking (see 7.3)
- Cross Domain Residual Transfer Learning for Person Re-identification (see 7.4)
- Face-based Attribute Classification (see 7.5)
- Face Attribute manipulation
- From attribute-labels to faces: face generation using a conditional generative adversarial network (see 7.6)
- Face analysis in structured light images (see 7.7)

#### 7.1.2. Semantic Activity Recognition

**Participants:** François Brémond, Antitza Dantcheva, Farhood Negin, Thanh Hung Nguyen, Michal Koperski, Srijan Das, Kaustubh Sakhalkar, Arpit Chaudhary, Abhishek Goel, Abdelrahman Abubakr, Abhijit Das, Yaohui Wang, S L Happy, Alexandra König, Guillaume Sacco, Philippe Robert, Soumik Mallick, Julien Badie, Monique Thonnat.

For this research axis, the contributions are :

- Deep-Temporal LSTM for Daily Living Action Recognition (see 7.8)
- A New Hybrid Architecture for Human Activity Recognition from RGB-D videos (see 7.10)
- Where to focus on for Human Action Recognition? (see 7.11)
- Online temporal detection of daily-living human activities in long untrimmed video streams (see 7.12)
- Activity Detection in Long-term Untrimmed Videos (see 7.13)
- Video based face analysis for health monitoring (see 7.14)
- Mobile biometrics (see 7.15)
- Comparing methods for assessment of facial dynamics in patients with major neurocognitive disorders (see 7.16)
- Combating the issue of low sample size in facial expression recognition (see 7.17)
- Serious exergames for Cognitive Stimulation (see 7.18)
- Fully Automatic Speech-Based Analysis of the Semantic Verbal Fluency Task (see 7.19)
- Language Modelling in the Clinical Semantic Verbal Fluency Task (see 7.19.2)
- Telephone-based Dementia Screening I: Automated Semantic Verbal Fluency Assessment (see 7.19.3)
- Automatic Detection of Apathy using Acoustic Markers extracted from Free Emotional Speech and using Automatic Speech Analysis (see 7.19.4)
- Monitoring the Behaviors of Retail Customers (see 7.20)

#### 7.1.3. Software Engineering for Activity Recognition

**Participants:** Sabine Moisan, Annie Ressouche, Jean-Paul Rigault, Ines Sarray, Daniel Gaffé, Julien Badie, François Brémond, Minh Khue Phan Tran.

The contributions for this research axis are:

- A Synchronous Approach to Activity Recognition (see 7.21)
- A Probabilistic Activity Description Language (see 7.22)

# 7.2. Late Fusion of Multiple Convolutional Layers for Pedestrian Detection

Participants: Ujjwal Ujjwal, François Brémond, Aziz Dziri [VEDECOM], Bertrand Leroy [VEDECOM].

One of the prominent problems in pedestrian detection is handling scale and occlusion. These problems are quite well aligned with the recent interests in autonomous vehicles. Successful detection of far-scale pedestrians can assist the vehicle in making safety maneuvers well ahead in time, thereby promoting a safer traffic environment. The same is true for surveillance systems in high security environment like airports and ports.

We propose a system design for pedestrian detection by leveraging the power of multiple convolutional layers explicitly (see Figure 5). We quantify the effect of different convolutional layers on the detection of pedestrians of varying scales and occlusion level. We show that earlier convolutional layers are better at handling small-scale and partially occluded pedestrians. We take cue from these conclusions and propose a pedestrian detection system design based on Faster-RCNN which leverages multiple convolutional layers by late fusion. In our design, we introduce height-awareness in the loss function to make the network emphasize on pedestrian heights which are misclassified during the training process. The proposed system design achieves a log-average miss-rate of 9.25% on the caltech-reasonable dataset. This is within 1.5% of the current state-of-art approach, while being a more compact system. The work was published in the 15<sup>th</sup> IEEE International Conference on Advanced Video and Signal-based Surveillance (AVSS)-2018 [51].

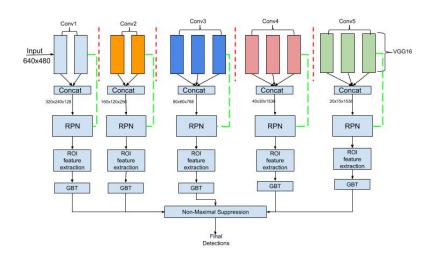


Figure 5. Block diagram of our proposed Multiple-RPN pedestrian detection system

# 7.3. Deep Learning applied on Embedded Systems for People Tracking

**Participants:** Juan Diego Gonzales Zuniga, Thi Lan Anh Nguyen, Francois Brémond, Serge Tissot [KON-TRON].

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#### Keywords: Deep Learning, Embedded Systems, Multiple Object Tracking

One of the main issues with people detection and tracking is the amount of resources it consumes for real time applications. Most architectures either require great amounts of memory or large computing time to achieve a state-of-the-art performance, these results are mostly achieved with dedicated hardware at data centers. The applications for an embedded hardware with these capabilities are limitless: automotive, security and surveillance, augmented reality and health-care just to name a few. But the state-of-the-art architectures are mostly focused on accuracy rather than resource consumption.

In our work, we have to consider improving the systems' accuracy and reducing resources for real-time applications. We are creating a shared effort of hardware adaptation and agnostic software optimization for all deep learning based solutions.

We here focus our work on two separated but linked problems.

First, we improve the feature representation of tracklets for the Multiple Object Tracking challenge. This is based on the concept of Residual Transfer Learning [44]. Second, we are creating a viable platform to run our algorithms on different target hardware, mainly, Intel Xeon Processors, FPGAs and AMD GPUs.

#### 7.3.1. Residual Transfer Learning :

We present a smart training alternative for transfer learning based on the concept of ResNet [65]. In ResNet, a layer learns the estimate residual between the input and output signals. We cast transfer learning as a residual learning problem, since the objective is to close the gap between the initial network and the desired one. Achieving this goal is done by adding residual units for a number of layers to an existing model that needs to be transferred from one task to another. The existing model can thus be able to perform a new task by adding and optimizing residual units as shown in Figure 6. The main advantage of using residual units for transfer learning is the flexibility in terms of modelling the difference between two tasks.

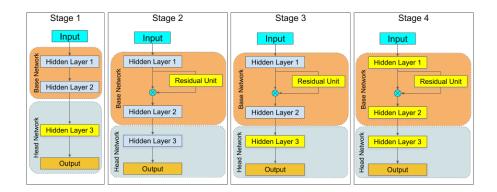


Figure 6. Training stages of Residual Transfer Learning method. Each stage only trains the layers shown in yellow, and fixes the layers in grey. The residual units are added at the second stage

#### 7.3.2. Deep Learning Platform on Multiple Target Hardware :

Deep learning algorithms need an extensive allocation of resources to be executed, most of the research is accomplished under NVIDIA GPU's. This is limiting because it reduces the possibilities on how to optimize certain blocks that directly depend on the hardware configuration. The main cause is the lack of a flexible platform that would support different targets: AMD GPUs, Intel Xeon processors and specialized FPGAs.

We work with two hardware based platforms; ROCm and Openvino. The ROCm stack, shown in Figure 7, allows us to perform a variety of layer computations on AMD GPUs. We have managed to import different deep learning networks such as VGG16, ResNet and Inception to AMD's Radeon graphics card. On the other hand, Openvino's main goal is to reduce the inference time of a network. For this solution, we count on the Openvino Optimizer, shown in Figure 8, which main goal is to transform the network model from Caffe or Tensorflow into an Inference Model for Intel's processors and FPGAs.

We also built docker images on top of the above mention platforms, this is done to speed the deployment stage by being operating system independent.

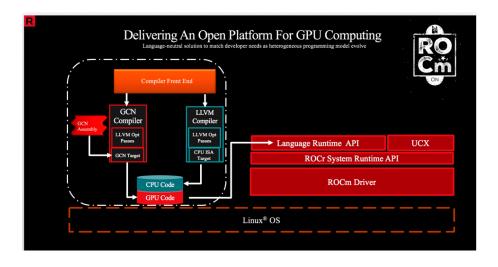


Figure 7. The ROCm System Runtime is language independent and makes heavy use of the Heterogeneous System Architecture.

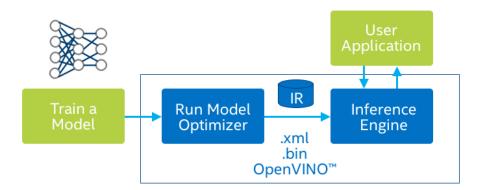


Figure 8. Openvino: When you run a pre-trained model through the Model Optimizer, your output is an Intermediate Representation of the network.

## 7.4. Cross Domain Residual Transfer Learning for Person Re-identification

Participants: Furqan Khan, Francois Brémond.

Keywords: multi-shot person re-identification, transfer learning, residual unit

Person re-identification (re-ID) refers to the retrieval task where the goal is to search for a given person (query) in disjoint camera views (gallery). Performance of appearance based person re-ID methods depends on the similarity metric and the feature descriptor used to build a person's appearance model from given image(s).

A novel way is proposed to transfer model weights from one domain to another using residual learning framework instead of direct fine-tuning. It also argues for hybrid models that use learned (deep) features and statistical metric learning for multi-shot person re-identification when training sets are small. This is in contrast to popular end-to-end neural network based models or models that use hand-crafted features with adaptive matching models (neural nets or statistical metrics). Our experiments demonstrate that a hybrid model with residual transfer learning can yield significantly better re-identification performance than an end-to-end model when training set is small. On iLIDS-VID [78] and PRID [67] datasets, we achieve rank1 recognition rates of 89.8% and 95%, respectively, which is a significant improvement over state-of-the-art.

## 7.4.1. Residual Transfer Learning

We use RTL to transfer a model trained on Imagenet [63] for object classification to perform person re-ID. We chose to use 16-layer VGG model due to its superior performance in comparison to AlexNet and overlooked ResNet for its extreme depth because our target datasets are small and do not warrant such a deep model for higher performance.

One advantage of using residual learning [66] for model transfer is that it allows more flexibility in terms of modeling the difference between two tasks through a number of residual units and their composition. We noted that when residual units are added to the network with a different network head, training loss is significantly higher in the beginning which pushes the network far away from pre-trained solution by trying to over compensate through residual units. To avoid this, we propose to train the network in 4 stages, with fourth stage being optional (Fig. 9). The proposed work has been published in [45].

- **Stage 1**: In the first stage, we replace original head of the network with a task specific head and initialize it randomly. At this stage, we do not add any residual units to the network and train only the parameters of the replaced head of the network. Thus only the head layers are considered to contribute to the loss. This allows the network to learn noisy high level representation for the desired task and decrease the network loss without affecting lower order layers.
- **Stage 2**: In the second stage, we add residual units to the network and initialize them randomly. Then we freeze all other layers, including the network head, and optimize the parameters of added residual units. As the head and other layers are fixed, residual units are considered as the source of loss. As we start with a reasonably low loss value, residual units are not forced to over compensate for the loss.
- Stage 3: In the third stage, we train the network by learning parameters of both added residual units and network head, thus allowing both the lower and higher order representations to adjust to the specific task.
- **Stage 4 (Optional)**: We noticed in our experiments on different datasets that the loss function generally gets low enough by the end of third stage. However, if needed, the whole network can be trained to further improve performance.

## 7.4.2. Conclusion

When using identity loss and large amount of training data, RTL gives comparable performance to direct finetuning of network parameters. However, the performance difference between two transfer learning approaches is considerably in favor of RTL when training sets are small. The reason is that when using RTL only a few parameters are modified to compensate for the residual error of the network. Still, the higher order layers of the network are prone to over-fitting. Therefore, we propose using hybrid models where higher order domain

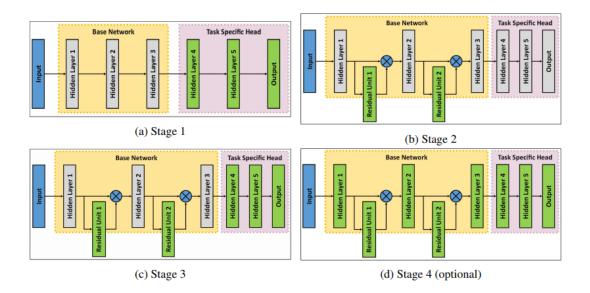


Figure 9. Residual Transfer Learning in 4 stages. During each stage only the selected layers (shown in green) are trained. Residual Units are added to the network after first stage of RTL.

specific layers are replaced with statistical metric learning. We demonstrate that the hybrid model performs significantly better on small datasets and gives comparable performance on large datasets. The ability of the model to generalize well from small amount of data is crucial for practical applications because frequent data collection in large amount for training is nit possible.

## 7.5. Face-based Attribute Classification and Manipulation

Participants: Abhijit Das, Antitza Dantcheva, Francois Brémond.

#### Keywords: Face, Attribute, GAN, Biometrics

Due to the biasness of face analytic datasets, with respect to factors such as age, gender, ethnicity, pose and resolution, systems based on a skewed training dataset are bound to produce skewed results. Further, it has been exhibited in the literature [59] that such biases may have serious impacts on performance in challenging situations where the outcome is critical. In order to progress toward balanced face recognition and attribute estimation, the 1st International Workshop on Bias Estimation in Face Analytics was organized in conjunction with ECCV 2018. The workshop also organized a challenge to introduce a well-balanced dataset across multiple factors: age, gender, ethnicity, pose and resolution and requested for algorithms to estimate biases.

We proposed a Multi-Task Convolutional Neural Network (MTCNN) algorithm that jointly learned [37] gender, age and ethnicity by a loss function involving joint dynamic loss weight adjustment and was successful, as well as relatively unbiased in estimating age, gender and ethnicity. Our algorithm was found to be the best algorithm focusing the aim of the competition and the above mentioned research problem.

#### 7.5.1. Generative Adversal Network (GAN)

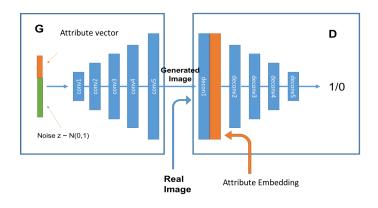
models are autoregressive models depending on the global information, which can be potentially affected by its employment on local feature/ attribute-based erasuring. In addition, these models are typically trained depending on the maximum likelihood to find the intense difference between the regression domains, as a result after a certain limit of learning it can produce very naive development in the interpolation of the regression carried out for the purpose of local attribute removal. Hence, to mitigate an aforementioned couple of pitfalls we propose a method for localizing the Cycle GAN (C-GAN) for local feature-based regression. We trained the C-GAN with domain-specific local feature and end model was recurrently imposed on the testing images. We experimented the Local C-GAN (L-C-GAN) on facial attribute (eyeglass and moustache/ bearded) auto-regression. Our qualitative performance on partial CelebA dataset and a couple of datasets we collected is promising. Moreover, ensuring the facial attributes have also been found to achieve better performance accuracy with respect to the presence of these attributes.

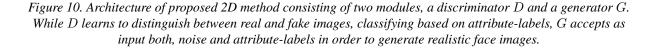
# 7.6. From Attribute-labels to Faces: Face Generation using a Conditional Generative Adversarial Network ,

Participants: Yaohui Wang, Antitza Dantcheva, Francois Brémond.

Keywords: Generative Adversarial Networks, Face generation

Facial attributes are instrumental in semantically characterizing faces. Automated classification of such attributes (i.e., age, gender, ethnicity) has been a well studied topic. We here seek to explore the inverse problem, namely given attribute-labels the *generation of attribute-associated faces*. The interest in this topic is fueled by related applications in law enforcement and entertainment. In this work, we propose two models for attribute-label based facial image and video generation incorporating 2D (see Figure 10) and 3D (see Figure 11) deep conditional generative adversarial networks (DCGAN). The attribute-labels serve as a tool to determine the specific representations of generated images and videos. While these are early results (see Figure 12 and 13), our findings indicate the methods' ability to generate realistic faces from attribute labels.





## 7.7. Face Analysis in Structured Light Images

Participants: Vikas Thamizharasan, Antitza Dantcheva, Francois Brémond.

Keywords: Structured light, Face analysis

The main objective has been to perform face analysis tasks like authentication, gender, age and ethnicity classification by generating low-dimensional face embedding from the raw data acquired from structured light (see Figure 14) sensors using deep learning techniques. In this context we studied depth/disparity map extraction (see Figure 15), as well as other models.

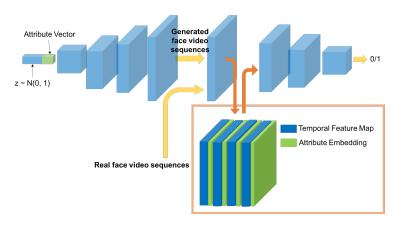


Figure 11. Architecture of proposed 3D model for face video generation

## 7.8. Deep-Temporal LSTM for Daily Living Action Recognition

Participants: Srijan Das, Michal Koperski, Francois Brémond, Gianpiero Francesca.

Keywords: Temporal sequences, Appearance, LSTM

We have proposed to improve the traditional use of RNNs by employing a many to many model for video classification. We analyzed the importance of modeling spatial layout and temporal encoding for daily living action recognition. Many RGB methods focus only on short term temporal information obtained from optical flow. Skeleton based methods on the other hand show that modeling long term skeleton evolution improves action recognition accuracy. In this work, we proposed a deep-temporal LSTM architecture (see fig. 16) which extends standard LSTM and allows better encoding of temporal information. In addition, we have proposed to fuse 3D skeleton geometry with deep static appearance. We validated our approach on publicly available datasets (CAD60, MSRDailyActivity3D and NTU-RGB+D), achieving competitive performance as compared to the state-of-the art. The proposed framework has been published in AVSS 2018 [39].

## 7.9. Spatio-Temporal Grids for Daily Living Action Recognition

Participants: Srijan Das, Kaustubh Sakhalkar, Michal Koperski, Francois Brémond.

Keywords: Spatio-temporal, Grids, Multi-modal

This work addresses the recognition of short-term daily living actions from RGB-D videos. Most of the existing approaches ignore spatio-temporal contextual relationships in the action videos. So, we have proposed to explore the spatial layout to better model the appearance. In order to encode temporal information, we divided the action sequence into temporal grids. We address the challenge of subject invariance by applying clustering on the appearance features and velocity features to partition the temporal grids. We validated our approach on four public datasets. The results show that our method is competitive with the state-of-the-art. The proposed architecture has been published in ICVGIP 2018 [40].

## 7.10. A New Hybrid Architecture for Human Activity Recognition from RGB-D videos

**Participants:** Srijan Das, Monique Thonnat, Kaustubh Sakhalkar, Michal Koperski, Francois Brémond, Gianpiero Francesca.

Keywords: Visual cues, Data fusion, RGB-D videos



(a) no glasses, female, black hair, smiling, young



(b) glasses, female, black hair, not smiling, old



(c) no glasses, male, no black hair, smiling, young



(d) glasses, male, no black hair, not smiling, old *Figure 12. Example images generated by the proposed 2D model.* 



(a) male, adolescent



(b) male, adult



(c) female, adolescent



(d) male, adult Figure 13. Chosen output samples from 3DGAN



Figure 14. Structured light. A calibrated camera and projector (typically both near infrared) are placed at a fixed, known baseline. The structured light pattern helps establish correspondence between observed and projected pixels. Depth is derived for each corresponding pixel through triangulation. The process is akin to two stereo cameras, but with the projector system replacing the second camera, and aiding the correspondence problem.

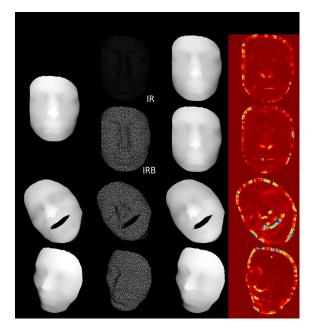


Figure 15. \*IR - Infrared image, IRB - Binarized Infrared image

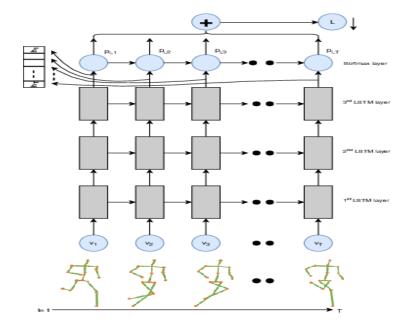


Figure 16. Framework of the deep-temporal LSTM proposed approach in [39]

Activity Recognition from RGB-D videos is still an open problem due to the presence of large varieties of actions. We have proposed a new architecture by mixing a high level handcrafted strategy and machine learning techniques. In order to address the problem of large variety of actions, we proposed a novel two level fusion strategy to combine motion, appearance and 3D pose information. For 3D pose information, we use the work published in AVSS 18 (described above). As similar actions are common in daily living activities, we also proposed a mechanism for similar action discrimination using dedicated SVMs. We validated our approach on four public datasets, CAD-60, CAD-120, MSRDailyActivity3D, and NTU-RGB+D improving the state-of-the-art results on them. The proposed architecture has been published in the industrial session of MMM 2019 [41].

## 7.11. Where to Focus on for Human Action Recognition?

**Participants:** Srijan Das, Arpit Chaudhary, Francois Brémond, Monique Thonnat. **Keywords:** Spatial attention, Body parts, End-to-end

We proposed a spatial attention mechanism based on 3D articulated pose to focus on the most relevant body parts involved in the action. For action classification, we proposed a classification network compounded of spatio-temporal subnetworks modeling the appearance of human body parts and RNN attention subnetwork implementing our attention mechanism. Furthermore, we trained our proposed network end-to-end using a regularized cross-entropy loss, leading to a joint training of the RNN delivering attention globally to the whole set of spatio-temporal features, extracted from 3D ConvNets. Our method outperforms the State-of-the-art methods on the largest human activity recognition dataset available to-date (NTU RGB+D Dataset) which is also multi-views and on a human action recognition dataset with object interaction (Northwestern-UCLA Multiview Action 3D Dataset). The proposed framework will be published in WACV 2019. Sample visual results displaying the attention scores attained for each body parts can be seen in fig. 17.

# 7.12. Online Temporal Detection of Daily-Living Human Activities in Long Untrimmed Video Streams

**Participants:** Abhishek Goel, Abdelrahman G. Abubakr, Michal Koperski, Francois Brémond. **keywords:** Daily-living activity recognition, Human activity detection, Video surveillance, Smarthome

Many approaches were proposed to solve the problem of activity recognition in short clipped videos, which achieved impressive results with hand-crafted and deep features. However, it is not practical to have clipped videos in real life, where cameras provide continuous video streams in applications such as robotics, video surveillance, and smart-homes. Here comes the importance of activity detection to help recognizing and localizing each activity happening in long videos. Activity detection can be defined as the ability to localize starting and ending of each human activity happening in the video, in addition to recognizing each activity label. A more challenging category of human activities is the daily-living activities, such as eating, reading, cooking, etc, which have low inter-class variation and environment where actions are performed are similar. In this work we focus on solving the problem of detection of daily-living activities in untrimmed video streams. We introduce new online activity detection pipeline that utilizes single sliding window approach in a novel way; the classifier is trained with sub-parts of training activities, and an online frame-level early detection is done for sub-parts of long activities during detection. Finally, a greedy Markov model based post processing algorithm is applied to remove false detection and achieve better results. We test our approaches on two daily-living datasets, DAHLIA and GAADRD, outperforming state of the art results by more than 10%. The proposed work has been published in [43].

## 7.12.1. The Work Flow of processing untrimmed videos is composed of three tasks:

- Feature extraction consists in extracting the Person-Centered CNN (PC-CNN) features as shown in fig. 18.
- **Classifier Training:** All training videos are first divided into relatively small windows of size W frames, which represent activity sub-videos (subparts). Then the features are generated for all these windows and the training is done with linear SVM classifier using all activities sub-videos.
- **Majority voting filtering**, as depicted in fig. 19, looks up for neighbors within a certain range that have the same label apply majority-voting between the labels

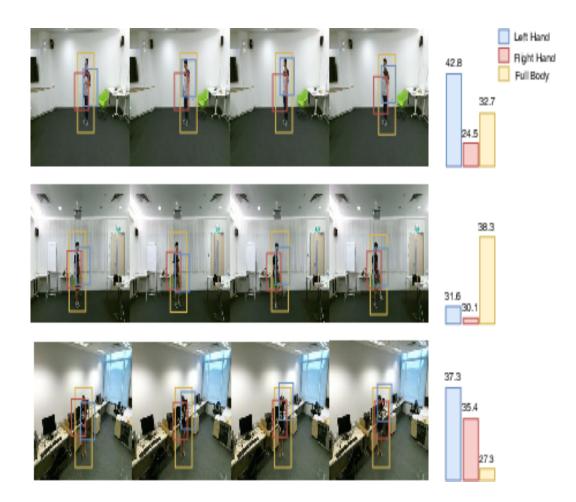


Figure 17. Example of video sequences with their respective attention scores. The action categories presented are drinking water with left hand (1st row), kicking (2nd row) and brushing hair with left hand (last row).



Figure 18. Extracting the Person-Centered CNN (PC-CNN) features

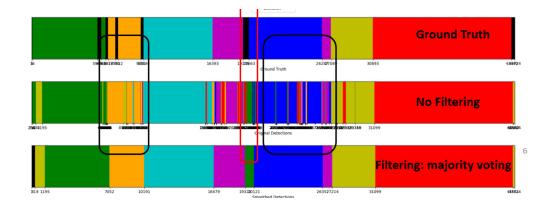


Figure 19. Post-filtering

# 7.13. Activity Detection in Long-term Untrimmed Videos by discovering sub-activities

**Participants:** Farhood Negin, Abhishek Goel, Abdelrahman G. Abubakr, Gianpiero Francesca, Francois Brémond.

Keywords: Activity detection, Semi-supervised learning, Sub-activity detection.

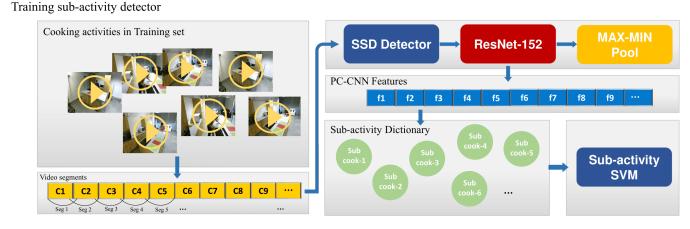


Figure 20. The process of extracting PC-CNN features and training of a weakly supervised sub-activity detector for the "Cooking" activity.

Detecting temporal delineation of activities is important to analyze large-scale videos. However, there are still challenges yet to be overcome in order to have an accurate temporal segmentation of activities. Detection of daily-living activities is even more challenging due to their high intra-class and low inter-class variations, complex temporal relationships of sub-activities performed in realistic settings. To tackle these problems, we

propose an online activity detection framework based on the discovery of sub-activities. We consider a long-term activity as a sequence of short-term sub-activities. Our contributions can be summarized as follows:

- We introduce a new online frame-level activity detection pipeline which uses single-sized window approach. A weakly supervised classifier is trained directly on sub-activities discovered by clustering and operates on test videos to capture sub-activities of long videos within a fixed temporal window.
- To alleviate the noisy detections especially in activity boundaries, we propose a novel greedy postprocessing method based on Markov models.
- We have extensively evaluated our proposed method on untrimmed videos from DAHLIA [68] and GAADRD [77] datasets and achieved state-of-the-art performances.

#### 7.13.1. Proposed Method:

Our framework produces frame-level activity labels in an online manner by two major steps followed by a novel greedy post-processing technique. In order to handle long activities, activities are decomposed into a sequence of fixed-length overlapping temporal clips. We then extract deep features from the clips. We suggested a person-centric feature (PC-CNN) based on SSD detector that satisfies required processing efficiency of online systems. We then proposed a weakly-supervised method for the discovery of sub-activities of long-term activities which benefits from clustering and model selection methods to find the optimal subactivities of the given activities. In order to characterize each activity with constituent sub-activities, we use K-means to cluster that activity's clips and construct a specific sub-activity dictionary. Therefore, we have one sub-activity dictionary for each main activity. We represent an activity sequence with sub-activity assignments using the trained dictionary. Then, for each activity class, we train a binary SVM classifier (one versus all) based on its sub-activities (Figure 20). The trained classifiers are then simultaneously used to produce framelevel activity labels with the help of a sliding window architecture. It should be noticed that unlike multiscale sliding window methods, we only use a single fixed-size temporal window thanks to recognition of fixed length sub-activities. Finally, assuming temporal progression of sub-activities, we developed a greedy algorithm based on Markov models to refine noisy sub-activity proposals in middle and boundary regions of long activities. We evaluated the proposed method on two daily-living activity datasets and achieved state-ofthe-art performances.

|        | performance. |         |      |                        |        |       |            |         |              |      |         |      |
|--------|--------------|---------|------|------------------------|--------|-------|------------|---------|--------------|------|---------|------|
|        | ELS          |         |      | Max Subgraph<br>Search |        |       | DOHT (HOG) |         | Sub Activity |      |         |      |
|        | FA_1         | F_score | IoU  | FA_1                   | F_scor | e IoU | FA_1       | F_score | IoU          | FA_1 | F_score | IoU  |
| View 1 | 0.18         | 0.18    | 0.11 | -                      | 0.25   | 0.15  | 0.80       | 0.77    | 0.64         | 0.85 | 0.81    | 0.73 |
| View 2 | 0.27         | 0.26    | 0.16 | -                      | 0.18   | 0.10  | 0.81       | 0.79    | 0.66         | 0.87 | 0.82    | 0.75 |
| View 3 | 0.52         | 0.55    | 0.39 |                        | 0.44   | 0.31  | 0.80       | 0.77    | 0.65         | 0.82 | 0.76    | 0.69 |

Table 1. The activity detection results obtained on the DAHLIA. Values in bold represent the best performance

Table 2. Detection results obtained on the GAADRD dataset.

| Method                           | FA_1 | F_score | IoU  |  |  |  |
|----------------------------------|------|---------|------|--|--|--|
| simple sliding window(HOG)       | 0.68 | 0.52    | 0.40 |  |  |  |
| simple sliding<br>window(PC-CNN) | 0.61 | 0.55    | 0.44 |  |  |  |

Tables 1 and 2 show the results of applying the developed frameworks on DAHLIA and GAADRD respectively. It can be noticed that in DAHLIA dataset (compared to [71], [61], [60]), we significantly outperformed state-of-the-art results in all of the categories except in camera view 3 when the F-Score metric is used. We reported the results of GAADRD dataset with the two types of features HOG and PC-CNN. As it can be seen, even with hand-crafted features our framework produces comparable results. In future work, we

are going to improve the sub-activity discovery algorithm by making it able to distinguish similar sub-activities in two different activities.

## 7.14. Video based Face Analysis for Health Monitoring

Participants: Abhijit Das, Antitza Dantcheva, Francois Brémond.

Keywords: Face, Attribute, GAN, Biometrics

Video based analysis in severely demented Alzheimer's Disease (AD) patients can be helpful for the analysis of their neuropsychiatric symptom such as apathy, depression. Even for the doctors it can be hard to know whether a person has depression or apathy. The main difference is that a person with depression will have feelings of sadness, be tearful, feel hopeless or have low self-esteem. Whereas, symptoms of person suffering from apathy can make the person's life less enjoyable. Therefore, a psychological protocol scenario can be used for video-based emotion analysis and facial movement can be used for discriminating apathetic person and non-apathetic person.

We proposed to use a) the facial expressions (neutral + 6 basic emotions: anger, disgust, happiness, surprise, sadness, fear) extracted using 50 layer Resnet, b) facial movements employing 68 facial landmark points, c) action unit intensity and frequency for AU 1, 2, 4, 5, 6, 7, 9, 10, 12, 14, 15, 17, 20, 23, 25, 26, and 45 using OpenFace and d) lip movements employing the 3D mouth open vector using the mean of upper lip and mean of bottom lip extracted from the facial landmarks detected around the lip as feature for each frame of the video. We post-process the features and calculated the amplitude, SD (Standard Deviations) and mean of each clip (10 seconds per clip) and these features were passed inputs to GRU. The GRU is connected to the Fully Connected layers, these fully connected features are mean pooled to get the apathy/non-apathy classification.

## 7.15. Mobile Biometrics

Participants: Abhijit Das, Antitza Dantcheva, Francois Brémond.

Keywords: Mobile biometrics

The prevalent commercial deployment of mobile biometrics as a robust authentication method on mobile devices has fueled increasingly scientific attention. Motivated by this, in this work [38] we seek to provide insight on recent development in mobile biometrics. We present parallels and dissimilarities of mobile biometrics and classical biometrics, enumerate related strengths and challenges. Further, we provide an overview of recent techniques in mobile bio-metrics, as well as application systems adopted by industry. Finally, we discuss open research problems in this field.

## 7.16. Comparing Methods for Assessment of Facial Dynamics in Patients with Major Neurocognitive Disorders

Participants: Yaohui Wang, Antitza Dantcheva, Francois Brémond.

Keywords: Face Analysis

Assessing facial dynamics in patients with major neurocognitive disorders and specifically with Alzheimer's disease (AD) has shown to be highly challenging. Classically such assessment is performed by clinical staff, evaluating verbal and non-verbal language of AD-patients, since they have lost a substantial amount of their cognitive capacity, and hence communication ability. In addition, patients need to communicate important messages, such as discomfort or pain. Automated methods would support the current healthcare system by allowing for telemedicine, *i.e.*, lesser costly and logistically inconvenient examination. In this work [52], we compare methods for assessing facial dynamics such as talking, singing, neutral and smiling in AD-patients, captured during music mnemotherapy sessions. Specifically, we compare 3D ConvNets (see Figure 21), Very Deep Neural Network based Two-Stream ConvNets (see Figure 22), as well as Improved Dense Trajectories. We have adapted these methods from prominent action recognition methods and our promising results suggest that the methods generalize well to the context of facial dynamics. The Two-Stream ConvNets in combination with ResNet-152 obtains the best performance on our dataset (Table 3), capturing well even minor facial dynamics and has thus sparked high interest in the medical community.

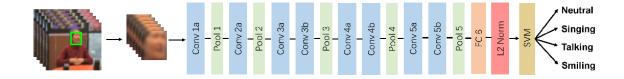
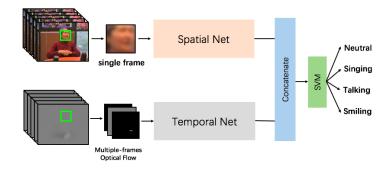
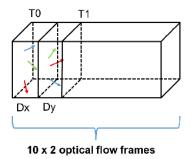


Figure 21. **C3D based facial dynamics detection:** For each video sequence, faces are detected and the face sequences are passed into a pre-trained C3D network to extract a 4096-dim feature vector for each video. Finally a SVM classifier is trained to predict the final classification result. We have blurred the faces of the subject in this figure, in order to preserve the patient's privacy.



(a) Two-Stream Architecture



(b) Stacked Optical Flow Field volume

Figure 22. (a) While the spatial ConvNet accepts a single RGB frame as input, the temporal ConvNet's input is the  $D_x$  and  $D_y$  of 10 consecutive frames, namely 20 input channels. Both described inputs are fed into the Two-stream ConvNets, respectively. We use in this work two variations of Very Deep Two Stream ConvNets, incorporating VGG-16 [76] ResNet-152 [65] for both streams respectively. (b) The optical flow of each frame has two components, namely  $D_x$  and  $D_y$ . We stack 10 times  $D_y$  after  $D_x$  for each frame to form a 20 frames length input volume.

| Table 3. Classification accuracies of C3D, Very Deep Two-Stream ConvNets, iDT, as well as fusion thereof |
|--|
| on the presented ADP-dataset. We report the Mean Accuracy (MA) associated to the compared methods.       |
| Abbreviations used: SNSpatial Net, TNTemporal Net.   |

| Method                                 | MA (%) |
|--|--------|
| C3D                                    | 67.4   |
| SN of Two-Stream ConvNets (VGG-16)     | 65.2   |
| TN of Two-Stream ConvNets (VGG-16)     | 69.9   |
| Two-Stream ConvNets (VGG-16)           | 76.1   |
| SN of Two-Stream ConvNets (ResNet-152) | 69.6   |
| TN of Two-Stream ConvNets (ResNet-152) | 75.8   |
| Two-Stream ConvNets (ResNet-152)       | 76.4   |
| iDT                                    | 61.2   |
| C3D + iDT                              | 71.1   |
| Two-Stream ConvNets (VGG-16) + iDT     | 78.9   |
| Two-Stream ConvNets (ResNet-152) + iDT | 79.5   |

# 7.17. Combating the Issue of Low Sample Size in Facial Expression Recognition

Participants: S L Happy, Antitza Dantcheva, Francois Brémond.

Keywords: Face analysis, Expression recognition

The universal hypothesis suggests that the six basic emotions - anger, disgust, fear, happiness, sadness, and surprise - are being expressed by similar facial expressions by all humans. While existing datasets support the universal hypothesis and contain images and videos with discrete disjoint labels of profound emotions, reallife data contain jointly occurring emotions and expressions of different intensities. Reliable data annotation is a major problem in this field, which results in publicly available datasets with low sample size. Transfer learning [73], [64] is usually used to combat the low sample size problem by capturing high level facial semantics learned on different tasks. However, models which are trained using categorical one-hot vectors often over-fit and fail to recognize low or moderate expression intensities. Motivated by the above, as well as by the lack of sufficient annotated data, we here propose a weakly supervised learning technique for expression classification, which leverages the information of unannotated data. In weak supervision scenarios, a portion of training data might not be annotated or wrongly annotated [79]. Crucial in our approach is that we first train a convolutional neural network (CNN) with label smoothing in a supervised manner and proceed to tune the CNN-weights with both labelled and unlabelled data simultaneously. The learning method learns the expression intensities in addition to classifying them into discrete categories. This bootstrapping of a fraction of unlabelled samples, replacing labelled data for model-update, while maintaining the confidence level of the model on supervised data improves the model performance.

| Test databases | Percentage of training data |        |        |  |  |
|----------------|-----------------------------|--------|--------|--|--|
|                | 25%                         | 50%    | 80%    |  |  |
| CK+ (test-set) | 88.79%                      | 91.29% | 95.16% |  |  |
| RaFD           | 64.25%                      | 65.25% | 78.46% |  |  |
| lifespan       | 35.13%                      | 40.51% | 60.83% |  |  |

Table 4. Cross database classification performance when using CK+ database for training.

#### 7.17.1. Experimental Results

Experiments were conducted on three publicly available expression datasets, namely CK+, RaFD, and lifespan. Substantial experiments on these datasets demonstrate large performance gain in cross-database performance,

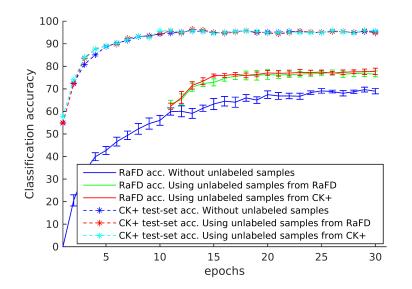


Figure 23. Cross-database experiments show significant performance improvement.

as well as show that the proposed method achieves to learn different expression intensities, even when trained with categorical samples. As can be seen in Fig. 23, when the model is trained on CK+ with unlabelled data, the model-performance improved by 11% in RaFD cross database evaluation. We observe that the use of unlabelled data from either CK+ or RaFD results in similar performances. Utilizing unlabelled images from CK+, the network sees varying expression-intensities and adapts to it. Table 4 reports the self and cross-database classification results with respect to varying number of training samples. Significant classification accuracy has been obtained with merely 25% of the training data. Use of a larger labelled training set strikingly boosts the cross-database performance. In future, we are planning to further improve the performance with unsupervised learning of expression patterns.

## 7.18. Serious Exergames for Cognitive Stimulation

Participants: Guillaume Sacco, Monique Thonnat.

**Keywords:** Neurocognitive disorders, Serious games, Geriatrics, Executive functions, Physical exercise, Cognitive training

A PhD thesis has been defended on the 8th of June at Nice University on this topic by Guillaume Sacco. This thesis presents a clinical and therapeutic approach aiming to create new care for patients with neurocognitive disorder. Serious exergames are serious video games integrating physical activity. Serious exergames could be tools to product enriched environment associating physical exercise and cognitive training. The aim of this thesis is to investigate whether serious exergames can contribute to the non-pharmacological management of neurocognitive disorders. In this thesis we have made two types of contributions. The first type are general contributions. One presents our integrative clinical approach associating physical exercise and cognitive training using serious exergames. The other one presents recommendations concerning the use of serious exergames. The second type of contributions are experimental. The first one aims to confirm a theoretical base of our clinical approach. The two other experiments assess the implementation of our approached in a population of patients with neurocognitive disorder. This year the integrative clinical approach associating physical exercise and cognitive training using serious exergames using serious exergames has been published [32] and presented at the International Conference on Gerontechnology ISG in Saint Petersburg, Florida, USA in May 2018.

## 7.19. Speech-Based Analysis for older people with dementia

Participants: Alexandra König, Philippe Robert, Nicklas Linz, Johannes Tröger, Jan Alexandersson.

**Keywords:** Alzheimer's disease, Dementia, Mild cognitive impairment, Neuropsychology, Assessment, Semantic verbal fluency, Speech recognition, Speech processing, Machine learning

#### 7.19.1. Fully Automatic Speech-Based Analysis of the Semantic Verbal Fluency Task:

Semantic verbal fluency (SVF) tests are routinely used in screening for mild cognitive impairment (MCI). In this task, participants name as many items as possible of a semantic category under a time constraint. Clinicians measure task performance manually by summing the number of correct words and errors. More fine-grained variables add valuable information to clinical assessment, but are time-consuming. Therefore, the aim of this study is to investigate whether automatic analysis of the SVF could provide measures as accurate as the manual ones and thus, support qualitative screening of neurocognitive impairment.

**Methods:** SVF data were collected from 95 older people with MCI (n = 47), Alzheimer's or related dementias (ADRD; n = 24), and healthy controls (HC; n = 24). All data were annotated manually and automatically with clusters and switches. The obtained metrics were validated using a classifier to distinguish HC, MCI, and ADRD.

**Results:** Automatically extracted clusters and switches were highly correlated (r = 0.9) with manually established values, and performed as well on the classification task, separating HC from persons with ADRD (area under curve [AUC] = 0.939) and MCI (AUC = 0.758).

**Conclusion:** The results show that it is possible to automate fine-grained analyses of SVF data for the assessment of cognitive decline [70].

## 7.19.2. Language Modelling in the Clinical Semantic Verbal Fluency Task:

We employed language modelling (LM) as a natural technique to model production in this task. Comparing different LMs, we show that perplexity of a person's SVF production predicts dementia well (F1 = 0.83). Demented patients show significantly lower perplexity, thus are more predictable. Persons in advanced stages of dementia differ in predictability of word choice and production strategy - people in early stages differ only in predictability of production strategy (Linz et al., 2018a).

# 7.19.3. Telephone-based Dementia Screening I: Automated Semantic Verbal Fluency Assessment:

Despite encouraging results, there are still two main issues in leveraging pervasive sensing technologies for automatic dementia screening: significant hardware costs or installation efforts and the challenge of an effective pattern recognition. Conversely, automatic speech recognition (ASR) and speech analysis have reached sufficient maturity and allow for low-tech remote telephone-based screening scenarios. Therefore, we examine the technological feasibility of automatically assessing a neuropsychological test—Semantic Verbal Fluency (SVF)—via a telephone-based solution. We investigate its suitability for inclusion into an automated dementia frontline screening and global risk assessment, based on concise telephone-sampled speech, ASR and machine learning classification. Results are encouraging showing an area under the curve (AUC) of 0.85. We observe a relatively low word error rate of 33% despite phone-quality speech samples and a mean age of 77 years of the participants. The automated classification pipeline performs equally well compared to the classifier trained on manual transcriptions of the same speech data. Our results indicate SVF as a prime candidate for inclusion into an automated telephone-screening system [50].

#### 7.19.4. Using Acoustic Markers extracted from Free Emotional Speech:

Apathy is a frequent neuropsychiatric syndrome in people with dementia. It leads to diminished motivation for physical, cognitive and emotional activity. Apathy is highly underdiagnosed since its criteria have been only recently established and rely heavily on the subjective evaluation of human observers. We analyzed speech samples from demented people with and without apathy. Speech was provoked by asking patients two emotional questions. Acoustic features were extracted and used in a classification task. The resulting models

show performances of AUC = 0.71 and AUC = 0.63. This is a decent first step into the direction of automatic detection of apathy from speech. Usefulness of stimuli to elicit free speech is found to depend on patients' gender [46].

#### 7.19.5. Using Automatic Speech Analysis:

Apathy is present in several psychiatric and neurological conditions and found to have a severe negative effect on patients' life. In older people, it can be a predictor of increased dementia risk. Current assessment methods seem insufficiently objective and sensitive, thus new diagnostic tools and broad-scale screening technologies are needed. This study is the first of its kind aiming to investigate whether automatic speech analysis could be used for characterization and detection of apathy.

**Methods:** A group of apathetic and non-apathetic patients (n = 60) was recorded while performing two short narrative speech tasks. Paralinguistic markers relating to prosodic, formant, source and temporal qualities of speech were automatically extracted, examined between the groups and compared to baseline assessments. Machine learning experiments were carried out to validate the diagnosis power of extracted markers.

**Results:** Correlations between apathy sub-scales and features revealed a relation between temporal aspects of speech and the subdomains of reduction in interest and initiative, as well as between prosody features and the affective domain. Group differences were found to vary for males and females, depending on the task. Differences in temporal aspects of speech were found to be the most consistent difference between apathetic and non-apathetic patients. Machine learning models trained on speech features achieved top performances of AUC = 0.88 for males and AUC = 0.77 for females (article under review).

An additional study in this context analyses transcripts of responses to emotional questions (positive and negative) for sentiment using a French emotion dictionary (FEEL) and for psycholinguistic properties (LIWC). Significant reductions in the number of words, the magnitude of sentiment, the overall sentiment and the range between sentiment in the positive and negative questions are found for the apathetic population. This effect is consistent between the positive and the negative stories. When training machine learning classifiers to detect apathy based on these features, the best model showed an AUC of 0.874 using only sentiment features. LIWC features mostly showed no predictive power. When ASR technology was introduced to automatically create transcripts, the performance of predictive models dropped slightly to AUC = 0.864. ASR errors were consistent over all categories of sentiment words. These results highlight the potential of computational linguistic analysis in screening for apathy (article under review).

## 7.20. Monitoring the Behaviors of Retail Customers

Participants: Soumik Mallick, Julien Badie, Francois Brémond.

Keywords: Ontology, Event detection, Multi-sensor data fusion, Real-time person tracking

The future shops will be connected and distributors as well as shopkeepers need to fulfill their promise to provide a personalized shopping experience to the customers, for example: advising and guiding customers in real time. It could not only enrich the productivity of the staffs but also increase the product sale. Implementing digital service and information in the store (like using beacons) is of primary importance. Sellers can keep their promise by providing the customer's contextual support tool in order to sell more product. To improve the performance of the store, this digital service can help to analyze customer displacement and the reaction to the product which can help to reduce the operational costs of the store by optimizing store process. It can also help to adjust store prices, merchandising and commercial operation. Thus connected digital store is a major level for new consumer services and an efficient way to manage the store.

We use multiple video cameras to detect customer in real-time inside the store. Furthermore, data are collected from different sensors like mobile phone, video camera, GPS location or Beacon. It helps to provide us with the trajectory information of the customer. A trajectory is composed of a set of points. The trajectory points are collected with the help of sensor API. Then, the calculation of distance of points in subsequent frames is performed. Every point has a minimum distance to a certain threshold of time. If there is a difference between a distance on a certain period of time that will be considered as a moving subject. For example, if we have 2 tracklets from different sensors (and generally with a different frequency of points), we cut both tracklets just to keep the intersection (in terms of time) and then apply Dynamic Time Warping (DTW) on this section. When we have the results for all tracklet pairs, we order them by distance and we decide to authorize to merge the data from the different sensors or not, with help of fusion algorithms to pass the information from the sensors to the ontology. After that, only one trajectory is sent to the ontology. Then we create a SPARQL request to extract trajectory-based events and execute it.

In this storeConnect project, we are investigating to improve the event recognition model. It will help to identify customer activity in the different zone inside the store as well as moving and stopping positions of the customer. Furthermore, inside the ontology, we want to add different attributes such as emotion, gender etc.

## 7.21. Synchronous Approach to Activity Recognition

Participants: Daniel Gaffé, Sabine Moisan, Annie Ressouche, Jean-Paul Rigault, Ines Sarray.

Activity Recognition aims at recognizing and understanding sequences of actions and movements of mobile objects (human beings, animals or artefacts), that follow the predefined model of an activity. We propose to describe activities as a series of actions, triggered and driven by environmental events.

Due to the large range of application domains (surveillance, safety, health care ...), we propose a generic approach to design activity recognition systems that interact continuously with their environment and react to its stimuli at run-time. Such recognition systems must satisfy stringent requirements: dependability, real time, cost effectiveness, security and safety, correctness, completeness ... To enforce most of these properties, our approach is to base the configuration of the system as well as its execution on formal techniques. We chose the *Synchronous Approach* which provides formal bases to perform static analysis, verification and validation, but also direct implementation.

Based on the synchronous approach, we designed a new user-oriented activity description language (named ADeL) to express activities and to automatically generate recognition automata. This language relies on two formal semantics, a behavioral and an equational one [48]. We also developed a component, called Synchronizer, to transform asynchronous sensor events into synchronous "instants", necessary for the synchronous approach. This year, we mainly worked on the ADeL compiler to generate synchronous automata, on the graphical tool of this language and on the Synchronizer component.

#### 7.21.1. ADeL Compilation:

To compile an ADeL program, we first transform it into an equation system which represents its synchronous automaton. Then we directly implement this equation system, transforming it into a Boolean equation system. This equation system provides an effective implementation of the initial ADeL program for our runtime recognition engine. The internal representation as Boolean equation systems also makes it possible to verify and validate ADeL programs, by generating a format suitable for a dedicated model checker such as the off-the-shelf NuSMV model-checker.

## 7.21.2. Synchronizer:

The role of the Synchronizer is to filter physical asynchronous events, to decide which ones may be considered as "simultaneous" and to aggregate the latter into logical instants. The sequence of these instants constitutes the logical time of our recognition systems. The runtime recognition engine interacts with the synchronizer and uses these instants to run the automata corresponding to the activities currently recognized. In general, no exact decision algorithm exists but several empirical strategies and heuristics may be used e.g., for determining instant boundaries. This year we completed the specification and implementation of a first version of the Synchronizer. It is parametrized by heuristics to manage events and data coming from various sensors, to define instant boundaries, and to cope with possible high level interruptions (preemptions).

Moreover, to facilitate the job of the synchronizer (to build the instants) and of the runtime engine (to wake up only the relevant automata), each automaton provides information about the awaited events at each state, i.e the events which may trigger transitions to a next state. The ADeL compiler has in charge to generate this information. In a first attempt, we computed statically all the awaited events in all states of an automaton. However, this approach implied to build the entire explicit automaton from an equation system, which was not realistic. Thus, this year we added specific equations to the equation systems of the operational semantics to compute the awaited events of each operator of the language. The information about next awaited events is now computed at runtine, when a state of the automaton is reached.

## 7.22. Probabilistic Activity Description Language

Participants: Elisabetta de Maria, Sabine Moisan, Jean-Paul Rigault.

Since the arrival of E. De Maria in the STARS team in September 2018, we work on the conception of a probabilistic framework for human behavior representation. The goal is to propose (i) a textual language for the description of activities which takes uncertainty into account; (ii) a formal probabilistic model to represent behaviors. Such a model will be tested and validated using experimental data coming from Alzheimer's patients. We will use temporal data resulting from different sensors and corresponding to patients playing with serious games. This will be the topic of T. L'Yvonnet's PhD starting in December. E. De Maria's main researches concern the investigation of the dynamic behavior of biological neuronal networks, using Leaky Integrate and Fire (LIF) neuronal networks, whose temporal dimension is crucial (the state of each neuron is computed taking into account not only present inputs but also past ones). This year, we used the PRISM language to model LIF neuronal networks as probabilistic reactive systems and we proposed an algorithm which aims at reducing the number of neurons and synaptical connections of these networks [42].

## **TITANE Project-Team**

# 7. New Results

## 7.1. Analysis

#### 7.1.1. Planar Shape Detection at Structural Scales

Participants: Hao Fang, Mathieu Desbrun, Florent Lafarge [contact].

Shape detection, abstraction, man-made objects, point clouds, surface reconstruction.

Interpreting 3D data such as point clouds or surface meshes depends heavily on the scale of observation. Yet, existing algorithms for shape detection rely on trial-and-error parameter tunings to output configurations representative of a structural scale. We present a framework to automatically extract a set of representations that capture the shape and structure of man-made objects at different key abstraction levels. A shape-collapsing process first generates a fine-to-coarse sequence of shape representations by exploiting local planarity. This sequence is then analyzed to identify significant geometric variations between successive representations through a supervised energy minimization. Our framework is flexible enough to learn how to detect both existing structural formalisms such as the CityGML Levels Of Details, and expert-specified levels of abstraction. Experiments on different input data and classes of man-made objects, as well as comparisons with existing shape detection methods, illustrate the strengths of our approach in terms of efficiency and flexibility. Figure 1 illustrates the goal of our method. This work has been published in the proceedings of CVPR [16].

## 7.1.2. Multi-task Deep Learning for Satellite Image Pansharpening and Segmentation Participants: Andrew Khalel, Onur Tasar, Yuliya Tarabalka [contact].

This work has been done in collaboration with Dr. Guillaume Charpiat (TAU team, Inria Saclay).

Segmentation, pansharpening, multi-task, joint learning

We proposed a novel multi-task framework to learn satellite image pansharpening and segmentation jointly. Our framework is based on encoder-decoder architecture, where both tasks share the same encoder but each one has its own decoder (see Fig. 2). We compare our framework against single-task models with different architectures. Results show that our framework outperforms all other approaches in both tasks.

### 7.1.3. Incremental Learning for Semantic Segmentation of Large-Scale Remote Sensing Data Participants: Onur Tasar, Pierre Alliez, Yuliya Tarabalka [contact].

#### This work has been done in collaboration with CNES and ACRI-ST.

Incremental learning, catastrophic forgetting, semantic segmentation, convolutional neural networks

In spite of remarkable success of the convolutional neural networks on semantic segmentation, they suffer from catastrophic forgetting: a significant performance drop for the already learned classes when new classes are added on the data, having no annotations for the old classes. We propose an incremental learning methodology, enabling to learn segmenting new classes without hindering dense labeling abilities for the previous classes, although the entire previous data are not accessible. The key points of the proposed approach are adapting the network to learn new as well as old classes on the new training data, and allowing it to remember the previously learned information for the old classes. For adaptation, we keep a frozen copy of the previously trained network, which is used as a memory for the updated network in absence of annotations for the former classes. The updated network minimizes a loss function, which balances the discrepancy between outputs for the previous classes from the memory and updated networks, and the mis-classification rate between outputs for the new classes from the updated network and the new ground-truth. For remembering, we either regularly feed samples from the stored, little fraction of the previous data or use the memory network, depending on

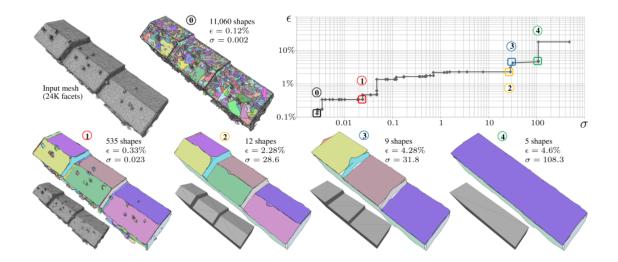


Figure 1. Planar shape detection at structural scales. Starting from 3D data (here a dense mesh generated by MultiView Stereo, top left), our algorithm produces a set of high-level representations with planar primitives (representations 1–4) describing the object at different representative structural scales (bottom). By progressively merging planar regions of an initial state (representation 0), one creates a sequence of representations whose further analysis allows for the extraction of a few structurally relevant representations (top right). Such shape representations can be used, for instance, as input for piecewise-planar reconstruction (see grey compact meshes). Note that each shape is displayed as a colored polygon computed as the  $\alpha$ -shape of its inliers projected onto the shape.

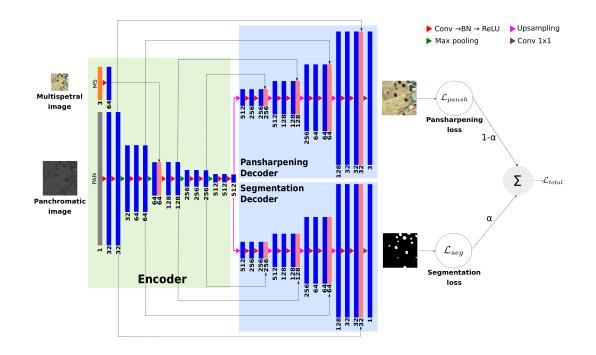


Figure 2. Overal framework for joint segmentation and pansharpening.

whether the new dat (see Fig. 3) are collected from completely different geographic areas or from the same city. Our experimental results prove that it is possible to add new classes to the network, while maintaining its performance for the previous classes, despite the whole previous training data are not available. This work was submitted to IEEE Transactions on Geoscience and Remote Sensing (TGRS) and is currently on arXiV [25].

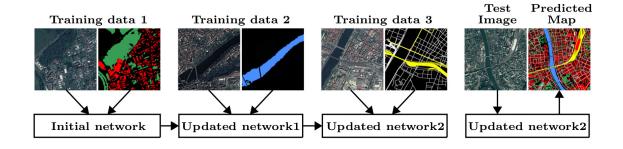


Figure 3. An example incremental learning scenario. Firstly, satellite images as well as their label maps for building and high vegetation classes are fed to the network. Then, from the second training data, the network learns water class without forgetting building and high vegetation classes. Finally, road and railway classes are taught to the network. Whenever new training data are obtained, we store only a small part of the previous ones for the network to remember. When a new test image comes, the network is able to detect all the classes.

# 7.1.4. Multimodal Image Alignment through a Multiscale Chain of Neural Networks with Application to Remote Sensing

Participants: Nicolas Girard, Yuliya Tarabalka [contact].

This work has been done in collaboration with Armand Zampieri and Dr. Guillaume Charpiat (TAO team, Inria Saclay).

Multimodal, Alignment, Registration, Remote sensing

We tackle here the problem of multimodal image non-rigid registration, which is of prime importance in remote sensing and medical imaging. The difficulties encountered by classical registration approaches include feature design and slow optimization by gradient descent. By analyzing these methods, we note the significance of the notion of scale. We design easy-to-train, fully-convolutional neural networks able to learn scale-specific features. Once chained appropriately, they perform global registration in linear time, getting rid of gradient descent schemes by predicting directly the deformation.

We show their performance in terms of quality and speed through various tasks of remote sensing multimodal image alignment. In particular, we are able to register correctly cadastral maps of buildings as well as road polylines onto RGB images, and outperform current keypoint matching methods (see Fig. 4). This work has been published in the proceedings of ECCV [20].

## 7.1.5. Aligning and Updating Cadaster Maps with Aerial Images by Multi-Task, Multi-Resolution Deep Learning

Participants: Nicolas Girard, Yuliya Tarabalka [contact].

This work has been done in collaboration with Dr. Guillaume Charpiat (TAO team, Inria Saclay).

Alignment, Registration, Multi-task, Multi-resolution

A large part of the world is already covered by maps of buildings, through projects such as OpenStreetMap. However when a new image of an already covered area is captured, it does not align perfectly with the buildings of the already existing map, due to a change of capture angle, atmospheric perturbations, human error when annotating buildings or lack of precision of the map data. Some of those deformations can be partially corrected, but not perfectly, which leads to misalignments. Additionally, new buildings can appear in the image. Leveraging multi-task learning, our deep learning model aligns the existing building polygons to the new image through a displacement output, and also detects new buildings that do not appear in the cadaster through a segmentation output (see Fig. 5). It uses multiple neural networks at successive resolutions to output a displacement field and a pixel-wise segmentation of the new buildings from coarser to finer scales. We also apply our method to buildings height estimation, by aligning cadaster data to the rooftops of stereo images.

## 7.2. Reconstruction

## 7.2.1. Kinetic Polygonal Partitioning of Images

Participants: Jean-Philippe Bauchet, Florent Lafarge [contact].

Polygons, image segmentation, object contouring, kinetic framework

Recent works showed that floating polygons can be an interesting alternative to traditional superpixels, especially for analyzing scenes with strong geometric signatures, as man-made environments. Existing algorithms produce homogeneously-sized polygons that fail to capture thin geometric structures and overpartition large uniform areas. We propose a kinetic approach that brings more flexibility on polygon shape and size. The key idea consists in progressively extending pre-detected line-segments until they meet each other. Our experiments demonstrate that output partitions both contain less polygons and better capture geometric structures than those delivered by existing methods. We also show the applicative potential of the method when used as preprocessing in object contouring. Figure 6 illustrates the goal of our method. This work has been published in the proceedings of CVPR [15].

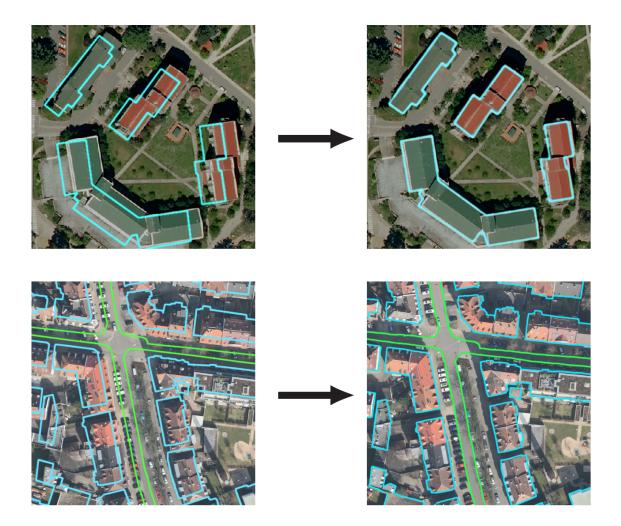


Figure 4. Multi-modal alignment.

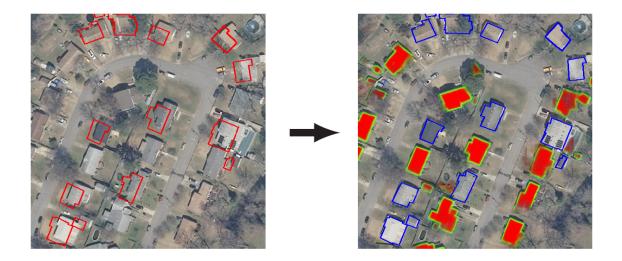


Figure 5. Multi-task learning with 2 tasks: multi-modal alignment and semantic segmentation.



Figure 6. Kinetic partitioning into polygons. Our algorithm decomposes an image (left) into a partition of convex polygons (right). While superpixel-based methods impose homogeneously-sized regions, our polygons are more meaningful, capturing both large components and thin lineic structures that compose, for instance, urban scenes.

## 7.2.2. Polygonization of Binary Classification Maps Using Mesh Approximation with Right Angle Regularity

Participants: Onur Tasar, Pierre Alliez, Yuliya Tarabalka [contact].

Work in collaboration with Emmanuel Maggiori.

Polygonization, vectorization, remote sensing, classification maps, mesh approximation, right angles

One of the most popular and challenging tasks in remote sensing applications is the generation of digitized representations of Earth's objects from satellite raster image data. A common approach to tackle this challenge is a two-step method that first involves performing a pixel-wise classification of the raster data, then vectorizing the obtained classification map. We propose a novel approach, which recasts the polygonization problem as a mesh-based approximation of the input classification map, where binary labels are assigned to the mesh triangles to represent the building class. A dense initial mesh is decimated and optimized using local edge and vertex-based operators in order to minimize an objective function that models a balance between fidelity to the classification map in  $\ell_1$  norm sense, right angle regularity for polygonized buildings, and final mesh complexity (see Fig. 7). Experiments show that adding the right angle objective yields better representations quantitatively and qualitatively than previous work and commonly used polygon generalization methods in remote sensing literature for similar number of vertices. This work was published at IGARSS [19].

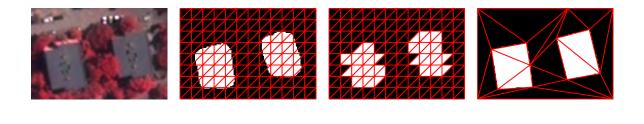


Figure 7. Input image and example labeled meshes. (a) Input image, (b) Initial fine lattice, (c) Initial and (d) Optimized labeled triangle meshes. The triangles labeled as building are indicated by white.

(c)

(d)

#### 7.2.3. End-to-End Learning of Polygons for Remote Sensing Image Classification

(b)

Participants: Nicolas Girard, Yuliya Tarabalka [contact].

High-resolution aerial images, polygon, vectorial, regression, deep learning, convolutional neural networks

While geographic information systems typically use polygonal representations to map Earth's objects, most state-of-the-art methods produce maps by performing pixelwise classification of remote sensing images, then vectorizing the outputs. This work studies if one can learn to directly output a vectorial semantic labeling of the image. We here cast a mapping problem as a polygon prediction task, and propose a deep learning approach which predicts vertices of the polygons outlining objects of interest. Experimental results on the Solar photovoltaic array location dataset show that the proposed network succeeds in learning to regress polygon coordinates, yielding directly vectorial map outputs (see Fig. 8). This work has been published in the proceedings of IGARSS [14].

## 7.3. Approximation

(a)

#### 7.3.1. Curved Optimal Delaunay Triangulation

Participants: Mathieu Desbrun, Pierre Alliez [contact].

Work in collaboration with Leman Feng (Ecole des Ponts ParisTech), Hervé Delingette (EPIONE) and Laurent Busé (AROMATH).

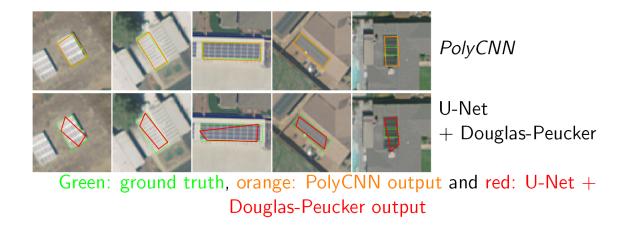


Figure 8. Results of polygon reconstruction with a deep neural network.

Higher-order meshing, Optimal Delaunay Triangulations, higher order finite elements, Bézier elements.

Meshes with curvilinear elements hold the appealing promise of enhanced geometric flexibility and higherorder numerical accuracy compared to their commonly-used straight-edge counterparts. However, the generation of curved meshes remains a computationally expensive endeavor with current meshing approaches: high-order parametric elements are notoriously difficult to conform to a given boundary geometry, and enforcing a smooth and non-degenerate Jacobian everywhere brings additional numerical difficulties to the meshing of complex domains. In this paper, we propose an extension of Optimal Delaunay Triangulations (ODT) to curved and graded isotropic meshes. By exploiting a continuum mechanics interpretation of ODT instead of the usual approximation theoretical foundations, we formulate a very robust geometry and topology optimization of Bézier meshes based on a new simple functional promoting isotropic and uniform Jacobians throughout the domain. We demonstrate that our resulting curved meshes can adapt to complex domains with high precision even for a small count of elements thanks to the added flexibility afforded by more control points and higher order basis functions (see Figure 9). This work has been published in the proceedings of ACM SIGGRAPH conference [12].

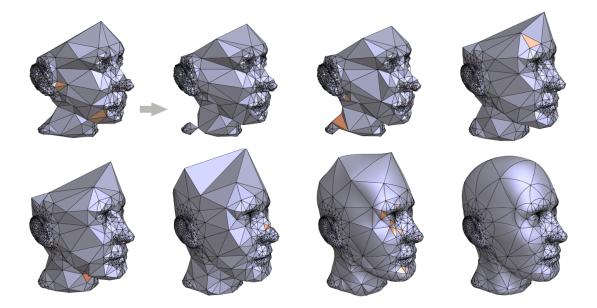


Figure 9. Generation of a curved optimal Delaunay triangulation.

## **WIMMICS Project-Team**

# 7. New Results

## 7.1. Users Modeling and Designing Interaction

### 7.1.1. User-centered Heuristics for the Control of Personal Data

Participants: Alain Giboin, Patrice Pena, Fabien Gandon.

This work (done in collaboration with Karima Boudaoud and Yoann Bertrand, SPARKS, I3S, in the context of the PadDOC FUI project) led to the elaboration and the evaluation of a set of user-centered heuristics and a procedure for designing and evaluating systems allowing the control of personal data. The elaboration of the heuristics was based on: (1) the transposal of Nielsen's heuristics and of Scapin and Bastien's ergonomic criteria to the control of personal data ; (2) the user centering of the Privacy-by-Design notion of integrated privacy; and (3) the integration of Altman's interaction approach to privacy.

## 7.1.2. Needs Analysis of the Target Users of the WASABI musical search platform

Participants: Alain Giboin, Isabelle Mirbel, Michel Buffa, Elmahdi Korfed.

In the context of the ANR project WASABI, we performed an analysis of the needs of the target users of the future WASABI platform. This analysis has been reported in an internal report.

## 7.1.3. Modeling the Users of Collaborative Ontology Building Environments Participant: Alain Giboin.

We undertook a study on the evolution of the user model of collaborative ontology building environments (COBEs). By a user model – or a contributor model – we refer to the representation that COBEs designers have of the users of their systems and more generally of the actors contributing to the building of ontologies. This study aimed at emphasizing the importance to get a better knowledge of potential COBE contributors in order to design collaborative tools better suited to these contributors. The study was published in [55]. In this paper, we describe: (1) the method we used to study the evolution of the user/contributor model; (2) the evolution of the model (in terms of user types, user characterizations, and user's environment characterizations); (3) the parallel evolutions of: (a) the methods of COBEs design, (b) the systems themselves, and (c) the methods of collaborative ontology building; we mention some evolution perspectives envisioned by the designers.

#### 7.1.4. Design of a User-Centered Evaluation Method for Exploratory Search Systems

Participants: Emilie Palagi, Alain Giboin, Fabien Gandon.

This work was undertaken in the context of the PhD of Emilie Palagi, in cooperation with Raphaël Troncy (EURECOM). Our method takes into account users' exploratory search (ES) behavior and is based on a cognitive model of an ES task. We specially work on Discovery Hub (Wimmics project – Inria) and 3cixty (EURECOM project) ESSs. During the third year of the PhD, we continued the evaluation of our model of exploratory search by comparing it to video records of seven other ES sessions on Discovery Hub, Frankenplace and 3cixty. We analyzed the videos with the same methodology: we wrote down the different chains of the different model's features used by the users in their ES session. For all the records we were able to identify the features of our model and extend our table of observed possible transitions between the model's features. From this analysis, we conclude that our model of ES can express the users' activity during an ES task. This work was partially published in [49].

Based on the ES model's features and the possible transitions between them, we designed two different evaluation and design methods of ES systems which do not necessarily involve users:

- Without users: Heuristics of ES and a procedure to use them. These heuristics are principles for the interaction design. The Heuristics of ES can be used several times along the design process of the ES system (in the design and evaluation phases). We presented the heuristics and evaluated them. This work was published in [48].
- With users: a guide for the elaboration of a customizable test protocol. The goal of the test is to analyze ES session records in order to find the model's features. In this guide, we give indications to customize the protocol and prepare users tests. We focused on two model-based elements of this customizable test protocol: a protocol for the elaboration of exploratory search tasks, and a video analysis grid for the evaluation of recorded exploratory search sessions.

#### 7.1.5. Supporting Learning Communities with Intelligent services

Participants: Oscar Rodríguez Rocha, Catherine Faron Zucker.

The Système Intelligent d'Enseignement en Santé 3.0 (SIDES 3.0), (Intelligent Health Education System 3.0), is a 3 years project funded by the French National Agency for Research (ANR) within the framework of the call for projects DUNE 2016. It builds upon a national Web platform, the Système Informatique D'Evaluation en Santé (SIDES) (Health Assessment Information System), used since 2013 by the faculties of medicine in France which enables them to perform all of their validation exams on tablets, providing them with automatic corrections. It contributes to the preparation of medical students to perform the Epreuves Classantes Nationales (ECN) informatisées (ECNi) (Computerized National Qualifying Events) which have been successfully held in France in June 2016 (8000 candidates simultaneously throughout France). The SIDES platform is administered by the 35 medicine faculties in France and is used by more than 70,000 students throughout their training. The system is also used to prepare students for ECNi. Over the last 3 years, more than 4 million clinical cases (made up of 15 questions each) have been performed by students (all activities combined).

Building on this success, the SIDES 3.0 project aims to upgrade the SIDES solution to an innovative solution providing the user with intelligent learning services based on a modelization of the pedagogical resources with Semantic Web models and technologies. It is coordinated by the *Université Numérique Thématique (UNT) en Santé et Sport*<sup>0</sup>. This structure offers an ideal national positioning for support and coordination of training centers (UFR) and also offers long-term financial sustainability. In this framework, we focus on developing and applying adaptive learning approaches to automatic quiz generation from existing questions, and quiz recommendation adapted to user profiles and learning contexts, to allow medical students to better achieve their educational objectives by answering quizzes [50], [51].

#### 7.1.6. Explainable Predictions Using Product Reviews

Participants: Elena Cabrio, Fabien Gandon, Nicholas Halliwell, Freddy Lecue, Serena Villata.

This is a joint work between Accenture and Wimmics team, funded by Accenture. The goal of this project is to design a recommender system that returns explainable predictions to the user, incorporating text from the product reviews in the explanation. To start, we have replicated results from current state of the art methods. We then gathered a dataset of Amazon books and corresponding reviews, and ran the current state of the art algorithm on our dataset. The next steps will be to build a deep learning model to outperform the current state of the art algorithm, and develop a method to explain the predictions to the user using the product reviews.

### 7.1.7. Argument Mining

Participants: Elena Cabrio, Fabien Gandon, Claude Frasson, Andrea Tettamanzi.

<sup>0</sup>http://www.uness.fr

We have published a survey paper about Argument Mining at IJCAI [61]. Argument mining is the research area aiming at extracting natural language arguments and their relations from text, with the final goal of providing machine-processable structured data for computational models of argument. This research topic has started to attract the attention of a small community of researchers around 2014, and it is nowadays counted as one of the most promising research areas in Artificial Intelligence in terms of growing of the community, funded projects, and involvement of companies. In this paper, we presented the argument mining tasks and we discussed the obtained results in the area from a data-driven perspective. An open discussion highlights the main weaknesses suffered by the existing work in the literature and proposes open challenges to be faced in the future.

Together with two colleagues from FBK Trento (Italy), we applied argumentation mining techniques, in particular relation prediction, to study political speeches in monological form, where there is no direct interaction between opponents. We argued that this kind of technique can effectively support researchers in history, social and political sciences, which must deal with an increasing amount of data in digital form and need ways to automatically extract and analyse argumentation patterns. We tested and discussed our approach based on the analysis of documents issued by R. Nixon and J. F. Kennedy during 1960 presidential campaign. We relied on a supervised classifier to predict argument relations (i.e., support and attack), obtaining an accuracy of 0.72 on a dataset of 1,462 argument pairs. The application of argument mining to such data allowed not only to highlight the main points of agreement and disagreement between the candidates' arguments over the campaign issues such as Cuba, disarmament and health-care, but also an in-depth argumentative analysis of the respective viewpoints on these topics. The results of this research have been published at AAAI [58].

In this direction, we have also, in collaboration with the Heron Lab of the University of Montreal, presented an empirical study about the relation between argumentative persuasion and emotions. Argumentative persuasion usually employs one of the three persuasion strategies: Ethos, Pathos or Logos. Several approaches have been proposed to model persuasive agents, however, none of them explored how the choice of a strategy impacts the mental states of the debaters and the argumentation process. We conducted a field experiment with real debaters to assess the impact of the mental engagement and emotions of the participants, as well as of the persuasiveness power of the arguments exchanged during the debate. Our results showed that the Pathos strategy is the most effective in terms of mental engagement. The results of this research have been published at FLAIRS [60].

Together with Souhila Kaci (LIRMM) and Leendert van der Torre (University of Luxembourg), we have proposed a formal framework to reason about preferences in abstract argumentation. Consider an argument A that is attacked by an argument B, while A is preferred to B. Existing approaches will either ignore the attack or reverse it. We introduced a new reduction of preference and attack to defeat, based on the idea that in such a case, instead of ignoring the attack, the preference is ignored. We compared this new reduction with the two existing ones using a principle-based approach for the four Dung semantics. The principle-based or axiomatic approach is a methodology to choose an argumentation semantics for a particular application, and to guide the search for new argumentation semantics. For this analysis, we also introduced a fourth reduction, and a semantics for preference-based argumentation based on extension selection. Our classification of twenty alternatives for preference-based abstract argumentation semantics using six principles suggests that our new reduction has some advantages over the existing ones, in the sense that if the set of preferences increases, the sets of accepted arguments increase as well. The results of this research have been published at COMMA [36].

Together with Celia da Costa Pereira (I3S) and Mauro Dragoni (FBK Trento), we presented SMACk, an opinion summary system built on top of an argumentation framework with the aim to exchange, communicate and resolve possibly conflicting viewpoints. SMACk allows the user to extract debated opinions from a set of documents containing user-generated content from online commercial websites, and to automatically identify the mostly debated positive aspects of the issue of the debate, as well as the mostly debated negative ones. The key advantage of such a framework is the combination of different methods, i.e., formal argumentation theory and natural language processing, to support users in making more informed decisions, e.g., in the context of online purchases. The results of this research have been published in the AI Communications journal [14].

## 7.2. Communities and Social Interactions Analysis

#### 7.2.1. Argumentation and Emotion Detection with Adaptive Sentiment Analysis

Participants: Vorakit Vorakitphan, Serena Villata, Elena Cabrio.

This PhD work just started in the context of the ANSWER project with Qwant search engine. One of the main objectives of the ANSWER project is to use emotion detection algorithms within text inquiries and sentiment analysis to provide powerful enhancements in the search results from Qwant search engine. The final goal is to extract effective and scalable indicators of sentiment, emotions, and argumentative relations in order to offer the users additional means to filter the results selected by the search engine. Powerful algorithms in state-of-art will be focused to define new criteria for filtering search results, i.e., the expression of a feeling in the answers found by the search engine. By doing as mentioned, textual elements to which we wish to associate a polarity will no longer be considered in their individuality but connected to each other by polarized relations to be analyzed in a higher level setting. Currently, the work progress is in the survey of state-of-the-art based on emotion detection algorithms and implementation of sentiment analysis. Then the next target, classification models with multi-label features based on emotion detection, will be deeply explored as a starting point of this research. Moreover, NLP related to emotional news content will be taken into account to build a novel dataset based on emotion annotation from news articles in sentence-level.

## 7.2.2. Cyberbullying Events Prevention

Participants: Pinar Arslan, Michele Corazza, Elena Cabrio, Serena Villata.

In the CREEP EIT project, we built an emotion detection classifier to automatically identify the emotion for user-generated texts such as Twitter and Instagram posts. The correlation analysis that we carried out to get a better understanding of the associations between emotions and cyberbullying instances unveiled that certain emotions (e.g., anger, joy) would be good indicative features to detect cyberbullying instances. Hence, our pipeline firstly reveals automatically detected emotion labels for social media texts to be used to detect cyberbullying instances. The automatically predicted emotion labels were used as one of the predictors for our cyberbullying detection classifier. As part of the project, we successfully built a classifier for offensive language in social media interactions for English, Italian and German using neural networks. This classifier was evaluated by participating in two shared tasks: Germeval (German offensive language detection) and Evalita (Italian hate speech detection). For the Germeval Challenge [29], two systems for predicting messagelevel offensive language in German tweets were used: one discriminates between offensive and not offensive messages, and the second performs a fine-grained classification by recognizing also classes of offense. Both systems are based on the same approach, which builds upon Recurrent Neural Networks used with the following features: word embeddings, emoji embeddings and social-network specific features. The model combines word-level information and tweet-level information to perform the classification tasks. Our best performing model ranked 7th out of 51 submitted runs on the binary classification task, 5th out of 25 for the fine-grained classification task. For the Evalita Challenge shared tasks [28], our submissions were based on three separate classes of models: a model using a recurrent layer, an ngram-based neural network and a LinearSVC. For the Facebook task and the two cross-domain tasks we used the recurrent model and obtained promising results, especially in the cross-domain setting. For Twitter, we used an ngram-based neural network and the Linear SVC-based model. Our system ranked 1st in the Facebook to Twitter dataset, 2nd in the Twitter to Facebook dataset, 3rd in the Facebook dataset and 4th on the Twitter dataset.

#### 7.2.3. Modeling of a Social Network of Service Providers

Participants: Molka Dhouib, Catherine Faron Zucker, Andrea Tettamanzi.

In the framework of a collaborative project with Silex France company and the CIFRE PhD thesis of Molka Dhouib, our aim is to model the social network of service providers and companies registered in the *software as a service* sourcing tool developed by Silex for the recommendation of the service providers that are best suited to meet the service requests expressed by companies. Our aim is to automate the matching of service requests and offers by reasoning on the social network of service providers and companies. We developed an automatic categorization of companies, service requests and service offers based on their textual descriptions. We conducted some experiments using state-of-the-art supervised Machine Learning techniques to classify

Silex textual data into predefined categories, and to choose the best vector representations of the textual descriptions of service offers and requests in the Silex platform, and the best Machine Learning algorithm. This work has been presented at the French conference on applications of Artificial Intelligence APIA2018 [31].

# 7.3. Vocabularies, Semantic Web and Linked Data based Knowledge Representation

## 7.3.1. Modeling a Vocabulary of Professional Skills and Fields of Activities

Participants: Molka Dhouib, Catherine Faron Zucker, Andrea Tettamanzi.

In the framework of the collaborative project with Silex France company aiming to model the social network of service providers and companies, as a preliminary step, we developed a dedicated vocabulary of competences and fields of activities to semantically annotate B2B service offers. We started with the study of existing reference taxonomies representing skills, professions and fields of activities and we formalized them in SKOS. Then we built a SKOS vocabulary from the internal Silex repositories. Finally we performed a semi-automatic alignment of these vocabularies. This work has been presented at the French conference on Knowledge Engineering IC 2018 [53].

## 7.3.2. Representing and Querying a Knowledge Graph on Pedagogical Resources

Participants: Géraud Fokou Pelap, Catherine Faron Zucker, Fabien Gandon, Olivier Corby.

In the framework of the EduMICS (Educative Models Interactions Communities with Semantics) joint laboratory (LabCom) between the Wimmics team and the Educlever company, we built a knowledge graph from the database of the Educlever platform describing learning resources, and related knowledge and skills. We deployed our proposed Semantic Web based solution within the industrial environment of Educlever, using Web services, and we showed the added value of Semantic Web modelling enabling to implement new functionalities with SPARQL queries on the knowledge graph. This work has been presented at the SemWeb.Pro 2018 day [56] and at the WEBIST conference [34].

## 7.3.3. A Learnable Crawler for Linked Open Data

Participants: Hai Huang, Fabien Gandon.

This work is supported by the ANSWER project in cooperation with Qwant company. It consists of designing a learnable Linked Data crawler featured by a prediction component which is able to predict whether a newly discovered URI contains RDF data or not.

As the Web of Linked Open Data is growing exponentially, crawling for Linked Data has become increasingly important. Unlike normal Web crawlers, a Linked Data crawler performs selectively to collect linked RDF (including RDFa) data on the Web. From the perspectives of throughput and coverage, given a newly discovered URI, the key issue of Linked Data crawlers is to decide whether this URI is desirable to download (if it contains RDF data). Current solutions adopt heuristic rules aiming to filter irrelevant URIs. Unfortunately, it would hurt the coverage of crawling. In this work, we developed a learnable Linked Data crawler featured by a prediction component which is able to predict whether a newly discovered URI contains RDF data or not. We extracted useful features from the context RDF graph of the URI. The prediction model is based on FTRL-proximal <sup>0</sup> online learning algorithm. We evaluated it through extensive experiments in comparison with a number of baseline methods and demonstrated its efficiency.

## 7.3.4. Argument Mining on Clinical Trials

Participants: Tobias Mayer, Serena Villata, Elena Cabrio.

<sup>&</sup>lt;sup>0</sup>FTRL: Follow The Regularized Leader

This work was done in the context of the PhD of Tobias Mayer, which is situated in the IADB project, "Intégration et Apprentissage sur les Données Biomédicales". We created a new annotated dataset of Randomized Controlled Tirals (RCT) about four different diseases (glaucoma, diabetes, hepatitis B, and hypertension), containing 976 argument components (697 containing evidence, 279 claims) together with a first approach for the argumentative component detection [39]. Empirical results are promising and show the portability of the proposed approach over different branches of medicine. Furthermore, we proposed a new sub-task of the argument component identification task: evidence type classification, which distinguishes the provided evidence on a more fine-grained level. To address it, we proposed a supervised approach and we tested it on our data set [40].

As a collaboration with "Base, Corpus, Language" (BCL) at UCA within the IADB project, we anonymized and cleaned clinical reports (from CHU Nice), built a "raw" French corpus from it and are currently working on transferring the above mentioned annotations and models to this data set.

### 7.3.5. Structure Detection in Song Lyrics

Participants: Michael Fell, Elena Cabrio, Fabien Gandon.

In the context of the WASABI ANR project, we work on the estimation of the structure of song lyrics. For this, we have built a predictive model that successfully segments song texts into their underlying paragraphs - a task called "Lyrics Segmentation". We have augmented existing state-of-the-art models for Lyrics Segmentation in two ways: (i) by applying convolutional neural networks to the task alongside of novel feature representations. This work resulted in a publication at the COLING conference [33]; (ii) by extending the feature representation with time-synchronized audio features, we improve the segmentation model performance. It can now also use audio cues when text cues are non-indicative; this improves segmentation performance. Our current endeavors aim at summarizing song texts so that journalists and musicologists can perform efficient searches under different perspectives (e.g. structure and semantic content).

#### 7.3.6. Legal Information, Privacy

Participants: Elena Cabrio, Serena Villata.

Together with Valentina Leone and Luigi di Caro (University of Torino), we presented the *InvestigatiOnt* tool which aims to ease the interaction of end users with legal ontologies in order to spread the use of machine-processable legal information as well as its understanding. This research is addressed in the context of the EU H2020 MIREL project. The results of this research have been published as demo paper at ISWC [71].

Together with Sabrina Kirrane (Vienna University of Economics and Business) and Matthieu d'Aquin (National University of Ireland Galway), we examined 78 articles from dedicated venues, the Privacy Online workshop series, two SPOT workshops, as well as the broader literature that connects the Semantic Web research domain with issues relating to privacy, security and/or policies. Specifically, we classified each paper according to three taxonomies (one for each of the aforementioned areas), in order to identify common trends and research gaps. We concluded by summarising the strong focus on relevant topics in Semantic Web research (e.g. information collection, information processing, policies and access control), and by highlighting the need to further explore under-represented topics (e.g., malware detection, fraud detection, and supporting policy validation by data consumers). The results of this research have been published in the Semantic Web journal [16].

## 7.3.7. Semantic Web for Biodiversity

Participants: Franck Michel, Catherine Faron Zucker.

The collaboration initiated with the French National Museum of Natural History of Paris (MNHN) is now giving rise to the development of an activity related to biodiversity data sharing and integration.

The TAXREF-LD linked data dataset, that we produced jointly with the MNHN, now appears in the Linked Open Data cloud <sup>0</sup> and is published on AgroPortal <sup>0</sup>, the ontology Web portal for agronomy and agriculture. At the Biodiversity Information Standards conference (TDWG 2018), we presented some insights in the modelling of biodiversity Linked Data [45], we demonstrated how SPARQL Micro-Services can help in the integration of heterogeneous biodiversity-related data sources [43]. We also presented a poster on the Bioschemas.org initiative [46], a W3C community group that seeks the definition and adoption of common biology-related markup. In this context, we have proposed a first specification of the Taxon term <sup>0</sup> whose adoption as part of the official Schema.org vocabulary is currently being discussed with Google.

We took part in the D2KAB ANR project submission that aims to turn agronomy and biodiversity data into semantically described, interoperable, actionable open-knowledge. The project has been accepted and is due to start in June 2019.

## 7.3.8. Integration of Heterogeneous Data Sources

Participants: Franck Michel, Catherine Faron Zucker, Fabien Gandon.

With the incentive of fostering the integration of Linked Data and non RDF data sources, we published two contributions this year, together with Johan Montagnat from I3S.

First, we proposed a generic method to bridge the gap between the Semantic Web and NoSQL worlds [42]. To avoid defining yet another SPARQL translation method for each and every database, a SPARQL query is translated into a pivot abstract query, spanning all database-independent steps. Only then, the abstract query is translated into the target database query language while taking into account the specific database capabilities and constraints.

Second, we defined the SPARQL Micro-Service architecture that harnesses the Semantic Web standards to enable automatic combination of Linked Data and data residing in Web APIs (aka. REST Web services). A SPARQL micro-service is a lightweight, task-specific SPARQL endpoint that provides access to a small, resource-centric virtual graph, while dynamically assigning dereferenceable URIs to Web API resources that do not have URIs beforehand. The graph is delineated by the Web API service being wrapped, the arguments passed to this service, and the restricted types of RDF triples that this SPARQL micro-service is designed to spawn.

This work was presented at the ESWC conference [42] and the LDOW workshop at the Web Conference [44]. We also conducted an experimentation where we dynamically augment biodiversity Linked Data with data from multiple Web APIs: Flickr, Biodiversity Heritage Library, Encyclopedia of Life, Macauley scientific media archive, and MusicBrainz [43].

## 7.3.9. Linked Data Script Language

Participant: Olivier Corby.

We have designed and implemented LDScript, a programming language compatible with SPARQL that enables users to write extension functions that are directly executable in SPARQL queries.

We have leveraged pattern matching for structured objects such as lists where we can retrieve first elements, intermediate sublist and last elements. We have defined event driven processing where the SPARQL interpreter emits events which are processed by LDScript functions. The function definitions are annotated with event names. This enables users to trace query execution, to overload SPARQL statements such as "order by, distinct" and to extend SPARQL with new statements implemented as functions. In particular we are able to overload SPARQL operators for extension datatypes such as romain numbers or values with units. We are also able to trap and overload SPARQL execution errors with specific LDScript functions. In addition, we have introduced a second order "eval" function that enables us to evaluate the arguments of expressions that caused an error.

<sup>&</sup>lt;sup>0</sup>http://lod-cloud.net/

<sup>&</sup>lt;sup>0</sup>http://agroportal.lirmm.fr/ontologies/TAXREF-LD/

<sup>&</sup>lt;sup>0</sup>http://bioschemas.org/devSpecs/Taxon/

LDScript has been extended in order to process SPARQL Update in addition to SPARQL Query. Hence LDScript can be used to implement Semantic Web services with the following statements: SPARQL Query and Update, OWL RL entailment, RDF transformation to HTML.

This a follow up work on the formalism that was originally published at ISWC 2017 [72].

## 7.3.10. Graphic Display for RDF Graphs

Participants: Olivier Corby, Erwan Demairy.

This work has been done in the context of an Inria funding for software development (ADT).

In order to perform Linked Data visualisation, we connected the D3.js graphic display library to the Corese Web server. We designed an STTL transformation that generates D3 graph format with stylesheet from RDF graph. The graph display is performed thanks to SVG code generated by D3. The graph display can be interactive, that is hypertext navigation can be associated with a click on graph nodes. We have setup a demo with HAL open data server<sup>0</sup>, see figure 1.

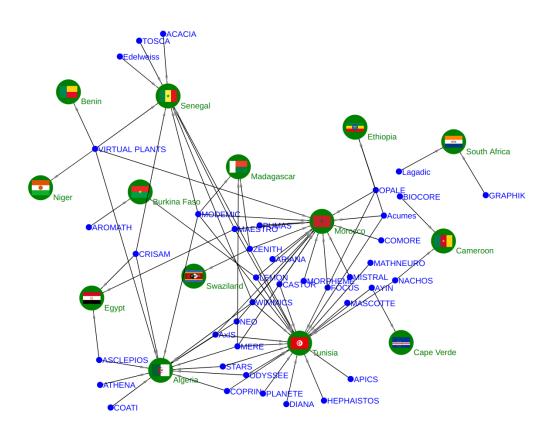


Figure 1. Inria Sophia Antipolis teams publishing with south American countries.

This work has been presented at the software development day at Inria Sophia Antipolis, November 14th.

<sup>0</sup>http://corese.inria.fr

## 7.3.11. Federated Query Scaler

Participant: Olivier Corby.

This work is done in the context of the *Federated Query Scaler* Inria exploratory research project (PRE) together with Olivier Dameron and Vijay Ingalalli from Dyliss team at Inria Rennes.

In this project, focused on SPARQL federated queries, Vijay Ingalalli designed a graph index for distributed SPARQL endpoints that enables us to predict whether joins between patterns can be performed within endpoints. We also wrote a compiler that generates a SPARQL query with service clauses from a federated query, that is a query annotated with several SPARQL endpoints URL.

We welcomed Vijay Ingalalli at Inria Sophia Antipolis, January 15-19, and Olivier Corby visited the Dyliss team in Rennes, March 4-6.

## 7.4. Analyzing and Reasoning on Heterogeneous Semantic Graphs

#### 7.4.1. Distributed Artificial Intelligence for Revisable Linked Data Management

Participants: Ahmed El Amine Djebri, Andrea Tettamanzi, Fabien Gandon.

The aim of this PhD thesis is to study and to propose original solutions to many key aspects: Knowledge Representation in case of uncertain, incomplete and reviewable data; Uncertainty Representation in a data source, with provenance; Distributed Knowledge Revision and Propagation; Reasoning over Uncertain, Incomplete and distributed data-sources. Starting from an open Web of Data, this work tries to give the users more objective, exhaustive and certain views and information about their queries, based on distributed data sources with different levels of certainty and trustworthiness. We proposed a vocabulary to formalize uncertainty representation, and a framework to handle uncertainty mapping to sentences and contexts. This work has been presented as a poster at ISWS [68].

#### 7.4.2. Learning Class Disjointness Axioms using Grammatical Evolution

Participants: Thu Huong Nguyen, Andrea Tettamanzi.

The aim of this research is to discover automatically class disjointness axioms from recorded RDF facts on the Web of Data. This may be regarded as a case of inductive reasoning and ontology learning. The instances, represented by RDF triples, play the role of specific observations, from which axioms can be extracted by generalization. We proposed the use of Grammatical Evolution, one type of evolutionary algorithm, for mining disjointness OWL2 axioms from an RDF data repository such as DBpedia. For the evaluation of candidate axioms against the DBpedia dataset, we adopt an approach based on possibility theory. We have submitted a paper to the conference EuroGP 2019.

## 7.4.3. Semantic Data for Image Recognition

Participants: Anna Bobasheva, Fabien Gandon.

This work is done in the context of the MonaLIA project with French Ministry of Culture, in collaboration with Frédéric Precioso, I3S, UCA. It consists of a preliminary study on image recognition of the Joconde database in connection with semantic data (JocondeLab).

The goal of this project is to exploit the cross-fertilization of recent advances in image recognition and semantic indexing on annotated image databases in order to improve the accuracy and the details of the annotation. The idea is, at first, to assess the potential of machine learning (including deep learning) and the semantic annotations on the Joconde database (350 000 illustrated artwork records from French museums). Joconde also contains metadata based on a thesaurus. In a previous project (JocondeLab) these metadata were formalized in Semantic Web formalism and were linking the iconographic Garnier thesaurus and DBpedia to the data of the Joconde database.

We developed SPARQL queries on Joconde database to extract the subset of images to train the Deep Learning classifier. We identified class subsets with enough labeled images for training, we balance number of images per class and we avoid images with intersected classes.

We tuned the pre-trained VGG16 implementation of the CNN classifier to classify the artwork images using well-known VGG16 with batch normalization [75] to train the classifier for the artwork images. We learned transfer from the training of the network on the ImageNet dataset to decrease the training time and we ran the classifier on many datasets and in different modes.

We developed another set of queries on the metadata to find the dependencies between the classification outcome and the artwork properties by applying statistical methods. We identified the usable (populated enough with reasonable number of categorical values) properties of the metadata. We used Recursive Feature Elimination (RFE) and Decision Tree to identify the top most statistically significant dependent variables and decision splitting values.

Results have been presented at a workshop of Ministry of Culture and Inria, November 22nd, at Bibliothèque Nationale de France in Paris.

#### 7.4.4. Hospitalization Prediction

Participants: Catherine Faron Zucker, Fabien Gandon, Raphaël Gazzotti.

HealthPredict is a project conducted in collaboration with the Département d'Enseignement de Recherche en Médecine Générale (DERMG) at Université Côte d'Azur and the SynchroNext company. It aims at providing a digital health solution for the early management of patients through consultation with their general practitioner and health care circuit. Concretely, it is a predictive Artificial Intelligence interface that allows us to cross the data of symptoms, diagnosis and medical treatments of the population in real time to predict the hospitalization of a patient. The first results of this project will be presented at the French EGC 2019 conference [54]. In this paper, we report and discuss the results of our first experiments on the database PRIMEGE PACA that contains more than 350,000 consultations carried out by 16 general practitioners. We propose and evaluate different ways to enrich the features extracted from electronic medical records with ontological resources before turning them into vectors used by Machine Learning algorithms to predict hospitalization.

#### 7.4.5. Fake News Detection

Participants: Jérôme Delobelle, Elena Cabrio, Serena Villata.

This work is part of the RAPID CONFIRMA (COntre argumentation contre les Fausses InfoRMAtion) DGA project aiming to automatically detect fake news and limit their diffusion. For this purpose, a framework will be developed to detect fake news, to reduce their propagation and to propose the best response strategies.

Thus, in addition to identifying the communities propagating these fake news, we will use methods from Natural Language Processing and Argumentation Theory to propose automatically extracted counter-arguments (adapted to target audience) from the existing reference press articles. These arguments allow to attack the false information detected in the fake news. Argument Mining techniques will make it possible to (1) analyse the argumentation in natural language, for example by looking for the argumentative structures, identifying the relations of support or attack between the arguments; (2) locate the data related to specific information (related to fake news) on the Web.

#### 7.4.6. Mining and Reasoning on Legal Documents

Participants: Cristian Cardellino, Milagro Teruel, Serena Villata.

Together with Cristian Cardellino, Fernando Cardellino, Milagro Teruel and Laura Alonso Alemany from Univ. of Cordoba, we have proposed a methodology to improve argument annotation guidelines by exploiting inter-annotator agreement measures. After a first stage of the annotation effort, we have detected problematic issues via an analysis of inter-annotator agreement. We have detected ill-defined concepts, which we have addressed by redefining high-level annotation goals. For other concepts, that are well-delimited but complex, the annotation protocol has been extended and detailed. Moreover, as can be expected, we showed that distinctions where human annotators have less agreement are also those where automatic analyzers perform worse. Thus, the reproducibility of results of Argument Mining systems can be addressed by improving inter-annotator agreement in the training material. Following this methodology, we are enhancing a corpus annotated

with argumentation, available online <sup>0</sup> together with guidelines and analyses of agreement. These analyses can be used to filter performance figures of automated systems, with lower penalties for cases where human annotators agree less. This research is addressed in the context of the EU H2020 MIREL project. The results of this research have been published at LREC [59].

Together with some colleagues from Data61 Queensland (Australia) and Antonino Rotolo (University of Bologna), we proposed a formal framework that can instantiate in agents' dialogues moral/rational criteria, such as the maximin principle, Pareto efficiency, and impartiality, which were used, e.g., by John Rawls' theory or rule utilitarianism. Most ethical systems define how the individuals ought, morally, act being part of a society. The process of elicitation of a moral theory governing the agents in a society requires them to express their own norms with the aim to find a moral theory on which all may agree upon. This research is addressed in the context of the EU H2020 MIREL project. The results of this research have been published at DEON [57].

### 7.4.7. Argumentation

Participants: Serena Villata, Andrea Tettamanzi.

In collaboration with Mauro Dragoni of FBK and Célia da Costa Pereira of I3S, we have proposed the SMACk System, combining argumentation and aspect-based opinion mining [14].

## 7.4.8. Agent-Based Recommender Systems

Participants: Amel Ben Othmane, Nhan Le Thanh, Andrea Tettamanzi, Serena Villata.

We have proposed a spatio-temporal extension for our multi-context framework for agent-based recommender systems (CARS), to which we have added representation and algorithms to manage uncertainty, imprecision, and approximate reasoning in time and space [47].

## 7.4.9. RDF Mining

Participants: Duc Minh Tran, Andrea Tettamanzi.

In collaboration with Dario Malchiodi of the University of Milan and Célia da Costa Pereira of I3S, we have studied the use of a prediction model as a surrogate of a possibilistic score for OWL axioms [38], [37].

In collaboration with Claudia d'Amato of the University of Bari, we made a comparison of rule evaluation metrics for EDMAR, our evolutionary approach to discover multi-relational rules from ontological knowledge bases exploiting the services of an OWL reasoner [52].

<sup>&</sup>lt;sup>0</sup>https://github.com/PLN-FaMAF/ArgumentMiningECHR

## **ZENITH Project-Team**

# 7. New Results

## 7.1. Query Processing

### 7.1.1. Top-k Query Processing Over Encrypted Data in the Cloud

Participants: Sakina Mahboubi, Reza Akbarinia, Patrick Valduriez.

Cloud computing provides users and companies with powerful capabilities to store and process their data in third-party data centers. However, the privacy of the outsourced data is not guaranteed by the cloud providers. One solution for protecting the user data against security attacks is to encrypt the data before being sent to the cloud servers. Then, the main problem is to evaluate user queries over the encrypted data.

In this work, we address the problem of top-k query processing over encrypted data. Top-k queries are important for many applications such as information retrieval, spatial data analysis, temporal databases, graph databases, etc. We consider two cases for top-k query processing over encrypted data: 1) centralized: the encrypted data are stored at a single node of a data center, which is useful if the database can fit at one node; 2) distributed: the encrypted data are partitioned and the partitions are encrypted and distributed across multiple nodes, which is useful if the database is very big.

In [52], we address the distributed case, and propose a system, called SD-TOPK, for top-k query processing over encrypted data distributed across several nodes of the cloud. SD-TOPK comes with a distributed top-k query processing algorithm that is executed in the nodes, and finds a set including the encrypted top-k data items. It also has an efficient filtering algorithm that removes most of the false positives included in the set returned by the top-k query processing algorithm. This filtering is done without needing to decrypt the data in the cloud.

In [51], we propose a complete system, called *BuckTop*, for the centralized case. BuckTop is able to efficiently evaluate top-k queries over encrypted data outsourced to a singe node, without having to decrypt it in that node. It includes a top-k query processing algorithm that works on the encrypted data stored in the cloud node, and returns a set that is proved to contain the encrypted data corresponding to the top-k results. We implemented BuckTop and compared its performance for processing top-k queries over encrypted data with that of the popular threshold algorithm (TA) over original (plaintext) data. The results show the effectiveness of BuckTop for outsourcing sensitive data in the cloud and answering top-k queries.

#### 7.1.2. Privacy Preserving Index for Range Query Processing in the Clouds

Participants: Reza Akbarinia, Esther Pacitti.

During the last decade, a large body of academic work has tackled the problem of outsourcing databases to an untrusted cloud while maintaining both privacy and SQL-like querying functionality (at least partially). Range query is an important kind of query that expresses a bounded restriction over the retrieved records. In the database management systems, these queries are usually answered by using efficient indexes. However, developing privacy preserving indexes for untrusted environments is very challenging.

In [55], we propose a differentially private index to an outsourced encrypted dataset. Efficiency is enabled by using a plaintext index structure to perform range queries. Security relies on both differential privacy (of the index) and semantic security (of the encrypted dataset). Our solution, called PINED-RQ, develops algorithms for building and updating the differentially private index. Compared to state-of-the-art secure index based range query processing approaches, PINED-RQ executes queries in the order of at least one magnitude faster. The security of PINED-RQ is proved and its efficiency is assessed by an extensive experimental validation.

## 7.1.3. Constellation Queries to Analyze Geometrical Patterns

Participants: Dennis Shasha, Patrick Valduriez.

Constellation queries are useful to analyze geometrical patterns. A geometrical pattern is a set of points with all pairwise distances (or, more generally, relative distances) specified. Finding matches to such patterns, i.e. constellations, has applications to spatial data in seismic, astronomical, and transportation contexts. Finding geometric patterns is a challenging problem as the potential number of sets of elements that compose shapes is exponentially large in the size of the dataset and the pattern. In [53], we propose algorithms to find patterns in large data applications using constellation queries. Our methods combine quadtrees, matrix multiplication, and bucket join processing. Our distributed experiments show that the choice of the composition algorithm (matrix multiplication or nested loops) depends on the freedom introduced in the query geometry through the distance additive factor. Three clearly identified blocks of threshold values guide the choice of the best composition algorithm. Answering complex constellation queries, i.e. isotropic and non-isotropic queries, is challenging because scale factors and stretch factors may take any of an infinite number of values. In [53], we propose practically efficient sequential and distributed algorithms for pure, isotropic, and non-isotropic constellation queries.

#### 7.1.4. Parallel Polyglot Query Processing

Participants: Boyan Kolev, Oleksandra Levchenko, Esther Pacitti, Patrick Valduriez.

The blooming of different cloud data stores has turned polystore systems to a major topic in the nowadays cloud landscape. Especially, as the amount of processed data grows rapidly each year, much attention is being paid on taking advantage of the parallel processing capabilities of the underlying data stores. To provide data federation, a typical polystore solution defines a common data model and query language with translations to API calls or queries to each data store. However, this may lead to losing important querying capabilities. The polyglot approach of the CloudMdsQL query language allows data store native queries to be expressed as inline scripts and combined with regular SQL statements in ad-hoc integration queries. Moreover, efficient optimization techniques, such as bind join, can still take place to improve the performance of selective joins. In [47], we introduce the distributed architecture of the LeanXcale query engine that processes polyglot queries in the CloudMdsQL query language, yet allowing native scripts to be handled in parallel at data store shards, so that efficient and scalable parallel joins take place at the query engine level. The experimental evaluation of the LeanXcale parallel query engine on various join queries illustrates well the performance benefits of exploiting the parallelism of the underlying data management technologies in combination with the high expressivity provided by their scripting/querying frameworks

## 7.2. Scientific Workflows

#### 7.2.1. In Situ Analysis of Simulation Data

Participants: Vitor Silva, Patrick Valduriez.

In situ analysis and visualization have been used successfully in large-scale computational simulations to visualize scientific data of interest, while data is in memory. Such data are obtained from intermediate (or final) simulation results, and once analyzed are typically stored in raw data files. However, existing in situ data analysis and visualization solutions (e.g. ParaView/Catalyst, VisIt) have limited online query processing and no support for dataflow analysis. The latter is a challenge for exploratory raw data analysis. In the context of the SciDISC associate team with Brazil [38], we propose a solution that integrates dataflow analysis with ParaView Catalyst for performing in-situ data analysis and monitoring dataflow from simulation runs [25].

In [21], we propose a solution (architecture and algorithms), called Armful, to combine the advantages of a dataflow-aware SWMS and raw data file analysis techniques to allow for queries on raw data file elements that are related but reside in separate files. Its main components are a raw data extractor, a provenance gatherer and a query processing interface, which are all dataflow-aware.

An instantiation of Armful is DfAnalyzer [34], a library of components to support online in-situ and intransit data analysis. DfAnalyzer components are plugged directly in the simulation code of highly optimized parallel applications with negligible overhead. With support of sophisticated online data analysis, scientists get a detailed view of the execution, providing insights to determine when and how to tune parameters or reduce data that does not need to be processed [35]. The source code of the DfAnalyzer implementation for Spark is available on github (github.com/hpcdb/RFA-Spark).

## 7.2.2. Scheduling of Scientific Workflows in Multisite Cloud

Participants: Esther Pacitti, Patrick Valduriez.

In [30], we consider the problem of efficient scheduling of a large SWf in a multisite cloud, i.e. a cloud with geo-distributed cloud data centers (sites). The reasons for using multiple cloud sites to run a SWf are that data is already distributed , the necessary resources exceed the limits at a single site, or the monetary cost is lower. In a multisite cloud, metadata management has a critical impact on the efficiency of SWf scheduling as it provides a global view of data location and enables task tracking during execution. Thus, it should be readily available to the system at any given time. While it has been shown that efficient metadata handling plays a key role in performance, little research has targeted this issue in multisite cloud. Then we propose to identify and exploit hot metadata (frequently accessed metadata) for efficient SWf scheduling in a multisite cloud, using a distributed approach. We implemented our approach within a scientific workflow management system, which shows that our approach reduces the execution time of highly parallel jobs up to 64% and that of the whole SWfs up to 55%.

#### 7.2.3. Distributed Management of Scientific Workflows for Plant Phenotyping

Participants: Gaetan Heidsieck, Christophe Pradal, Esther Pacitti, Patrick Valduriez.

In the last decade, high-throughput phenotyping platforms have allowed acquisition of quantitative data on thousands of plants required for genetic analyses in well-controlled environmental conditions. The seven facilities of Phenome produce 200 terabytes of data annually, which are heterogeneous (images, time courses), multiscale (from the organ to the field) and originate from different sites. Hence, the major problem becomes the automatic analysis of these massive datasets and the ability to reproduce large and complex in-silico experiments.

In [31], we propose a solution (infrastructure) to distribute the computation of scientific workflows on very large grid computing facilities (EGI/France Grilles) to the 3D reconstruction, segmentation and tracking of plant organs. This infrastructure, InfraPhenoGrid, is based on OpenAlea, SciFloware and SON, a set of software and technology developed in the team. We have used this solution in [27] to dissect the genetic and environmental influence of biomass accumulation in complex multi-genotype maize canopies.

## 7.3. Data Analytics

#### 7.3.1. Massively Distributed Indexing of Time Series

**Participants:** Djamel-Edine Yagoubi, Reza Akbarinia, Boyan Kolev, Oleksandra Levchenko, Florent Masseglia, Patrick Valduriez, Dennis Shasha.

Indexing is crucial for many data mining tasks that rely on efficient and effective similarity query processing. Consequently, indexing large volumes of time series, along with high performance similarity query processing, have became topics of high interest. For many applications across diverse domains though, the amount of data to be processed might be intractable for a single machine, making existing centralized indexing solutions inefficient.

In [36], we consider the problem of finding highly correlated pairs of time series across multiple sliding windows. Doing this efficiently and in parallel could help in applications such as sensor fusion, financial trading, or communications network monitoring, to name a few. We have developed a parallel incremental random vector/sketching approach, called ParCorr, to this problem and compared it with the state-of-the-art nearest neighbor method iSAX. Whereas iSAX achieves 100% recall and precision for Euclidean distance, the sketching approach is, empirically, at least 10 times faster and achieves 95% recall and 100% precision on real and simulated data. For many applications this speedup is worth the minor reduction in recall. Our method scales up to 100 million time series and scales linearly in its expensive steps (but quadratic in the less expensive ones).

In [48], we propose a demonstration of our sketch-based solution to efficiently perform both the parallel indexing of large sets of time series and a similarity search on them. Because our method is approximate, we explore the tradeoff between time and precision. A video showing the dynamics of the demonstration can be found at http://parsketch.gforge.inria.fr/video/parSketchdemo\_720p.mov.

#### 7.3.2. Parallel Mining of Maximally Informative k-Itemsets in Data Streams

Participants: Mehdi Zitouni, Reza Akbarinia, Florent Masseglia.

The discovery of informative itemsets is a fundamental building block in data analytics and information retrieval. While the problem has been widely studied, only few solutions scale. This is particularly the case when the dataset is massive, or the length k of the informative itemset to be discovered is high.

In [63], we address the problem of mining maximally informative k-itemsets (miki) in data streams based on joint entropy. We propose PentroS, a highly scalable parallel miki mining algorithm. PentroS renders the mining process of large volumes of incoming data very efficient. It is designed to take into account the continuous aspect of data streams, particularly by reducing the computations of need for updating the miki results after arrival/departure of transactions to/from the sliding window. PentroS has been extensively evaluated using massive real-world data streams. Our experimental results confirm the effectiveness of our proposal which allows excellent throughput with high itemset length.

## 7.3.3. Spatio-Temporal Data Mining

Participants: Esther Pacitti, Florent Masseglia.

The problem of discovering spatiotemporal sequential patterns affects a broad range of applications. Many initiatives find sequences constrained by space and time. We address in [40] an appealing new challenge for this domain: find tight space-time sequences, i.e., find within the same process: i) frequent sequences constrained in space and time that may not be frequent in the entire dataset and ii) the time interval and space range where these sequences are frequent. The discovery of such patterns along with their constraints may lead to extract valuable knowledge that can remain hidden using traditional methods since their support is extremely low over the entire dataset. Our contribution is a new Spatio-Temporal Sequence Miner (STSM) algorithm to discover tight space-time sequences.

## 7.4. Machine Learning for High-dimensional Data

### 7.4.1. Uncertainty in Fine-grained Classification

Participants: Titouan Lorieul, Alexis Joly.

Uncertainty is critical when considering classification problems that involve thousands of domain specific labels. A picture of a plant, for instance, contains only a partial information that is usually not sufficient to determine its scientific name with certainty. We first work on the modelling of such uncertainty in the context of crowdsourcing systems involving experts as well as non expert annotators. We rely on Bayesian inference to learn the annotators' confusion and to optimally assign them new items to be validated. In particular, we work on a non-parametric version of this model allowing to combine annotators' suggestions even when the number of possible labels is undetermined and might change over time [33]. In mirror to this research, we also work on the uncertainty of automatic classifiers, in particular deep convolutional neural networks trained on massive amounts of plant images. We conduct an experimental study aimed at evaluating quantitatively the intrinsic data ambiguity of image-based plant observations [64], and we started working on new methods for estimating the uncertainty of ensembles of deep neural networks by fitting a Dirichlet distribution on the set of their predictions. Besides, we study the use of different taxonomic levels as a source of potential reduction in prediction uncertainties [66].

## 7.4.2. Species Distribution Modelling based on Citizen Science Data

Participants: Christophe Botella, Alexis Joly.

Species distribution models (SDM) are widely used for ecological research and conservation purposes. Given a set of species occurrence, the aim is to infer its spatial distribution over a given territory. Because of the limited number of occurrences of specimens, this is usually achieved through environmental niche modeling approaches, i.e. by predicting the distribution in the geographic space on the basis of a mathematical representation of their known distribution in environmental space (= realized ecological niche). The environment is in most cases represented by climate data (such as temperature, and precipitation), but other variables such as soil type or land cover can also be used. In [24], we study for the first time the relevance of a species distribution model computed from automatically identified plant observations made by citizens rather than from classical inventories made by experts. The results show that the resulting models have a great potential for the early detection of new invasions. In [65] and [60], we propose a deep learning approach to species distribution modelling in order to improve the predictive effectiveness in the context of massive amount of occurrence data. Non-linear prediction models have been of interest for SDM for more than a decade but our study is the first one bringing empirical evidence that deep, convolutional and multilabel models might participate to resolve the limitations of SDM.

#### 7.4.3. Evaluation of Species Identification and Prediction Algorithms

Participants: Alexis Joly, Hervé Goëau, Christophe Botella, Jean-Christophe Lombardo.

We ran a new edition of the LifeCLEF evaluation campaign [45] with the involvement of 13 research teams worldwide. The main novelties and outcomes of the 2018-th edition are the following:

- **GeoLifeCLEF**: a new challenge [71] dedicated to the location-based prediction of species based on spatial occurrences and environmental data tensors. The evaluation concludes that deep environmental convolutional neural networks perform better than spatial models or ponctual environmental models.
- Man vs. Machine plant identification: To evaluate how far automated identification systems are from the best possible performance, we organize a challenge involving 19 deep-learning systems implemented by 4 different research teams and 9 of the best expert botanists of the French flora. The main outcome of this work is that the performance of state-of-the-art deep learning models is now very close to the most advanced human expertise.
- **Bird sounds identification**: the 2018-the edition of the BirdCLEF challenge reveals impressive identification performance when considering bird sounds recorded by the Xeno-Canto community. Identifying birds in raw, multi-directional soundscapes, however, remains a very challenging task.

# 7.4.4. Towards the Recognition of The World's Flora: When HPC Meets Deep Learning

Participants: Hervé Goëau, Jean-Christophe Lombardo, Alexis Joly.

Automated identification of plants and animals have improved considerably in the last few years, in particular thanks to the recent advances in deep learning. In 2017, a challenge on 10,000 plant species (PlantCLEF) resulted in impressive performances with accuracy values reaching 90%. One of the most popular plant identification application, Pl@ntNet, nowadays works on 18K plant species. It accounts for million of users all over the world and already has a strong societal impact in several domains including education, landscape management and agriculture. Now, the big challenge is to train such systems at the scale of the world's biodiversity. Therefore, we built a training set of about 12M images illustrating 300K species of plants. Training a convolutional neural network on such a large dataset can take up to several months on a single node equipped with four recent GPUs. Moreover, to select the best performing architecture and optimize the hyper-parameters, it is often necessary to train several of such networks. Overall, this becomes a highly intensive computational task that has to be distributed on large HPC infrastructures. Therefore, we experiment two french national supercomputers through an access offered by GENCI (Occigen@CINES, a 3.5 Pflop/s Tier-1 cluster based on Broadwell-14cores@2.6Ghz nodes and Joliot-Curie»@TGCC, a BULL-Sequana-X1000 cluster integrating 1656 nodes Intel Skylake8168-24cores@2.7GHz). To implement the synchronized stochastic gradient descent on the CPU cluster Joliot-Curie, we are using the deep learning framework Intel CAFFE coupled with Intel MLSL library (in the context of a collaboration with Intel).

### 7.4.5. Evaluation of Music Separation Techniques

Participants: Antoine Liutkus, Fabian-Robert Stöter.

After the groundbreaking advent of deep learning, we feel the music processing community needs to step back and think about what had been accomplished and what remains challenging in the problems of musical signal processing and filtering. Therefore, we give a complete overview of the state of the art in music demixing in [32] comprising more than 350 references, as well as two chapters in dedicated books [68], [67]. These references may be considered as complete overviews of the state of the art in music demixing. Furthermore, we introduce the topic to non-expert researchers and engineers in [26].

Apart from this effort in presenting the most recent advances in music processing to the community, we organize yearly a systematic evaluation of state of the art. We report the results of the 2018 Signal Separation Evaluation Campaign in [58], gathering a record number of participants. A perceptual evaluation of the results obtained through this campaign is presented in [59], in collaboration with researchers from the Surrey University.

#### 7.4.6. Robust Probabilistic Models for Time-series

Participants: Antoine Liutkus, Fabian-Robert Stöter.

Processing large amounts of data for denoising or analysis comes with the need to devise models that are robust to outliers and that permit efficient inference. For this purpose, we advocate the use of non-Gaussian models for this purpose, which are less sensitive to data-uncertainty. Most of our effort on this topic is split in two subtasks.

First, we develop new filtering methods that go beyond least-squares estimation. In collaboration with researchers from RWTH, Aachen, Germany, we introduce a new model based on mixtures of Gaussians for filtering in [50]. It combines tractability with a better account of phase consistency for complex data. Along with researchers from IRISA, Rennes and Telecom ParisTech, we also work on filtering  $\alpha$ -stable processes [44], [46], [57], which enjoy important applications in robust signal processing.

Second, we work on large amounts of musical archives. This includes an original way to scale up interference reduction in live musical recordings in collaboration with the managers of the Montreux Jazz Festival data at EPFL (Switzerland).